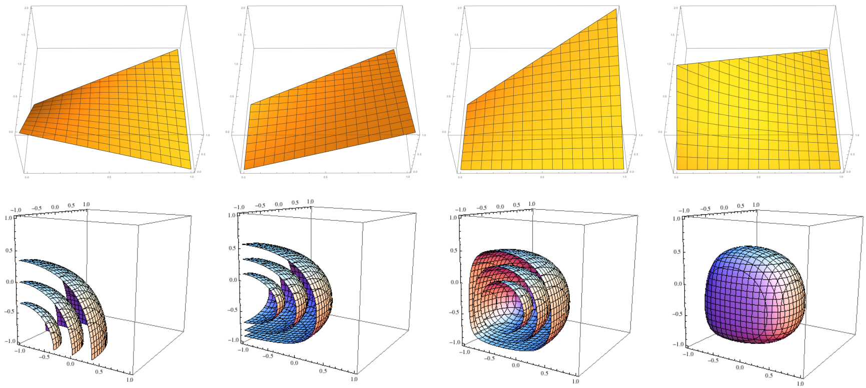
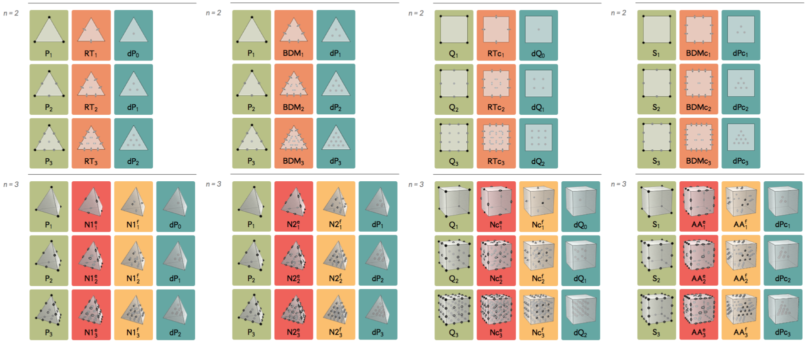
A Plethora of Basis Functions for Quadrilaterals and Hexahedra

Andrew Gillette - University of Arizona



The ‘Periodic Table of the Finite Elements’

ARNOLD, LOGG, “Periodic table of the finite elements,” *SIAM News*, 2014.

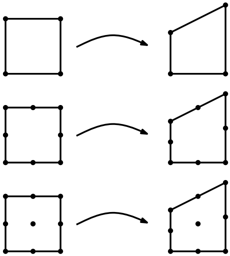


- Classification of many common conforming finite element types.
- Squares and cubes occupy the right half of the table.
- The right-most column is the “serendipity” family of finite elements.

Serendipity elements struggle with reference mapping

Quadratic serendipity elements, mapped non-affinely, are only expected to converge at the rate of *linear* elements.

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



	$\|\|u - u_h\|\|_{L^2}$	$\|\|\nabla(u - u_h)\|\|_{L^2}$
linear	$O(h^2)$	$O(h)$
quadratic serendipity	$O(h^2)$	$O(h)$
quadratic tensor prod.	$O(h^3)$	$O(h^2)$

Extensions to vector-valued and higher dimensions:

ARNOLD, BOFFI, FALK, "Quadrilateral $H(\text{div})$ Finite Elements," *SINUM*, 2005.
ARNOLD, BOFFI, BONIZZONI, "Finite element differential forms on curvilinear cubic meshes," *Numer. Math.*, 2014

Open source finite element software

FEniCS primarily supports simplicial elements

deal.ii primarily supports quad/hex elements

ALNÆS ET AL. "The FEniCS Project Version 1.5" *Archive of Numerical Software* 2015
BANGERTH ET AL. "The deal.ii Library, Version 8.4," *Journal of Num. Math.*, 2016

Neither package supports serendipity elements!

