From Squares and Cubes to Quads and Hexes: Recent Advances in Conforming Finite Elements

Andrew Gillette - University of Arizona

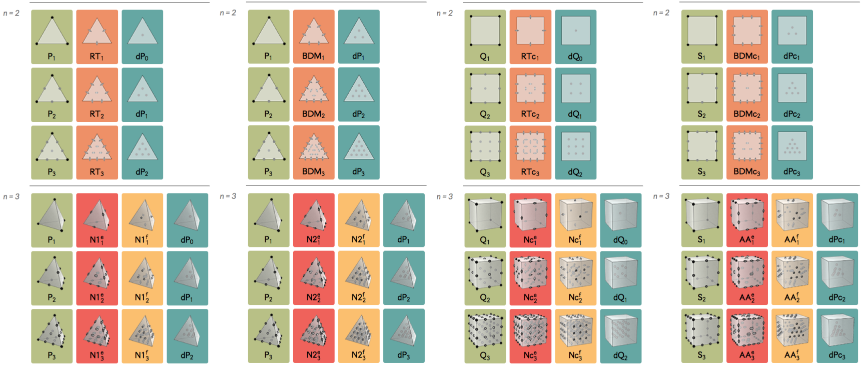


Table of Contents

Outline

1. Squares and cubes: finite element classification
2. Trimmed serendipity spaces: a new family on squares and cubes
3. Quads and Hexes: theory, software, meshing
4. Application priorities? A lesson from cardiac electrophysiology

Classification of conforming methods

Conforming finite element method types can be broadly classified by three integers:

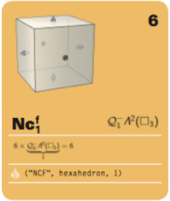
n	$\to$	the spatial dimension of the domain
r	$\to$	the order of error decay
k	$\to$	the differential form order of the solution space

An element type is defined in part by its **degrees of freedom**. Typically:

the more degrees of freedom, the greater the computational cost of the method

Ex: $\mathcal{Q}_1^-\Lambda^2(\square_3)$ is an element for

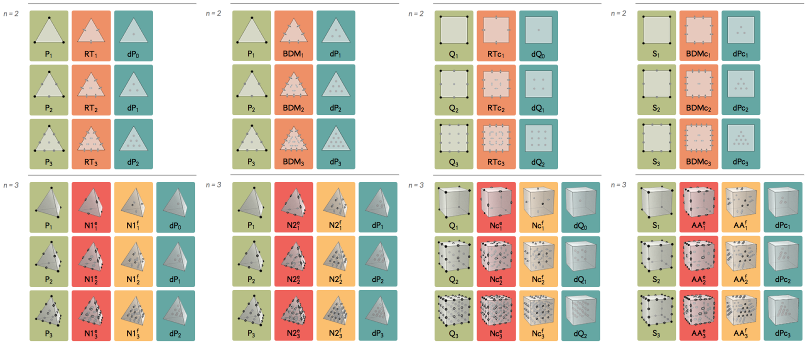
$n = 3$	$\to$	domains in $\mathbb{R}^3$
$r = 1$	$\to$	linear order of error decay
$k = 2$	$\to$	conformity in $\Lambda^2(\mathbb{R}^3) \rightsquigarrow H(\text{div})$



$\mathcal{Q}_1^-\Lambda^2(\square_3)$ is part of the $\mathcal{Q}^-$ 'column' of elements,
is defined on geometry $\square_3$ (i.e. a cube),
has a **6** dimensional space of test functions,
and has an associated set of **6** degrees of freedom
that are unisolvent for the test function space.

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.

$n \quad \rightarrow \quad$ Domains in $\mathbb{R}^2$ (top half) and in $\mathbb{R}^3$ (bottom half)
$r \quad \rightarrow \quad$ Order $1, 2, 3$ of error decay (going down columns)
$k \quad \rightarrow \quad$ Conformity type $k = 0, \ldots, n$ (going across a row)

Geometry types: Simplices (left half) and cubes (right half).

An abbreviated reading list (50 years of theory!)

RAVIART, THOMAS, "A mixed finite element method for 2nd order elliptic problems" *Lecture Notes in Mathematics*, 1977 ← *3254 citations, including 38 from 2018!*

NÉDÉLEC, "Mixed finite elements in $\mathbb{R}^3$," *Numerische Mathematik*, 1980

BREZZI, DOUGLAS JR., MARINI, "Two families of mixed finite elements for second order elliptic problems," *Numerische Mathematik*, 1985

NÉDÉLEC, "A new family of mixed finite elements in $\mathbb{R}^3$," *Numerische Mathematik*, 1986

ARNOLD, FALK, WINTHER "Finite element exterior calculus, homological techniques, and applications," *Acta Numerica*, 2006

CHRISTIANSEN, "Stability of Hodge decompositions in finite element spaces of differential forms in arbitrary dimension," *Numerische Mathematik*, 2007

ARNOLD, FALK, WINTHER "Finite element exterior calculus: from hodge theory to numerical stability," *Bulletin of the AMS*, 2010

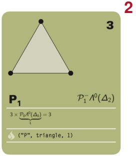
ARNOLD, AWANOU "The serendipity family of finite elements ", *Found. Comp Math*, 2011

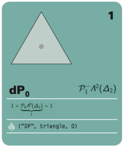
ARNOLD, AWANOU "Finite element differential forms on cubical meshes", *Math Comp.*, 2013

ARNOLD, BOFFI, BONIZZONI "Finite element differential forms on curvilinear meshes and their approximation properties," *Numerische Mathematik*, 2014

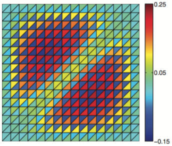
Stable pairs of elements for mixed methods

Picking elements from the table for a mixed method for the Poisson problem:

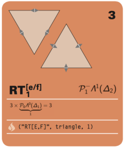


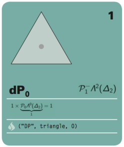


$\subset H^1 \times H^1$ $\subset L^2$ $\Rightarrow$

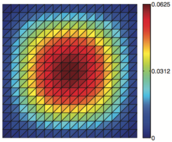


Unstable method





$\subset H(\text{div})$ $\subset L^2$ $\Rightarrow$



Provably stable method

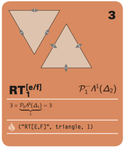
converges to

$u = x(1-x)y(1-y)$

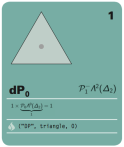
Example and images on right from:

ARNOLD, FALK, WINTHER "Finite Element Exterior Calculus..." *Bulletin of the AMS*, 47:2, 2010.

