

Serendipity Finite Element Methods for Cardiac Electrophysiology Models

Andrew Gillette

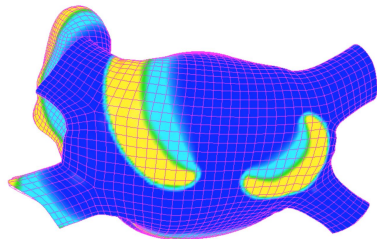
Department of Mathematics
University of California, San Diego

<http://ccom.ucsd.edu/~agillette/>

Monodomain Equations for Electrophysiology

Numerical approximation of solutions to the **monodomain equations** allows the simulation of electrical propagation on patient-specific cardiac geometries.

Find $u, v : \Omega \rightarrow \mathbb{R}$ such that



$$\frac{ds}{dt} = F(s, v) \quad \text{in } \Omega$$

$$\frac{\lambda}{1 + \lambda} \nabla \cdot (M_i \nabla v) = v_t + I(v, s) \quad \text{in } \Omega$$

$$-\frac{1}{1 + \lambda} \nabla \cdot (M_i \nabla v) = \nabla \cdot (M_i \nabla u) \quad \text{in } \Omega$$

$$(M_i \nabla v) \cdot \hat{n} = 0 \quad \text{on } \partial\Omega$$

$$(M_i \nabla u) \cdot \hat{n} = 0 \quad \text{on } \partial\Omega$$

v = transmembrane potential

u = extracellular potential

s = state of ionic currents

$F(v, s)$ = voltage-dependent state update

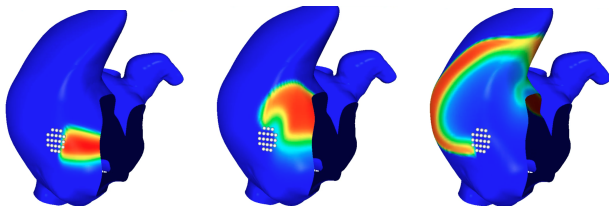
$I(v, s)$ = ionic current across membrane

M_i, M_e = intra-, extra-cellular conductivity tensors, satisfying $M_e = \lambda M_i$

Application Motivations and Challenges

Scientific and clinical motivations:

- Provide models of electrical activity at spatial and temporal resolutions beyond MRI and EKG data.
- Allow patient-specific modeling for 'real-time' simulations during surgery.
- Analyze 'spiral waves' that occur during atrial fibrillation:



[show videos]

Competing theories of the biophysical nature of this phenomenon have been proposed; computational simulations and mathematical analysis can provide evidence for or against treatment strategies (e.g. where to cauterize heart cells)

Application Motivations and Challenges

Computational challenges:

- Survey of various codes on a 'benchmark problem' revealed large discrepancies in the estimation of activation time, a basic measure of accuracy.
- In the application context,

$$\text{Péclet number} = \frac{k \cdot h^2}{6 \cdot D} = \frac{(\text{reaction rate}) \cdot (\text{mesh element length})^2}{6 \cdot (\text{diffusivity constant})} > 1$$

which can lead to Gibbs type phenomena of spurious oscillations. This can be overcome either by using many mesh elements (small h values) or higher order methods, both of which can be computationally expensive.

- Using different functions for geometry and function approximation is expensive; unified methods are needed.

Serendipity finite element methods help address these challenges.

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- 1 Geometric Decompositions for Serendipity FEM
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What is a serendipity finite element method?