Remainder of this talk

- Recent advances and current uses of quad/hex meshes
- Techniques for finite elements on general quad/hex meshes
- Lessons from an application of serendipity elements for cardiac electrophysiology

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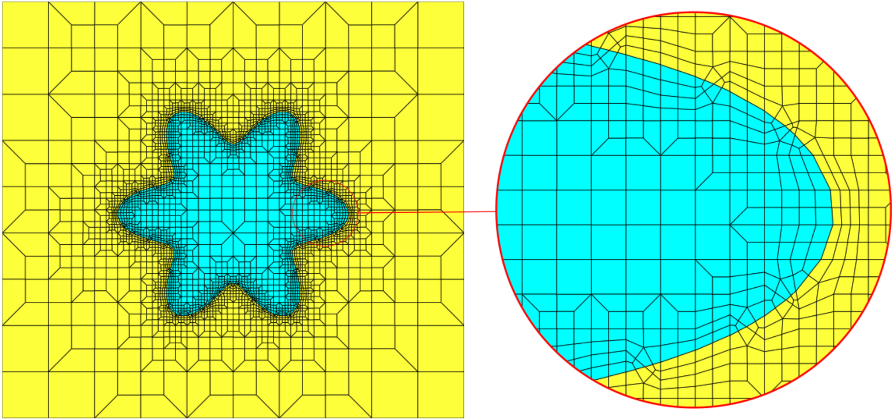
Outline

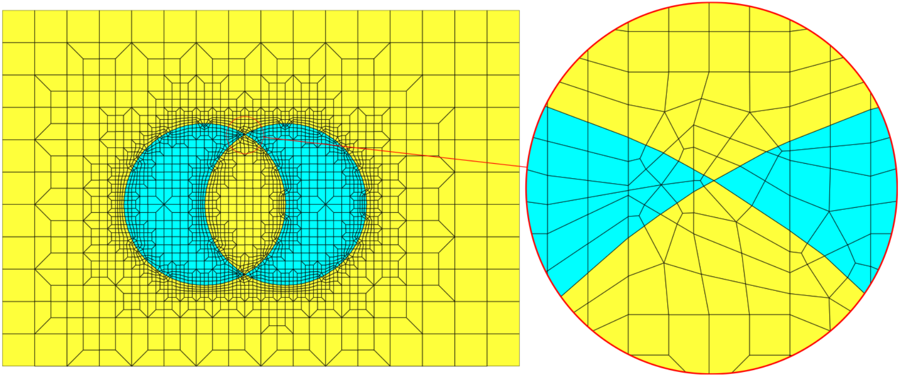
Recent advances in quad meshing



An all-quad mesh conforming to a given curve.

RUSHDI ET AL. “All-quad meshing without cleanup,” *Computer-Aided Design*, 2017

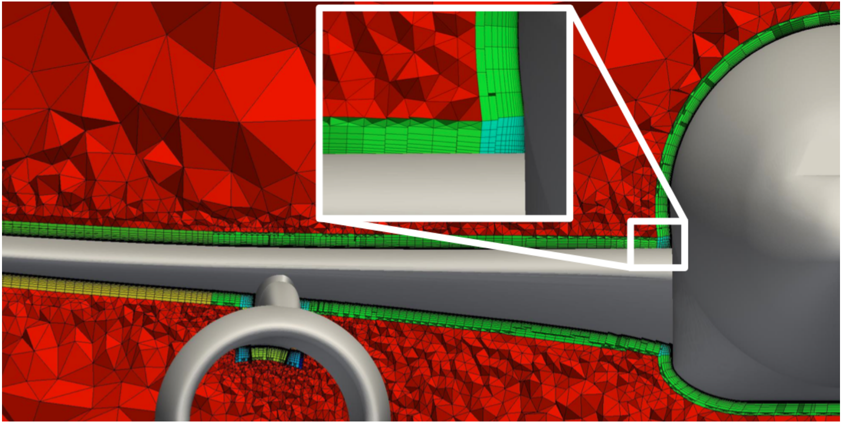
Recent advances in quad meshing



An all-quad mesh conforming to a given curve.

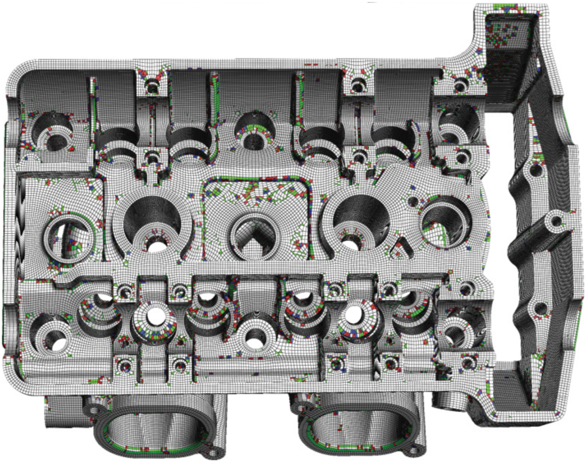
RUSHDI ET AL. "All-quad meshing without cleanup," *Computer-Aided Design*, 2017