Method selection and cochain complexes

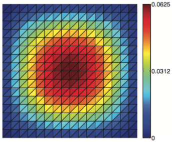


$\subset H(\mathrm{div})$



$\subset L^2$

$\Rightarrow$



Provably stable method

converges to

$$\mathrm{u} = x(1-x)y(1-y)$$

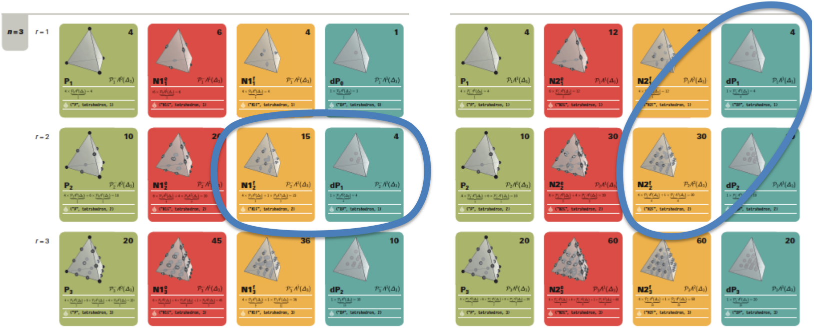
Stable pairs of elements for mixed Hodge-Laplacian problems are found by choosing consecutive spaces in compatible discretizations of the L^2 deRham Diagram.

$$H^1 \xrightarrow[\text{grad}]{\nabla} H(\mathrm{curl}) \xrightarrow[\text{curl}]{\nabla\times} H(\mathrm{div}) \xrightarrow[\text{div}]{\nabla\cdot} L^2$$

	H^1	$H(\mathrm{curl})$	$H(\mathrm{div})$	L^2
vector Poisson	σ	μ		
Maxwell's eqn's		h	b	
Darcy / Poisson			$\mathbf{u}$	p

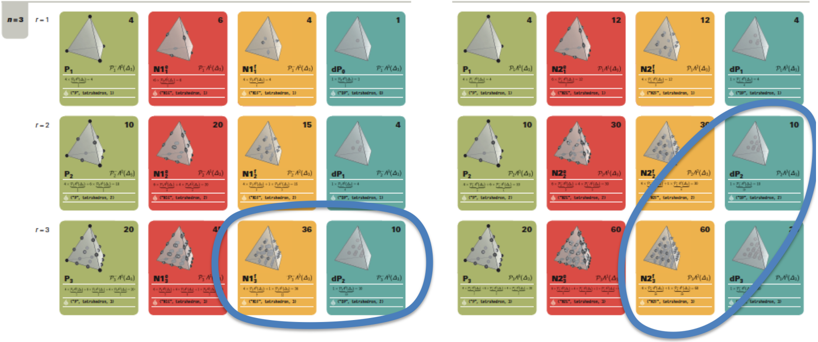
The Periodic Table of Finite Elements lets us 'read off' stable pairs visually.

Stable pairs for tetrahedral meshes



Problem: Darcy / Poisson
Dimension: $n = 3$
Mesh type: tetrahedral
Convergence: quadratic ($r = 2$)

Stable pairs for tetrahedral meshes

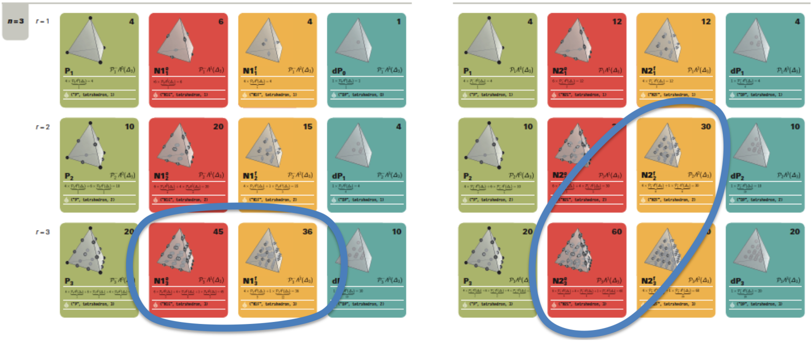


Problem: Darcy / Poisson
Dimension: $n = 3$
Mesh type: tetrahedral
Convergence: cubic ($r = 3$)

Stable pairs for tetrahedral meshes

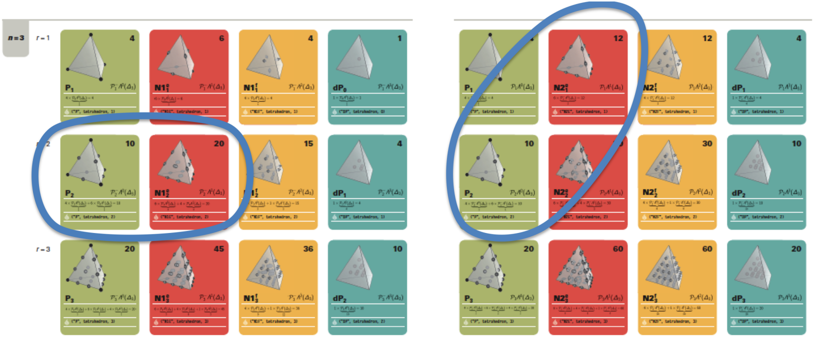
Problem: Maxwell's
Dimension: $n = 3$
Mesh type: tetrahedral
Convergence: quadratic ($r = 2$)

Stable pairs for tetrahedral meshes



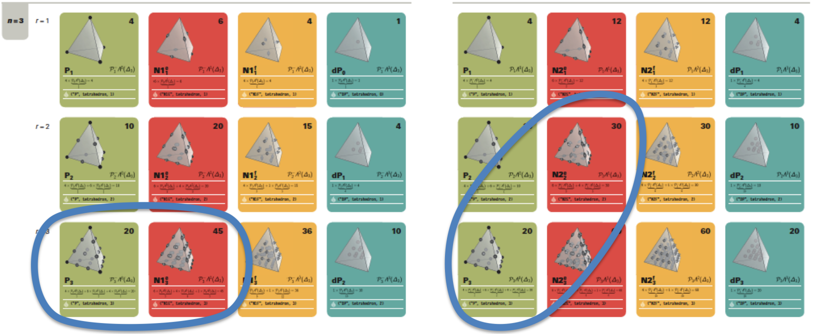
Problem: Maxwell's
Dimension: $n = 3$
Mesh type: tetrahedral
Convergence: cubic ($r = 3$)

Stable pairs for tetrahedral meshes



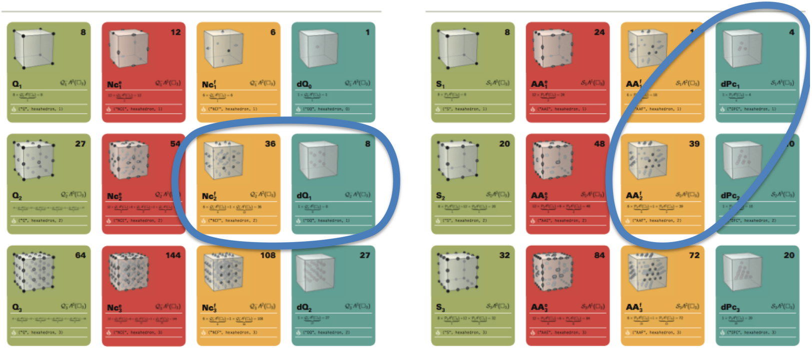
Problem: vector Poisson
Dimension: $n = 3$
Mesh type: tetrahedral
Convergence: quadratic ($r = 2$)