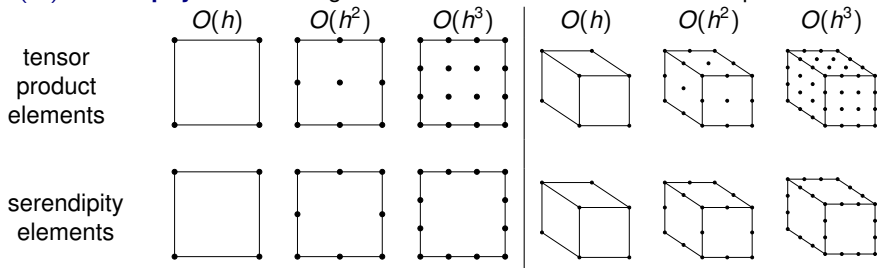
Goal: Efficient, accurate approximation of the solution to a PDE over $\Omega \subset \mathbb{R}^n$.

Standard $O(h^r)$ **tensor product** finite element method in \mathbb{R}^n :

- Mesh Ω by n -dimensional cubes of side length h .
- Set up a linear system involving $(r + 1)^n$ degrees of freedom (DoFs) per cube.
- For unknown continuous solution u and computed discrete approximation u_h :

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

A $O(h^r)$ **serendipity** FEM converges at the **same rate** with **fewer DoFs** per element:



Example: For $O(h^3)$, $d = 3$, 50% fewer DoFs → $\approx 50\%$ smaller linear system

What is a geometric decomposition?

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

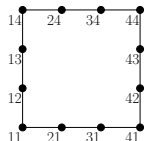
$$\{1, x, y, x^2, y^2, xy, x^3, y^3, x^2y, xy^2, x^3y, xy^3\}$$

monomials



$$\{\vartheta_{11}, \vartheta_{14}, \vartheta_{41}, \vartheta_{44}, \vartheta_{12}, \vartheta_{13}, \vartheta_{42}, \vartheta_{43}, \vartheta_{21}, \vartheta_{31}, \vartheta_{24}, \vartheta_{34}\}$$

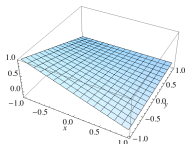
basis functions



domain points

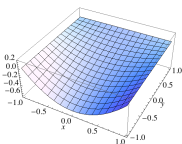
→ Previously known basis functions employ Legendre polynomials

→ These functions bear no symmetrical correspondence to the domain points



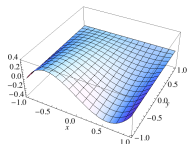
$$\frac{1}{4}(x-1)(y-1)$$

vertex



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

edge (quadratic)



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

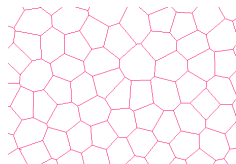
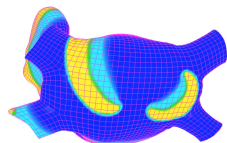
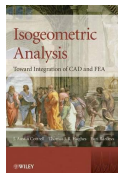
edge (cubic)

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

A 'canonical' geometric decomposition can aid in higher order generalizations.

Motivations and Related Topics

Goal: Construct geometric decompositions of serendipity spaces using linear combinations of standard tensor product functions. **Focus:** Cubic Hermites.



- **Isogeometric analysis:** Finding basis functions suitable for both domain description and PDE approximation avoids the expensive computational bottleneck of re-meshing.

COTTRELL, HUGHES, BAZILEVS *Isogeometric Analysis: Toward Integration of CAD and FEA*, Wiley, 2009.

- **Modern mathematics:** Finite Element Exterior Calculus, Discrete Exterior Calculus, Virtual Element Methods. . .

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

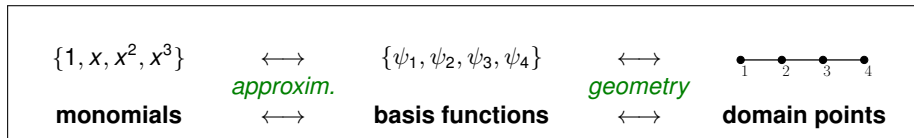
DA VEIGA, BREZZI, CANGIANI, MANZINI, RUSSO *Basic Principles of Virtual Element Methods*, M3AS, 2013.

- **Flexible Domain Meshing:** Serendipity type elements for Voronoi meshes provide computational benefits without need of tensor product structure.