Volume meshing for Computational Fluid Dynamics



*Hyrbid hex / pyramid / prism / tet mesh for CFD, using **ITI Transcendata** software.*
(from a keynote address at Geometric Modeling and Processing 2015)

Recent advances in hex-dominant meshing



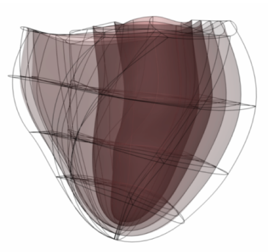
→ A hex-dominant mesh with ≈1.3 million cells, including ≈1 million hexahedra.

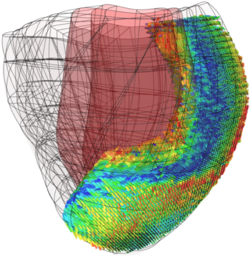
→ Re-meshed from a mesh of ≈ 10 million tetrahedra.

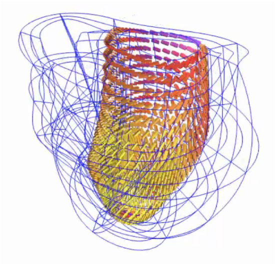
SOKOLOV ET AL. “Hexahedral-Dominant Meshing,” *ACM Trans. Graphics*, 2016

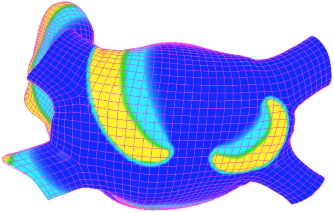
Established models use hexahedral meshes

All-hex meshes of a specific patient's heart are generated and used to create simulations of electrophysical phenomena.







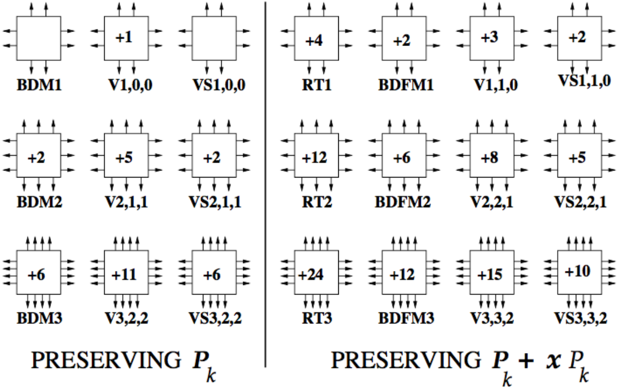


McCulloch research group, *Continuity* software
National Biomedical Computation Resource
UC San Diego
2006–2017

Outline

1. Serendipity elements in theory and software
2. Recent advances and current uses of quad/hex meshes
3. Techniques for finite elements on general quad/hex meshes
4. An application of serendipity elements for cardiac electrophysiology

The virtual element technique



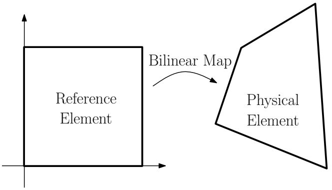
→ Analogues of conforming finite element spaces on squares can be treated as virtual elements.

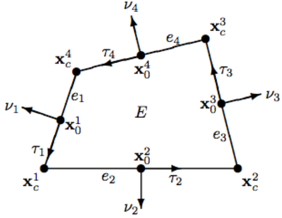
→ Explicit basis functions are not needed to implement the method.

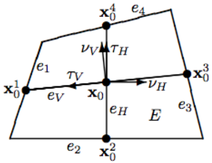
→ Related polygonal element methods (HHO, HDG, WG. . .) may offer similar approaches.

BEIRÃO DA VEIGA, BREZZI, MARINI, RUSSO "Serendipity face and edge VEM spaces" *Rendiconti Lincei-Matematica e Applicazioni*, 2017.

The Arbogast-Correa technique







A finite element space on a general quadrilateral is built in two parts:

- Apply Piola mapping to functions associated to boundary of reference element.
- Define functions on the physical element corresponding to interior degrees of freedom in a way that ensures relevant polynomial approximation properties.