Stable pairs for tetrahedral meshes



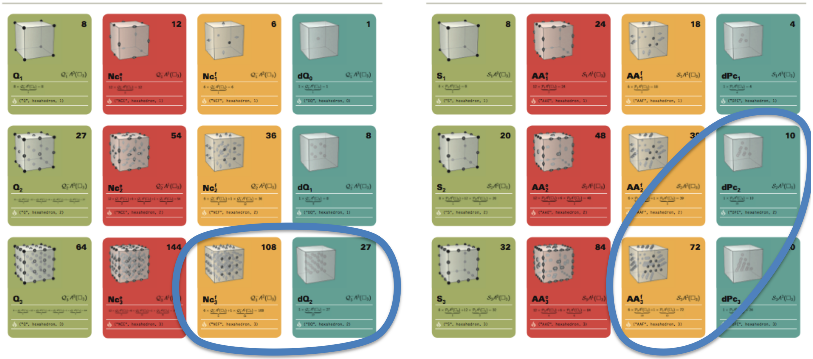
Problem: vector Poisson
Dimension: $n = 3$
Mesh type: tetrahedral
Convergence: cubic ($r = 3$)

Stable pairs for cubical meshes



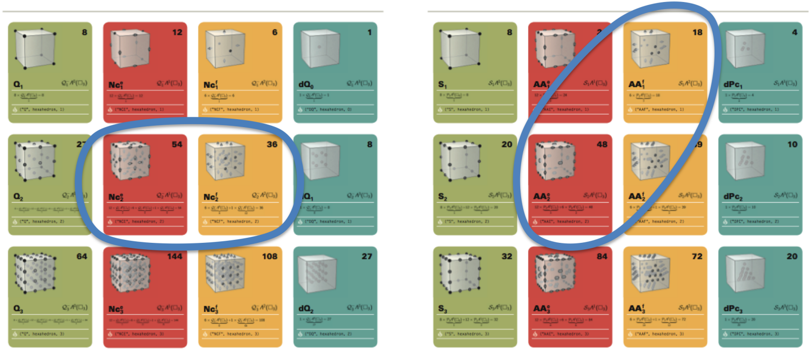
Problem:	Darcy / Poisson
Dimension:	$n = 3$
Mesh type:	cubes
Convergence:	quadratic ($r = 2$)

Stable pairs for cubical meshes



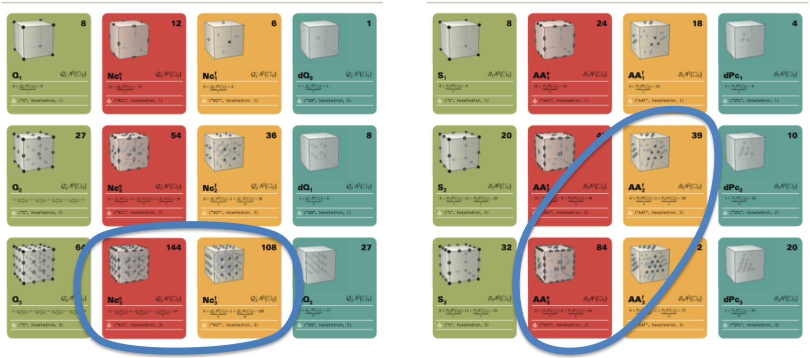
Problem:	Darcy / Poisson
Dimension:	$n = 3$
Mesh type:	cubes
Convergence:	cubic ($r = 3$)

Stable pairs for cubical meshes



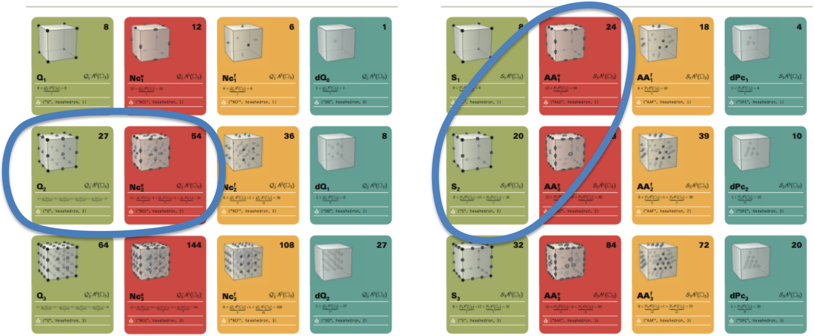
Problem:	Maxwell's
Dimension:	$n = 3$
Mesh type:	cubes
Convergence:	quadratic ($r = 2$)

Stable pairs for cubical meshes



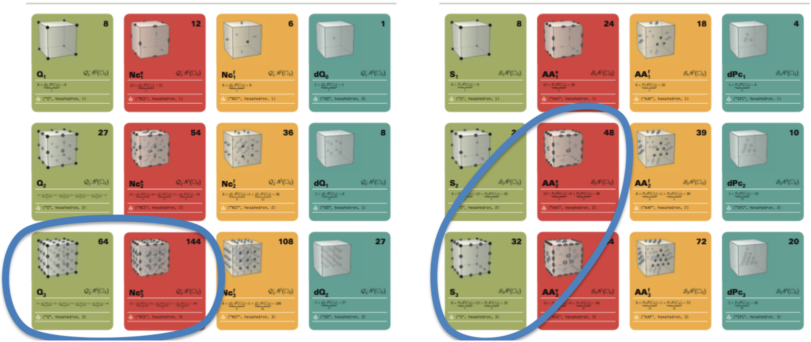
Problem: Maxwell's
Dimension: $n = 3$
Mesh type: cubes
Convergence: cubic ($r = 3$)

Stable pairs for cubical meshes



Problem: vector Poisson
Dimension: $n = 3$
Mesh type: cubes
Convergence: quadratic ($r = 2$)

Stable pairs for cubical meshes



Problem: vector Poisson
Dimension: $n = 3$
Mesh type: cubes
Convergence: cubic ($r = 3$)

Exact cochain complexes found in the table

On an n-simplex in $\mathbb{R}^n$:

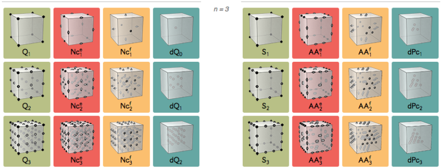
$$\mathcal{P}_r^-\Lambda^0 \to \mathcal{P}_r^-\Lambda^1 \to \cdots \to \mathcal{P}_r^-\Lambda^{n-1} \to \mathcal{P}_r^-\Lambda^n$$ **'trimmed' polynomials**

$$\mathcal{P}_r\Lambda^0 \to \mathcal{P}_{r-1}\Lambda^1 \to \cdots \to \mathcal{P}_{r-n+1}\Lambda^{n-1} \to \mathcal{P}_{r-n}\Lambda^n$$ **polynomials**