RAND, G., BAJAJ *Quadratic Serendipity Finite Elements on Polygons Using Generalized Barycentric Coordinates*, Mathematics of Computation, in press.

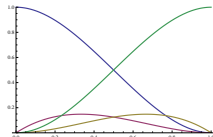
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Cubic Hermite Geometric Decomposition: 1D



Cubic Hermite Basis
on $[0, 1]$

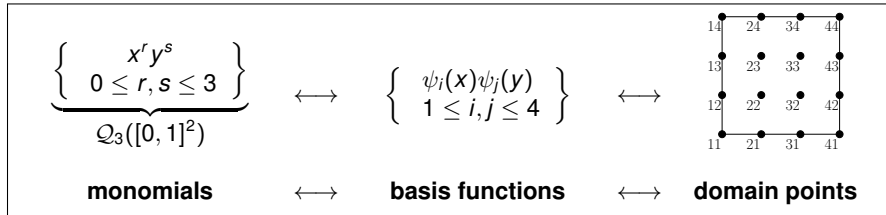
$$\begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{bmatrix} := \begin{bmatrix} 1 - 3x^2 + 2x^3 \\ x - 2x^2 + x^3 \\ x^2 - x^3 \\ 3x^2 - 2x^3 \end{bmatrix}$$



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

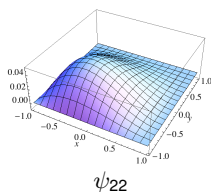
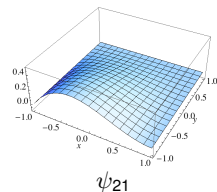
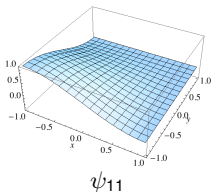
Geometry: $u = u(0)\psi_1 + u'(0)\psi_2 - u'(1)\psi_3 + u(1)\psi_4$, $\forall u \in \underbrace{\mathcal{P}_3([0, 1])}_{\text{cubic polynomials}}$

Cubic Hermite Geometric Decomposition: 2D



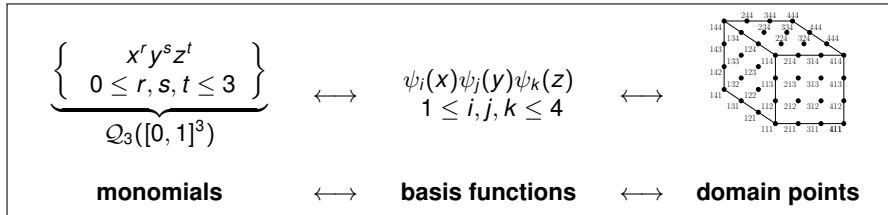
Approximation: $x^r y^s = \sum_{i=1}^4 \sum_{j=1}^4 \varepsilon_{r,i} \varepsilon_{s,j} \psi_{ij}$, for $0 \leq r, s \leq 3$, $\varepsilon_{r,i}$ as in 1D.

Geometry:



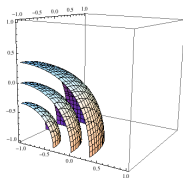
$$u = u|_{(0,0)} \psi_{11} + \partial_x u|_{(0,0)} \psi_{21} + \partial_y u|_{(0,0)} \psi_{12} + \partial_x \partial_y u|_{(0,0)} \psi_{22} + \dots, \quad \forall u \in \mathcal{Q}_3([0, 1]^2)$$

Cubic Hermite Geometric Decomposition: 3D

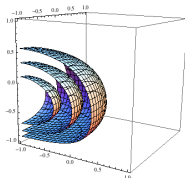


Approximation: $x^r y^s z^t = \sum_{i=1}^4 \sum_{j=1}^4 \sum_{k=1}^4 \varepsilon_{r,i} \varepsilon_{s,j} \varepsilon_{t,k} \psi_{ijk}$, for $0 \leq r, s, t \leq 3$, $\varepsilon_{r,i}$ as in 1D.