ARBOGAST, CORREA "Two families of H(div) mixed finite elements on quadrilaterals of minimal dimension," *SIAM J. Numerical Analysis*, 2016

The generalized barycentric coordinate technique

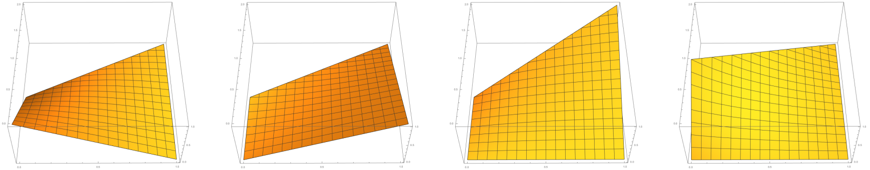
Let P be a convex polytope with vertex set V. We say that

$$\lambda_{\mathbf{v}} : P \to \mathbb{R} \quad \text{are} \quad \textbf{generalized barycentric coordinates (GBCs)} \text{ on } P$$

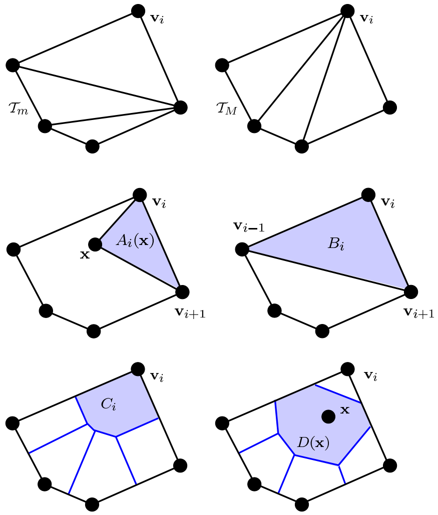
if they satisfy $\lambda_{\mathbf{v}} \geq 0$ on P and $L = \sum_{\mathbf{v}\in V} L(\mathbf{v}_{\mathbf{v}})\lambda_{\mathbf{v}}, \quad \forall\, L : P \to \mathbb{R}$ linear.

Familiar properties are implied by this definition:

$$\underbrace{\sum_{\mathbf{v}\in V} \lambda_{\mathbf{v}} \equiv 1}_{\text{partition of unity}} \qquad \underbrace{\sum_{\mathbf{v}\in V} \mathbf{v}\lambda_{\mathbf{v}}(\mathbf{x}) = \mathbf{x}}_{\text{linear precision}} \qquad \underbrace{\lambda_{\mathbf{v}_i}(\mathbf{v}_j) = \delta_{ij}}_{\text{interpolation}}$$



Many barycentric coordinates are available . . .



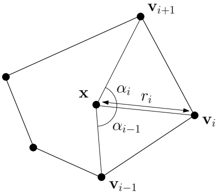
- Triangulation
  ⇒ FLOATER, HORMANN, KÓS, *A general construction of barycentric coordinates over convex polygons*, 2006

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

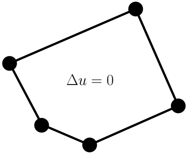
- Wachspress
  ⇒ WACHSPRESS, *A Rational Finite Element Basis*, 1975.
  ⇒ WARREN, *Barycentric coordinates for convex polytopes*, 1996.

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

Many barycentric coordinates are available . . .



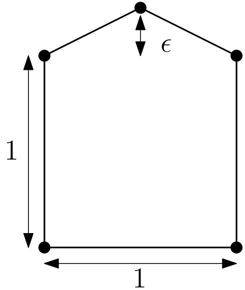
- Mean value
  ⇒ FLOATER, *Mean value coordinates*, 2003.
  ⇒ FLOATER, KÓS, REIMERS, *Mean value coordinates in 3D*, 2005.