On an n-dimensional cube in $\mathbb{R}^n$:

$$\mathcal{Q}_r^-\Lambda^0 \to \mathcal{Q}_r^-\Lambda^1 \to \cdots \to \mathcal{Q}_r^-\Lambda^{n-1} \to \mathcal{Q}_r^-\Lambda^n$$ **tensor product**

$$\mathcal{S}_r\Lambda^0 \to \mathcal{S}_{r-1}\Lambda^1 \to \cdots \to \mathcal{S}_{r-n+1}\Lambda^{n-1} \to \mathcal{S}_{r-n}\Lambda^n$$ **serendipity**



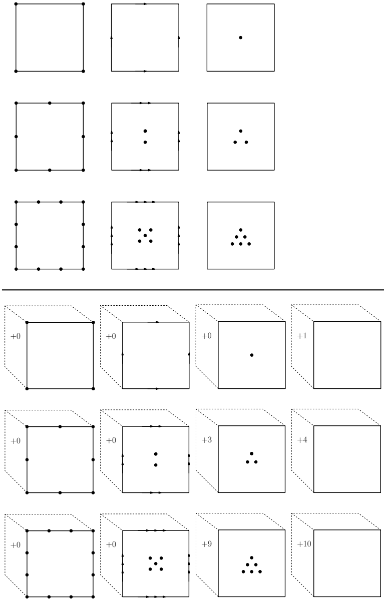
The 'minus' spaces proceed across rows of the PToFE (***r* is fixed**) while the 'regular' spaces proceed along diagonals (***r* decreases**)

Mysteriously, the degree of freedom count for mixed methods from the $\mathcal{P}_r^-$ spaces is smaller than those from the $\mathcal{P}_r$ spaces, while the opposite is true for the $\mathcal{Q}_r^-$ and $\mathcal{S}_r$ spaces.

Outline

1. Squares and cubes: finite element classification
2. Trimmed serendipity spaces: a new family on squares and cubes
3. Quads and Hexes: theory, software, meshing
4. Application priorities? A lesson from cardiac electrophysiology

The 5th column: Trimmed serendipity spaces



A new column for the PToFE:
the **trimmed serendipity** elements.

$\boxed{\mathcal{S}_r^- \Lambda^k(\square_n)}$ denotes

approximation order r,
subset of k-form space $\Lambda^k(\Omega)$,
use on meshes of n-dim'l cubes.

Defined for any $n \geq 1$, $0 \leq k \leq n$, $r \geq 1$

Identical or analogous properties to all the other colummns in the table.

The advantage of the $\mathcal{S}_r^- \Lambda^k$ spaces is that they have fewer degrees of freedom for mixed methods than their tensor product and serendipity counterparts.

G., KLOEFKORN "Trimmed Serendipity Finite Element Differential Forms" *Mathematics of Computation*, to appear.
See `arXiv:1607.00571`

Key properties of the trimmed serendipity spaces

$$\mathcal{Q}_r^-\Lambda^0 \to \mathcal{Q}_r^-\Lambda^1 \to \cdots \to \mathcal{Q}_r^-\Lambda^{n-1} \to \mathcal{Q}_r^-\Lambda^n$$ **tensor product**

$$\mathcal{S}_r\Lambda^0 \to \mathcal{S}_{r-1}\Lambda^1 \to \cdots \to \mathcal{S}_{r-n+1}\Lambda^{n-1} \to \mathcal{S}_{r-n}\Lambda^n$$ **serendipity**

$$\mathcal{S}_r^-\Lambda^0 \to \mathcal{S}_r^-\Lambda^1 \to \cdots \to \mathcal{S}_r^-\Lambda^{n-1} \to \mathcal{S}_r^-\Lambda^n$$ **trimmed serendipity**

Subcomplex: $d\mathcal{S}_r^-\Lambda^k \subset \mathcal{S}_r^-\Lambda^{k+1}$

Exactness: The above sequence is exact.
i.e. the image of incoming map = kernel of outgoing map

Inclusion: $\mathcal{S}_r\Lambda^k \subset \mathcal{S}_{r+1}^-\Lambda^k \subset \mathcal{S}_{r+1}\Lambda^k$

Trace: $\mathrm{tr}_f\mathcal{S}_r^-\Lambda^k(\mathbb{R}^n) \subset \mathcal{S}_r^-\Lambda^k(f)$, for any $(n-1)$-hyperplane f in $\mathbb{R}^n$

Special cases:
$\mathcal{S}_r^-\Lambda^0 = \mathcal{S}_r\Lambda^0$
$\mathcal{S}_r^-\Lambda^n = \mathcal{S}_{r-1}\Lambda^n$
$\mathcal{S}_r^-\Lambda^k + d\mathcal{S}_{r+1}\Lambda^{k-1} = \mathcal{S}_r\Lambda^k$.

Replace '$\mathcal{S}$' by '$\mathcal{P}$' $\rightsquigarrow$ key properties about the first two columns for $\mathcal{P}_r^-\Lambda^k$ and $\mathcal{P}_r\Lambda^k$!

Dimension count and comparison

Formula for counting degrees of freedom of $\mathcal{S}_r^- \Lambda^k(\square_n)$:

$$\sum_{d=k}^{\min\{n,\lfloor r/2\rfloor+k\}} 2^{n-d}\binom{n}{d}\left(\binom{r-d+2k-1}{r-d+k-1}\binom{r-d+k-1}{d-k}+\binom{r-d+2k}{k}\binom{r-d+k-1}{d-k-1}\right)$$

	k	r=1	2	3	4	5	6	7
n=2	0	4	8	12	17	23	30	38
	1	4	10	17	26	37	50	65
	2	1	3	6	10	15	21	28
n=3	0	8	20	32	50	74	105	144
	1	12	36	66	111	173	255	360
	2	6	21	45	82	135	207	301
	3	1	4	10	20	35	56	84
n=4	0	16	48	80	136	216	328	480
	1	32	112	216	392	656	1036	1563
	2	24	96	216	422	746	1227	1910
	3	8	36	94	200	375	644	1036
	4	1	5	15	35	70	126	210

Mixed Method dimension comparison 1

Mixed method for Darcy problem:
$$\begin{aligned} \mathbf{u} + K\nabla p &= 0 \\ \operatorname{div}\ \mathbf{u} - f &= 0 \end{aligned}$$

We compare degree of freedom counts among the three families for use on meshes of affinely-mapped squares or cubes, when a conforming method with (at least) order r decay in the approximation of p, $\mathbf{u}$, and div $\mathbf{u}$ is desired.