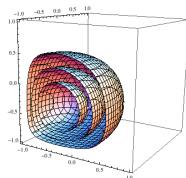
Geometry: Contours of level sets of the basis functions:



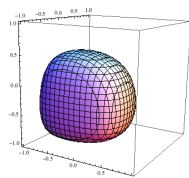
ψ_{111}



ψ_{112}



ψ_{212}



ψ_{222}

Two families of finite elements on cubical meshes

$\mathcal{Q}_r^- \Lambda^k([0, 1]^n) \rightarrow$ 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](#)

$\mathcal{S}_r \Lambda^k([0, 1]^n) \rightarrow$ 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.

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

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

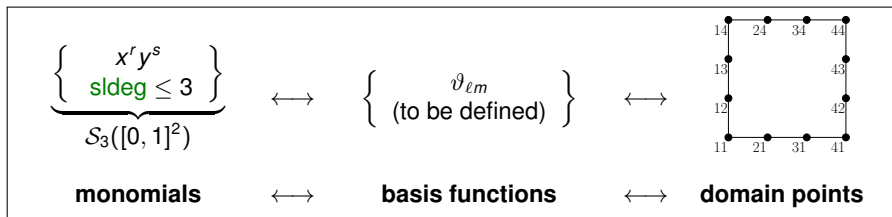
$\mathcal{Q}_r^- \Lambda^k$ and $\mathcal{S}_r \Lambda^k$ and have the **same** key mathematical properties needed for FEEC
(degree, inclusion, trace, subcomplex, unisolvence, commuting projections)

but for fixed $k \geq 0, r, n \geq 2$ the serendipity spaces have **fewer** degrees of freedom

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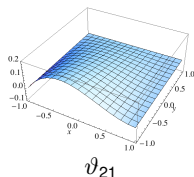
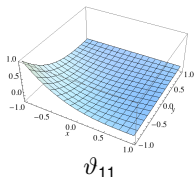
Cubic Hermite Serendipity Geom. Decomp: 2D

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



Approximation: $x^r y^s = \sum_{\ell m} \varepsilon_{r,i} \varepsilon_{s,j} v_{\ell m}$, for *superlineardegree*($x^r y^s$) ≤ 3

Geometry:



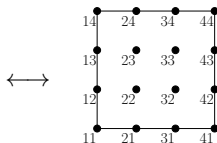
$$\begin{aligned}
 u &= u|_{(0,0)} v_{11} \\
 &+ \partial_x u|_{(0,0)} v_{21} \\
 &+ \partial_y u|_{(0,0)} v_{12} \\
 &+ \dots \\
 \forall u &\in \mathcal{S}_3([0, 1]^2)
 \end{aligned}$$

Cubic Hermite Serendipity Geom. Decomp: 2D

Proof Overview:

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

V = vertices (11, 14, ...)
 E = edges (12, 13, ...)
 D = interior (22, 23, ...)



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

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

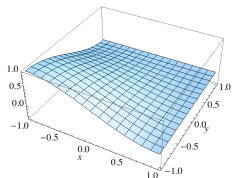
- 2 Define a 12×16 matrix \mathbb{H} with entries $h_{ij}^{\ell m}$ so that $\ell m \in V \cup E$, $ij \in V \cup E \cup D$.
- 3 Define the serendipity basis functions $\vartheta_{\ell m}$ via

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

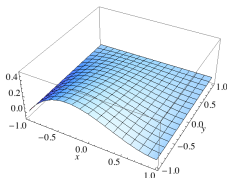
and show that the **approximation** and **geometry** properties hold.