- Harmonic
  ⇒ WARREN, SCHAEFER, HIRANI, DESBRUN, *Barycentric coordinates for convex sets*, 2007.
  ⇒ CHRISTIANSEN, *A construction of spaces of compatible differential forms on cellular complexes*, 2008.
  ⇒ Similar to virtual elements

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

Large angle experiment



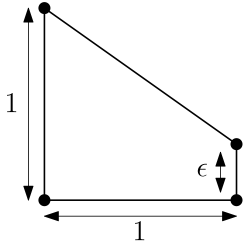
On a ***single*** element with a large angle:

- Set boundary values on domain shown from
  $$u(x, y) = 0.77223(x - 0.331)^2 + 1.1123(y + 0.177344)^2$$
- Compute harmonic (**hm**), Wachspress (**wa**), mean value (**mv**), discrete harmonic (**dh**), moving least squares (**ls-***), and maximum entropy (**me-***) coordinates as $\epsilon \to 0$
- Report $\left|u_h^{hm}\right|_{H^1}$ and $\left|u_h^{hm} - u_h^*\right|_{H^1}$

ϵ	**hm**	**wa**	**mv**	**dh**	**ls-1**	**ls-2**	**ls-3**	**me-t**	**me-u**
0.1600	1.3e0	2.6e-1	6.0e-2	2.3e-1	1.8e-1	2.2e-2	5.4e-2	7.9e-2	5.1e-1
0.0400	1.3e0	1.3e0	1.1e-1	1.5e0	3.6e-1	5.4e-2	1.2e-1	1.6e-1	2.2e0
0.0100	1.3e0	3.1e0	1.3e-1	3.9e0	4.4e-1	6.5e-2	1.4e-1	1.9e-1	5.1e0
0.0025	1.3e0	6.4e0	1.3e-1	8.3e0	4.5e-1	6.7e-2	1.4e-1	2.0e-1	9.3e0
0.0000	1.3e0	-	1.3e-1	-	4.5e-1	6.8e-2	1.5e-1	2.0e-1	-

Only *some* coordinates lose interpolation quality as the geometry degenerates.
(in this case, **wa**, **dh**, and **me-u**).

Short edge experiment

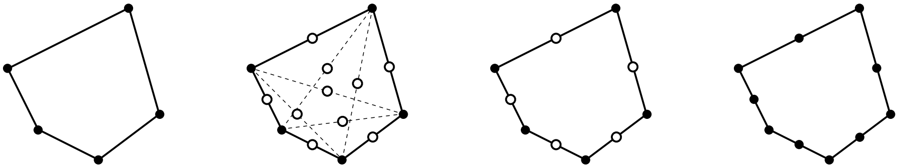


On a quadrilateral with a very short edge:

ϵ	**hm**	**wa**	**mv**	**dh**	**ls-1**	**ls-2**	**ls-3**	**me-t**	**me-u**
0.1600	7.5e-1	1.1e-1	4.0e-2	2.3e-1	2.2e-1	3.4e-2	6.5e-2	2.5e-1	7.3e-1
0.0400	8.5e-1	3.9e-2	1.2e-2	8.3e-2	9.0e-2	1.3e-2	2.9e-2	9.6e-2	4.6e-1
0.0100	8.9e-1	1.2e-2	3.2e-3	1.6e-1	2.9e-2	4.3e-3	1.0e-2	3.0e-2	2.5e-1
0.0025	9.1e-1	3.3e-3	6.7e-4	3.7e-3	7.9e-3	1.2e-3	3.2e-3	8.9e-3	9.9e-2

In this case, *none* of the coordinates lose interpolation quality as the geometry degenerates!

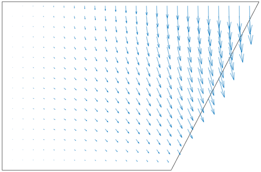
Higher order and vector-valued GBC elements

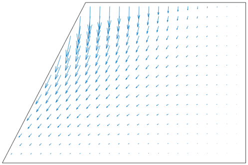


$\{\lambda_i\}$ —pairwise products→ $\{\lambda_a\lambda_b\}$ —$\mathbb{A}$→ $\{\xi_{ij}\}$ —$\mathbb{B}$→ $\{\psi_{ij}\}$

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

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

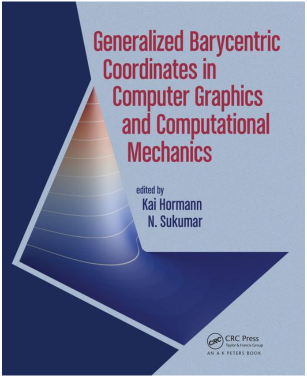




Can also do Whitney-like constructions: $\{\lambda_i \nabla \lambda_j\}$

G, RAND, BAJAJ, "Construction of Scalar and Vector Finite Element Families on Polygonal and Polyhedral Meshes," *CMAM*, 2016.