Total # of degrees of freedom on a square ($n = 2$):

r	$\lvert\mathcal{Q}_r^-\Lambda^1\rvert + \lvert\mathcal{Q}_r^-\Lambda^2\rvert$	$\lvert\mathcal{S}_r\Lambda^1\rvert + \lvert\mathcal{S}_{r-1}\Lambda^2\rvert$	$\lvert\mathcal{S}_r^-\Lambda^1\rvert + \lvert\mathcal{S}_r^-\Lambda^2\rvert$
1	4+1 = 5	8+1 = 9	4+1 = 5
2	12+4 = 16	14+3 = 17	10+3 = 13
3	24+9 = 33	22+6 = 28	17+6 = 23

Total # of degrees of freedom on a cube ($n = 3$):

r	$\lvert\mathcal{Q}_r^-\Lambda^2\rvert + \lvert\mathcal{Q}_r^-\Lambda^3\rvert$	$\lvert\mathcal{S}_r\Lambda^2\rvert + \lvert\mathcal{S}_{r-1}\Lambda^3\rvert$	$\lvert\mathcal{S}_r^-\Lambda^2\rvert + \lvert\mathcal{S}_r^-\Lambda^3\rvert$
1	6+1 = 7	18+1 = 19	6+1 = 7
2	36+8 = 44	39+4 = 43	21+4 = 25
3	108+27 = 135	72+10 = 82	45+10 = 55

Mixed Method dimension comparison 2

Mixed method for Darcy problem:

$$\begin{aligned} \mathbf{u} + K\nabla p &= 0 \\ \operatorname{div}\ \mathbf{u} - f &= 0 \end{aligned}$$

The number of interior degrees of freedom is reduced from tensor product, to serendipity, to trimmed serendipity:

\# of **interior** degrees of freedom on a square ($n = 2$):

r	$\lvert\mathcal{Q}_r^-\Lambda_0^1\rvert + \lvert\mathcal{Q}_r^-\Lambda_0^2\rvert$	$\lvert\mathcal{S}_r\Lambda_0^1\rvert + \lvert\mathcal{S}_{r-1}\Lambda_0^2\rvert$	$\lvert\mathcal{S}_r^-\Lambda_0^1\rvert + \lvert\mathcal{S}_r^-\Lambda_0^2\rvert$
1	0+1 = 1	0+1 = 1	0+1 = 1
2	4+4 = 8	2+3 = 5	2+3 = 5
3	12+9 = 21	6+6 = 12	5+6 = 11

\# of **interior** degrees of freedom on a cube ($n = 3$):

r	$\lvert\mathcal{Q}_r^-\Lambda_0^2\rvert + \lvert\mathcal{Q}_r^-\Lambda_0^3\rvert$	$\lvert\mathcal{S}_r\Lambda_0^2\rvert + \lvert\mathcal{S}_{r-1}\Lambda_0^3\rvert$	$\lvert\mathcal{S}_r^-\Lambda_0^2\rvert + \lvert\mathcal{S}_r^-\Lambda_0^3\rvert$
1	0+1 = 1	0+1 = 1	0+1 = 1
2	12+8 = 20	3+4 = 7	3+4 = 7
3	54+27 = 81	12+10 = 22	9+10 = 19

Mixed Method dimension comparison 3

Mixed method for Darcy problem:
$$\begin{aligned} \mathbf{u} + K\nabla p &= 0 \\ \text{div } \mathbf{u} - f &= 0 \end{aligned}$$

Assuming interior degrees of freedom could be dealt with efficiently (e.g. by static condensation), trimmed serendipity elements *still* have the fewest DoFs:

\# of **interface** (edge) degrees of freedom on a square ($n = 2$):

r	$\lvert\mathcal{Q}_r^-\Lambda^1(\partial\square_2)\rvert$	$\lvert\mathcal{S}_r\Lambda^1(\partial\square_2)\rvert$	$\lvert\mathcal{S}_r^-\Lambda^1(\partial\square_2)\rvert$
1	4	8	4
2	8	12	8
3	12	16	12

\# of **interface** (edge+face) degrees of freedom on a cube ($n = 3$):

r	$\lvert\mathcal{Q}_r^-\Lambda^2(\partial\square_3)\rvert$	$\lvert\mathcal{S}_r\Lambda^2(\partial\square_3)\rvert$	$\lvert\mathcal{S}_r^-\Lambda^2(\partial\square_3)\rvert$
1	6	18	6
2	24	36	18
3	54	60	36

Decomposition by polynomial subspace

$\mathcal{S}_r^-\Lambda^k(\square_n)$ is a space of differential k-forms whose coefficients are polynomials in $\mathbb{R}^n$.

$$\mathcal{S}_r^-\Lambda^k = \mathcal{P}_r^-\Lambda^k \oplus \mathcal{J}_r\Lambda^k \oplus d\mathcal{J}_r\Lambda^{k-1}$$

Polynomial coefficients in each summand:

$\mathcal{P}_r^-\Lambda^k$: anything up to degree $r-1$ and some degree r

$\mathcal{J}_r\Lambda^k$: certain polynomials whose degree is between $r+1$ and $r+n-k-1$

$d\mathcal{J}_r\Lambda^{k-1}$: certain polynomials whose degree is between r and $r+n-k-2$

The "regular" serendipity space has an analogous decomposition:

$$\mathcal{S}_r\Lambda^k = \mathcal{P}_r\Lambda^k \oplus \mathcal{J}_r\Lambda^k \oplus d\mathcal{J}_{r+1}\Lambda^{k-1}$$

– – – – – – – – – – – – –

This decomposition provides a direct sum into some precise but elaborate subspaces:

$$\mathcal{J}_r\Lambda^k(\mathbb{R}^n) := \sum_{l\geq 1} \kappa\mathcal{H}_{r+l-1,l}\Lambda^{k+1}(\mathbb{R}^n),$$

where $\mathcal{H}_{r,l}\Lambda^k(\mathbb{R}^n) := \left\{\omega \in \mathcal{H}_r\Lambda^k(\mathbb{R}^n) \mid \text{ldeg}\ \omega \geq l\right\},$

where $\text{ldeg}(x^\alpha dx_\sigma) := \#\{i \in \sigma^* \ : \ \alpha_i = 1\}.$

Decomposition by Cubical Geometry

We can also decompose $\mathcal{S}_r^- \Lambda^k(\square_n)$ by the subspace of "zero trace":

$$\mathcal{S}_r^- \Lambda^k = \mathcal{S}_r^- \Lambda^k_{\mathbf{0}} \oplus \left(\mathcal{S}_r^- \Lambda^k_{\mathbf{0}}\right)^\perp$$

We use this decomposition to prove that $\mathcal{S}_r^- \Lambda^\bullet(\square_n)$ is a **minimal compatible finite element system** containing $\mathcal{P}_{r-1}\Lambda^\bullet(\square_n)$.

– – – – – – – – – – – – – –

A computational basis for $\mathcal{S}_r^- \Lambda^k_{\mathbf{0}}$ would aid in the construction of bases for $\mathcal{S}_r^- \Lambda^k$.

Building such a basis is non-trvial. Consider

$$\alpha := \begin{array}{r} (z-1)(y^2-1)\ dx \\ +y(x+1)(z-1)\ dy \\ +(x+1)(y^2-1)\ dz \end{array} \qquad \beta := \begin{array}{r} (z-1)(y^2-1)\ dx \\ -2y(x+1)(z-1)\ dy \\ +(x+1)(y^2-1)\ dz \end{array}$$

Both α and β have a natural association to the approximation of y on the edge

$\{x=1, z=-1\}$, and both are elements of $\mathcal{Q}_2\Lambda^1(\square_3)$. But *only* β is in $\mathcal{S}_1\Lambda^1(\square_3)$!