Hermite Style Serendipity Functions (2D)

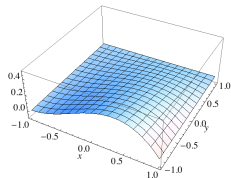
$$[\vartheta_{\ell m}] = \begin{bmatrix} \vartheta_{11} \\ \vartheta_{14} \\ \vartheta_{41} \\ \vartheta_{44} \\ \vartheta_{12} \\ \vartheta_{13} \\ \vartheta_{42} \\ \vartheta_{43} \\ \vartheta_{21} \\ \vartheta_{31} \\ \vartheta_{24} \\ \vartheta_{34} \end{bmatrix} = \begin{bmatrix} -(x-1)(y-1)(-2+x+x^2+y+y^2)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



ϑ_{11}



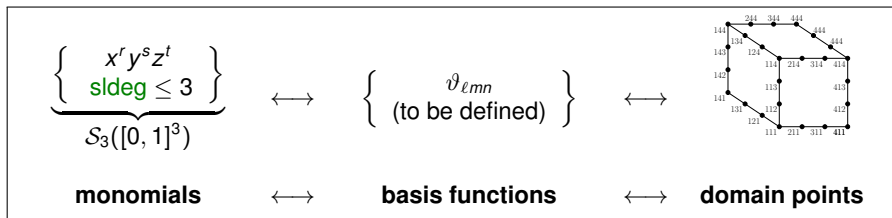
ϑ_{21}



ϑ_{31}

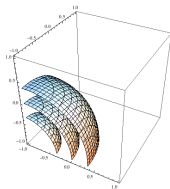
Cubic Hermite Serendipity Geom. Decomp: 3D

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

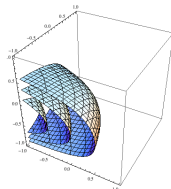


Approximation: $x^r y^s z^t = \sum_{\ell mn} \varepsilon_{r,i} \varepsilon_{s,j} \varepsilon_{t,k} \vartheta_{\ell mn}$, for $\text{superlineardegree}(x^r y^s z^t) \leq 3$

Geometry:



ϑ_{111}



ϑ_{112}

$$\begin{aligned}
 u &= u|_{(0,0,0)} \vartheta_{111} \\
 &+ \partial_x u|_{(0,0,0)} \vartheta_{211} \\
 &+ \partial_y u|_{(0,0,0)} \vartheta_{121} \\
 &+ \partial_z u|_{(0,0,0)} \vartheta_{112} \\
 &+ \dots \\
 \forall u &\in \mathcal{S}_3([0, 1]^3)
 \end{aligned}$$

Cubic Hermite Serendipity Geom. Decomp: 3D

Proof Overview:

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

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

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

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

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

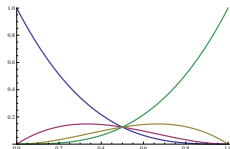
and show that the **approximation** and **geometry** properties hold.

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

Cubic Bernstein Serendipity Geom. Decomp: 2D, 3D

**Cubic
Bernstein Basis**
on $[0, 1]$

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

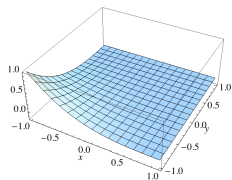


Theorem [G, 2012]: Bernstein-like geometric decompositions of $\mathcal{S}_3([0, 1]^2)$ and $\mathcal{S}_3([0, 1]^3)$ exist.

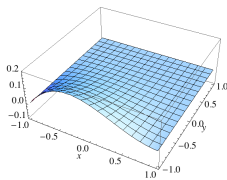
$$[\xi_{\ell m}] = \begin{bmatrix} \xi_{11} \\ \xi_{14} \\ \vdots \\ \xi_{24} \\ \xi_{34} \end{bmatrix} = \begin{bmatrix} (x-1)(y-1)(-2-2x+x^2-2y+y^2) \\ -(x-1)(y+1)(-2-2x+x^2+2y+y^2) \\ \vdots \\ (x-1)^2(x+1)(y+1) \\ -(x-1)(x+1)^2(y+1) \end{bmatrix} \cdot \frac{1}{16}$$