Other applications of GBCs



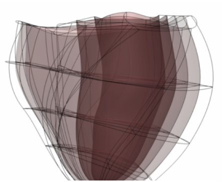
- Shape quality metrics and analysis
- Discrete Laplacians
- Mesh parameterization
- Shape deformation
- Self-supporting surfaces
- Extreme deformations
- BEM-based FEM
- Virtual element methods
- . . . *and much more!*

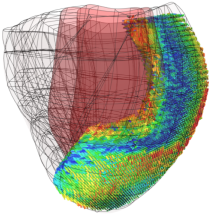
Book available October 31, 2017 from CRC Press.

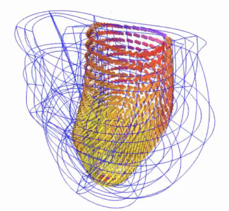
Outline

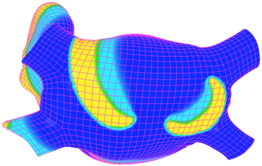
Returning to the cardiac electrophysiology example...

- An established code at UCSD uses ***cubic tensor product*** Hermite-style basis functions to carry out finite element simulations.
- Would an analogous serendipity basis help here, even without accounting for the non-affine geometry mappings?









McCulloch research group, *Continuity* software
National Biomedical Computation Resource
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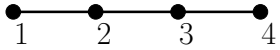
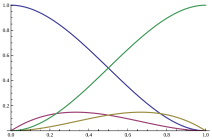
2006–2017

Cubic Hermite Geometric Decomposition: 1D

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

Cubic Hermite Basis on [0, 1]

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

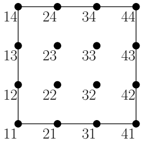


Approximation: $x^r = \sum_{i=1}^{4} \varepsilon_{r,i}\psi_i$, for $r = 0, 1, 2, 3$, where $[\varepsilon_{r,i}] = \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & -1 & 1 \\ 0 & 0 & -2 & 1 \\ 0 & 0 & -3 & 1 \end{pmatrix}$

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

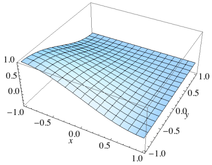
$$\underbrace{\left\{\begin{array}{c} x^r y^s \\ 0 \le r, s \le 3 \end{array}\right\}}_{\mathcal{Q}_3([0,1]^2)} \longleftrightarrow \left\{\begin{array}{c} \psi_i(x)\psi_j(y) \\ 1 \le i, j \le 4 \end{array}\right\} \longleftrightarrow$$



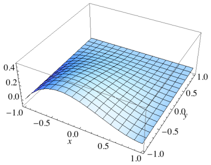
monomials $\longleftrightarrow$ **basis functions** $\longleftrightarrow$ **domain points**

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.

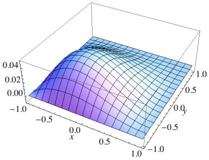
Geometry:



ψ_{11}



ψ_{21}

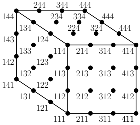


ψ_{22}

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

Cubic Hermite Geometric Decomposition: 3D

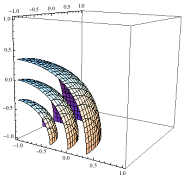
$$\underbrace{\left\{ \begin{array}{c} x^r y^s z^t \\ 0 \le r, s, t \le 3 \end{array} \right\}}_{\mathcal{Q}_3([0,1]^3)} \quad \longleftrightarrow \quad \begin{array}{c} \psi_i(x)\psi_j(y)\psi_k(z) \\ 1 \le i, j, k \le 4 \end{array} \quad \longleftrightarrow$$



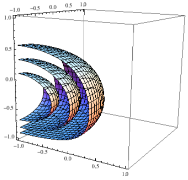
monomials $\longleftrightarrow$ **basis functions** $\longleftrightarrow$ **domain points**

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 $0 \le r, s, t \le 3$, $\varepsilon_{r,i}$ as in 1D.