Decompositions shared insight

Why is $\beta \in \mathcal{S}_1\Lambda^1(\square_3)$?

$$\beta = \begin{array}{r} (z-1)(y^2-1)\,dx \\ -2y(x+1)(z-1)\,dy \\ +(x+1)(y^2-1)\,dz \end{array}$$

$$= \underbrace{\begin{array}{r} y^2z\,dx \\ -2xyz\,dy \\ xy^2\,dz \end{array} + \begin{array}{r} -y^2\,dx \\ 2xy\,dy \\ 0\,dz \end{array} + \begin{array}{r} 0\,dx \\ -2yz\,dy \\ y^2\,dz \end{array}}_{\text{basis elements for } d\mathcal{J}_2\Lambda^0} + \underbrace{\begin{array}{r} (-z+1)\,dx \\ 2y\,dy \\ (-x-1)\,dz \end{array}}_{\in\mathcal{P}_1\Lambda^1}.$$

From the polynomial subspace decompositions:

$$\beta \in d\mathcal{J}_2\Lambda^0 \oplus \mathcal{P}_1\Lambda^1 \quad \subset \mathcal{S}_1\Lambda^1$$

$$\beta \in d\mathcal{J}_2\Lambda^0 \oplus \mathcal{P}_1\Lambda^1 \quad \subset \mathcal{S}_2^-\Lambda^1$$

Full report on this approach coming soon!

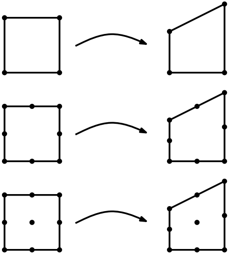
Outline

1. Squares and cubes: finite element classification
2. Trimmed serendipity spaces: a new family on squares and cubes
3. Quads and Hexes: theory, software, meshing
4. Application priorities? A lesson from cardiac electrophysiology

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

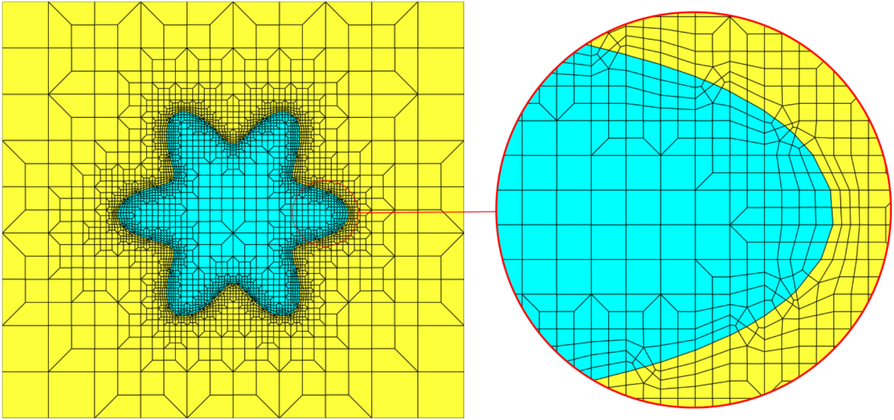


	$\|\|u - u_h\|\|_{L^2}$	$\|\|\nabla(u - u_h)\|\|_{L^2}$
linear	$O(h^2)$	$O(h)$
quadratic serendipity	$O(h^2)$	$O(h)$
quadratic tensor prod.	$O(h^3)$	$O(h^2)$

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

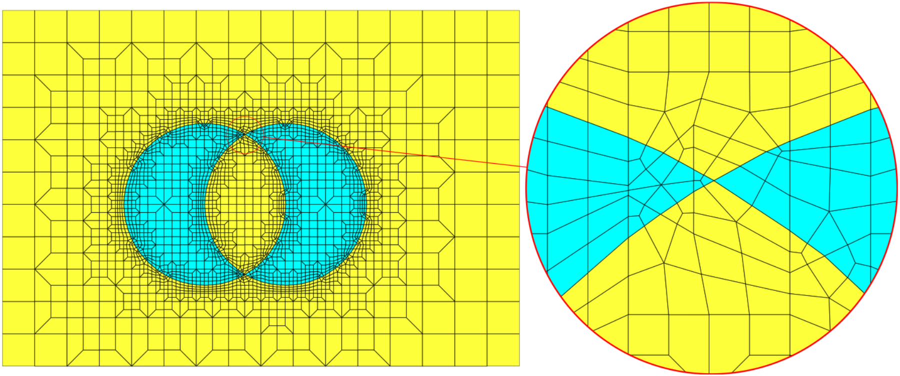
Recent advances in quad meshing



An all-quad mesh conforming to a given curve.

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

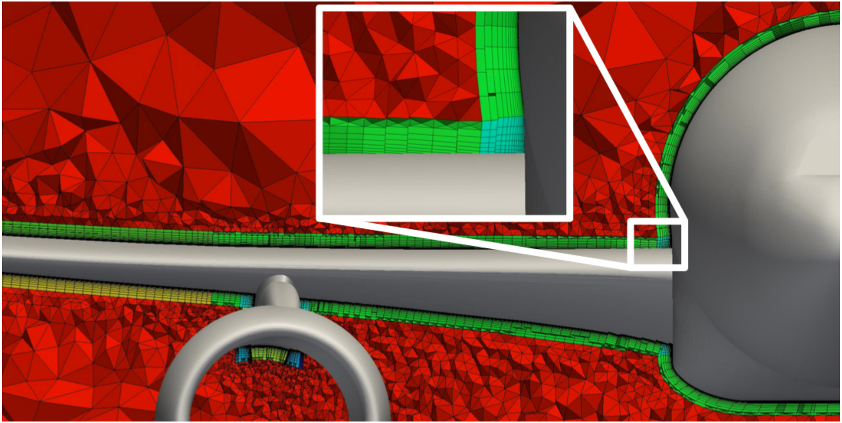
Recent advances in quad meshing



An all-quad mesh conforming to a given curve.

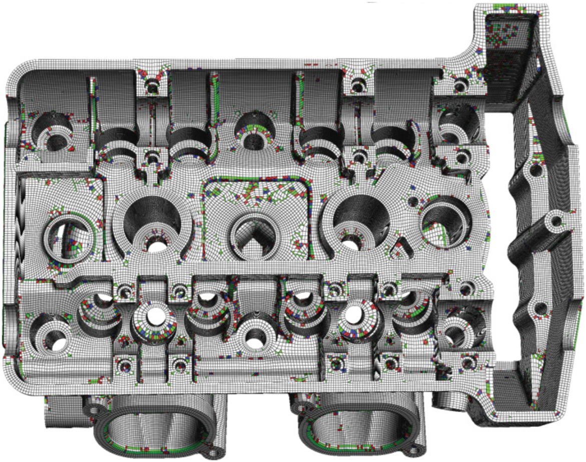
RUSHDI ET AL. "All-quad meshing without cleanup," *Computer-Aided Design*, 2017

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

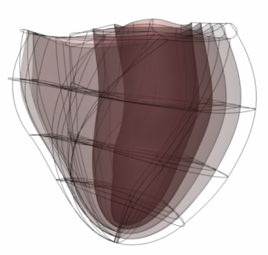


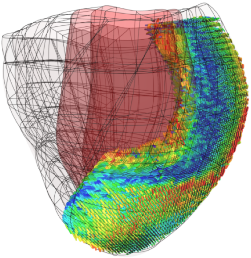
→ A hex-dominant mesh with ≈1.3 million cells, including ≈1 million hexahedra.
→ Re-meshed from a mesh of ≈ 10 million tetrahedra.