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

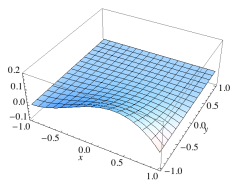
Bernstein Style Serendipity Functions (2D)



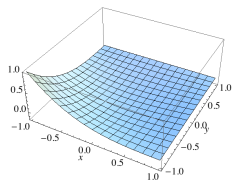
β_{11}



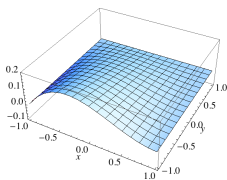
β_{21}



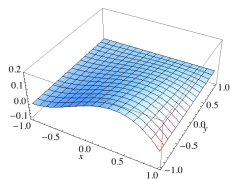
β_{31}



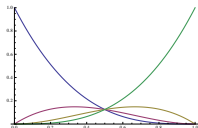
ξ_{11}



ξ_{21}



ξ_{31}

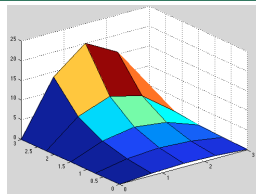


Bicubic Bernstein functions (top) and Bernstein-style serendipity functions (bottom).

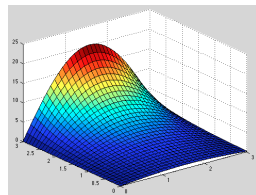
→ Note boundary agreement with Bernstein functions.

Computational Evidence

Serendipity cubic Hermite-like method implemented in Matlab to solve Poisson's equation with exact solution $u(x, y) = \sin(x) e^y$



$n = 2$



$n = 32$

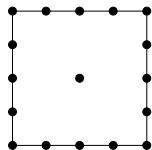
n	$\ u - u_h\ _{L^2}$		$\ \nabla(u - u_h)\ _{L^2}$	
	error	rate	error	rate
2	2.89e-1		1.44e+0	
4	1.32e-2	4.4	1.62e-1	3.1
8	6.90e-4	4.3	1.82e-2	3.2
16	3.83e-5	4.2	2.09e-3	3.1
32	2.22e-6	4.1	2.48e-4	3.1

Confirms the expected **cubic** order *a priori* error estimate

$$\underbrace{\|u - u_h\|_{H^1(\Omega)}}_{\text{approximation error}} \leq \underbrace{C h^3 \|u\|_{H^4(\Omega)}}_{\text{optimal error bound}}, \quad \forall u \in H^4(\Omega),$$

- 1 Geometric Decompositions for Serendipity FEM
- 2 The Cubic Tensor Product Case
- 3 The Cubic Serendipity Space Case
- 4 Future Directions**

Serendipity spaces for large r



Let $p(x, y) := (1 + x)(1 - x)(1 - y)(1 + y)$.

Observe $p \in \mathcal{P}_4 \subset \mathcal{S}_4$, but $p \equiv 0$ on $\partial([0, 1]^2)$.

When $r > 3$, there are interior domain points for the serendipity spaces as characterized in

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

	1	2	3	4	5	6	7	$r \geq 2n$
$n = 2$								
$\dim Q_r$	4	9	16	25	36	49	64	$r^2 + 2r + 1$
$\dim S_r$	4	8	12	17	23	30	38	$\frac{1}{2}(r^2 + 3r + 6)$
$n = 3$								
$\dim Q_r$	8	27	64	125	216	343	512	$r^3 + 3r^2 + 3r + 1$
$\dim S_r$	8	20	32	50	74	105	144	$\frac{1}{6}(r^3 + 6r^2 + 29r + 24)$

- Thus, when $r \geq 2n$, the expected computational savings by serendipity methods is **50% in 2D** and **83% in 3D**.
- I am currently pursuing related theoretical results with Snorre Christiansen and Michael Floater (both from U. Oslo).

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