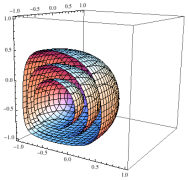
Geometry: Contours of level sets of the basis functions:



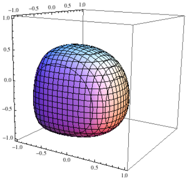
ψ_{111}



ψ_{112}

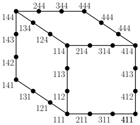


ψ_{212}



ψ_{222}

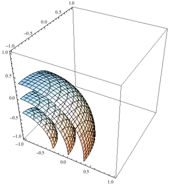
$$\underbrace{\left\{\begin{array}{c} x^r y^s z^t \\ \text{sldeg} \leq 3 \end{array}\right\}}_{\mathcal{S}_3([0,1]^3)} \longleftrightarrow \left\{\begin{array}{c} \vartheta_{\ell mn} \\ \text{(defined in paper)} \end{array}\right\} \longleftrightarrow$$



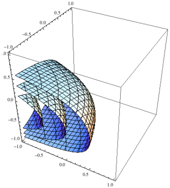
monomials $\longleftrightarrow$ **basis functions** $\longleftrightarrow$ **domain points**

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}

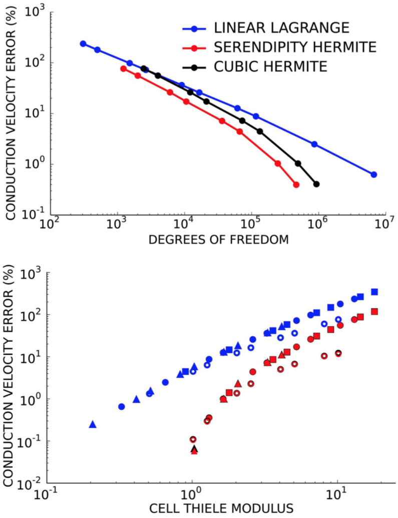


ϑ_{112}

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

G., "Hermite and Bernstein style basis functions..." *Proc. Approx. Theory XIV*, 2014.

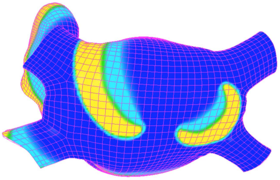
Cardiac electrophysiology example

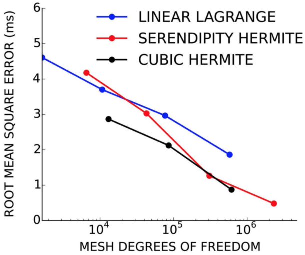


Benchmark electrophysiology experiments:

- Simulate electrical propagation in a 20x7x3 mm domain of cardiac tissue, governed by a monodomain equation (reaction-diffusion PDE).
- For error in the quantity of interest (conduction velocity), a cubic serendipity element with Hermite-like basis functions presented the best results in terms of per-DoF cost.
- Further, the dimensionless parameter cell Thiele modulus was found to be a good predictor of this error, with both cubic order elements (red and black) performing similarly. *Shapes and fills identify model and diffusivity choices.*

Cardiac electrophysiology example





Patient-specific geometry experiments:

- Goal is to accurately and efficiently estimate "activation times" for the electrical propagating through the heart (*eventually: in the OR while the patient is sedated!*)
- Solution with tensor product cubic elements with Hermite-like functions on the finest resolution mesh was taken to be a "fully converged" solution
- For error in the quantity of interest (RMS error in activation time) both cubic order elements had smaller error than linear elements, in terms of per-DoF cost.
- The results provide proof-of-concept for the use of higher order serendipity elements on coarse meshes of patient-specific geometry, to clinically-relevant levels of precision in estimates of physical quantities of interest.

A takeaway message

VINCENT, GONZALES, G., VILLONGCO, PEZZUTO, OMENS, HOLST, MCCULLOCH
"High-order interpolation methods for cardiac monodomain simulations,"
Frontiers in Physiology 2015.

- Measurements of error and computational cost that practitioners care about in regards to quad/hex elements may be different than those studied by the math community.
- Additional implementations of quad/hex techniques are needed in order to see widespread adoption of methods that align with the supporting theory.

Acknowledgments

Thanks to the organizers for the invitation to speak!

Research Funding

Supported in part by the National Science Foundation grant DMS-1522289.

Collaborators on this work

Chandrajit Bajaj	UT Austin	computer science
Alexander Rand	CD-adapco	industry
Matthew Gonzales	UC San Diego	bioengineering
Kevin Vincent	UC San Diego	bioengineering

Slides and Pre-prints

http://math.arizona.edu/~agillette/