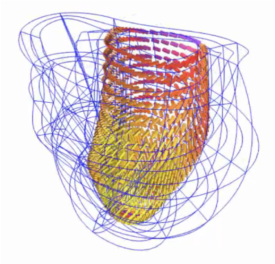
SOKOLOV ET AL. "Hexahedral-Dominant Meshing," *ACM Trans. Graphics*, 2016

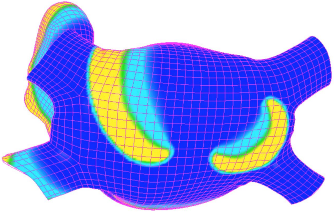
Established models use hexahedral meshes

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

Open source finite element software

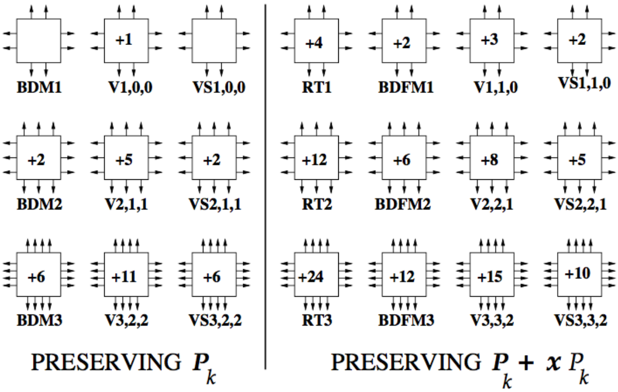
FEniCS primarily supports simplicial elements

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!

The virtual element technique



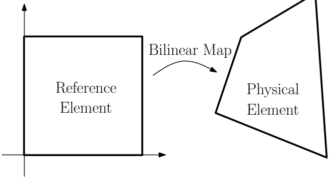
→ Analogues of conforming finite element spaces on squares can be treated as virtual elements.

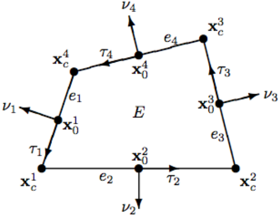
→ Explicit basis functions are not needed to implement the method.

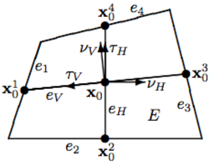
→ Related polygonal element methods (HHO, HDG, WG. . .) may offer similar approaches.

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

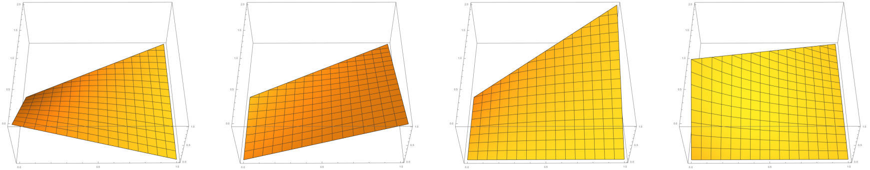
Let P be a convex polytope with vertex set V. We say that

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

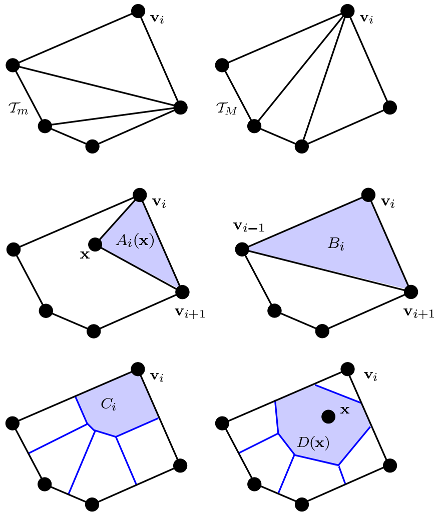
if they satisfy $\quad \lambda_{\mathbf{v}} \geq 0$ on P and $\displaystyle L = \sum_{\mathbf{v} \in V} L(\mathbf{v}_{\mathbf{v}})\lambda_{\mathbf{v}}, \quad \forall\, L : P \to \mathbb{R}$ linear.

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 . . .



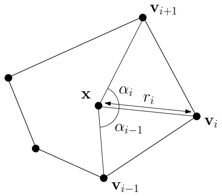
- Triangulation
  ⇒ FLOATER, HORMANN, KÓS, *A general construction of barycentric coordinates over convex polygons*, 2006

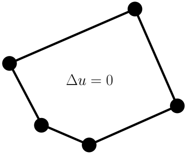
$$0 \leq \lambda_i^{\mathcal{T}_m}(\mathbf{x}) \leq \lambda_i(\mathbf{x}) \leq \lambda_i^{\mathcal{T}_M}(\mathbf{x}) \leq 1$$

- 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 . . .



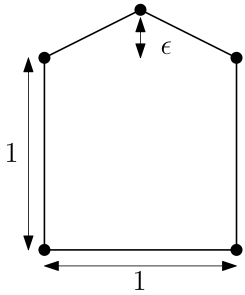


- Mean value
  ⇒ FLOATER, *Mean value coordinates*, 2003.
  ⇒ FLOATER, KÓS, REIMERS, *Mean value coordinates in 3D*, 2005.

- 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



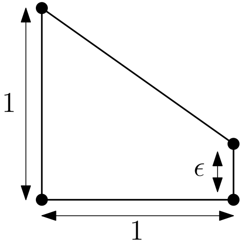
On a ***single*** element with a large angle:

- 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 $\left|u_h^{\text{hm}}\right|_{H^1}$ and $\left|u_h^{\text{hm}} - u_h^*\right|_{H^1}$

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

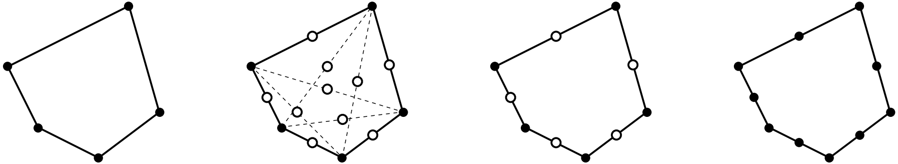


On a quadrilateral with a very short edge:

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!

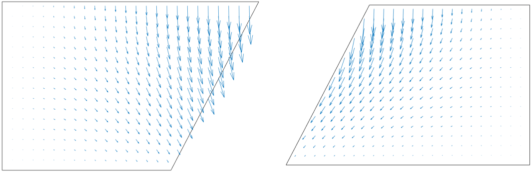
Higher order and vector-valued GBC elements



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

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

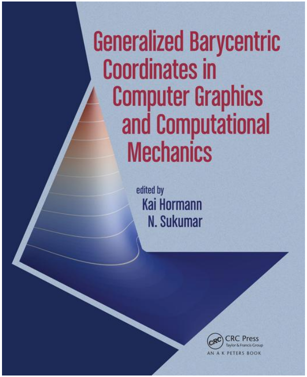
Rand, G, Bajaj, "Quadratic Serendipity Finite Element on Polygons Using Generalized Barycentric Coordinates," *Math. Comp.*, 2011.



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!*

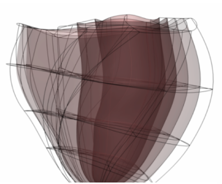
Book available from CRC Press (2017).

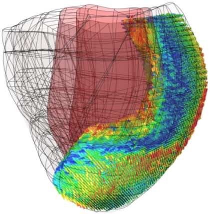
Chapter 2: G., RAND "Shape quality for generalized barycentric interpolation."

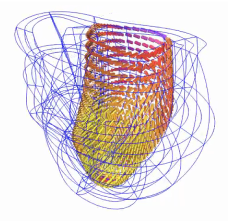
Outline

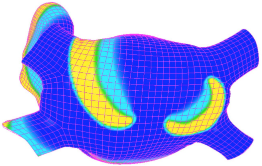
Returning to the cardiac electrophysiology example...

- 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?



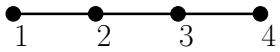






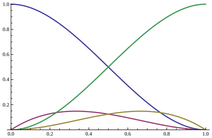
McCulloch research group, *Continuity* software
National Biomedical Computation Resource
UC San Diego
2006–2017

Cubic Hermite Geometric Decomposition: 1D

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

Cubic Hermite Basis on $[0, 1]$

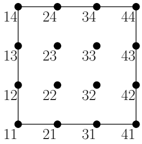
$$\begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{bmatrix} := \begin{bmatrix} 1 - 3x^2 + 2x^3 \\ x - 2x^2 + x^3 \\ x^2 - x^3 \\ 3x^2 - 2x^3 \end{bmatrix}$$



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

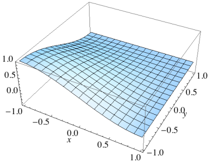
$$\underbrace{\left\{ \begin{array}{c} x^r y^s \\ 0 \le r,s \le 3 \end{array} \right\}}_{\mathcal{Q}_3([0,1]^2)} \quad \longleftrightarrow \quad \left\{ \begin{array}{c} \psi_i(x)\psi_j(y) \\ 1 \le i,j \le 4 \end{array} \right\} \quad \longleftrightarrow$$



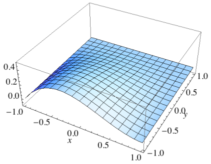
monomials $\longleftrightarrow$ **basis functions** $\longleftrightarrow$ **domain points**

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.

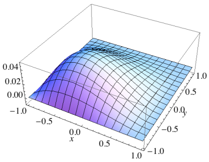
Geometry:



ψ_{11}



ψ_{21}

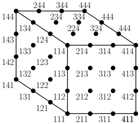


ψ_{22}

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

Cubic Hermite Geometric Decomposition: 3D

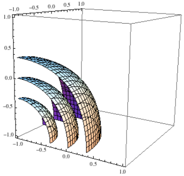
$$\underbrace{\left\{ \begin{array}{c} x^r y^s z^t \\ 0 \leq r, s, t \leq 3 \end{array} \right\}}_{\mathcal{Q}_3([0,1]^3)} \longleftrightarrow \begin{array}{c} \psi_i(x)\psi_j(y)\psi_k(z) \\ 1 \leq i, j, k \leq 4 \end{array} \longleftrightarrow$$



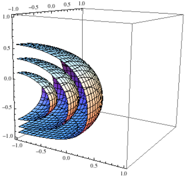
monomials $\longleftrightarrow$ **basis functions** $\longleftrightarrow$ **domain points**

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.

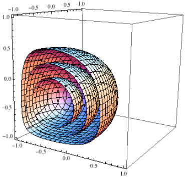
Geometry: Contours of level sets of the basis functions:



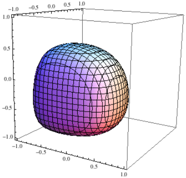
ψ_{111}



ψ_{112}



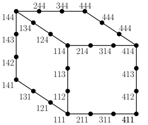
ψ_{212}



ψ_{222}

Cubic Hermite Serendipity Geom. Decomp: 3D

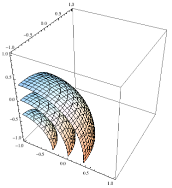
$$\underbrace{\left\{ \begin{array}{c} x^r y^s z^t \\ \text{sldeg} \le 3 \end{array} \right\}}_{\mathcal{S}_3([0,1]^3)} \longleftrightarrow \left\{ \begin{array}{c} \vartheta_{\ell mn} \\ \text{(defined in paper)} \end{array} \right\} \longleftrightarrow$$



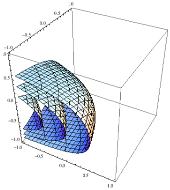
monomials $\longleftrightarrow$ **basis functions** $\longleftrightarrow$ **domain points**

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 $(x^r y^s z^t) \le 3$

Geometry:



ϑ_{111}



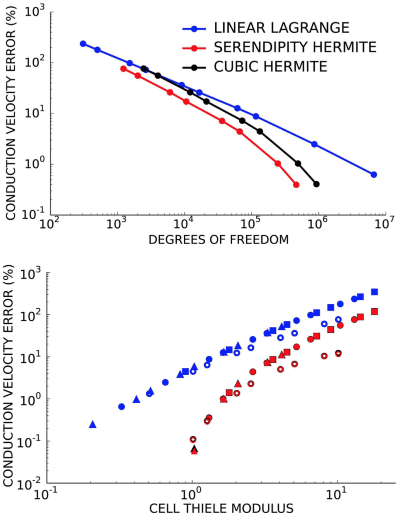
ϑ_{112}

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

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

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

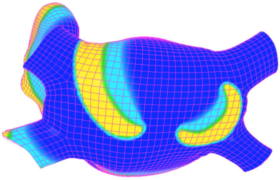
Cardiac electrophysiology example

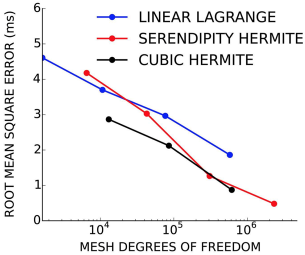


Benchmark electrophysiology experiments:

- 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 for the invitation to speak!

Collaborators on this work

Tyler Kloefkorn	AAAS STP Fellow, hosted at NSF
Chandrajit Bajaj	UT Austin
Alexander Rand	CD-adapco
Matthew Gonzales	UC San Diego
Kevin Vincent	UC San Diego

Research Funding

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

Slides and Pre-prints

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