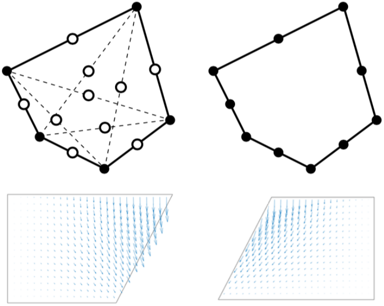
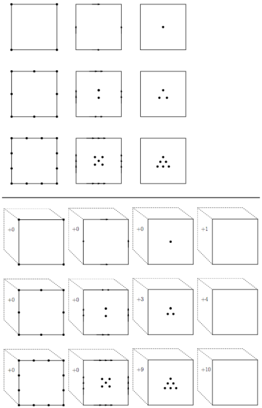
Serendipity Elements: Old and New

Andrew Gillette - University of Arizona

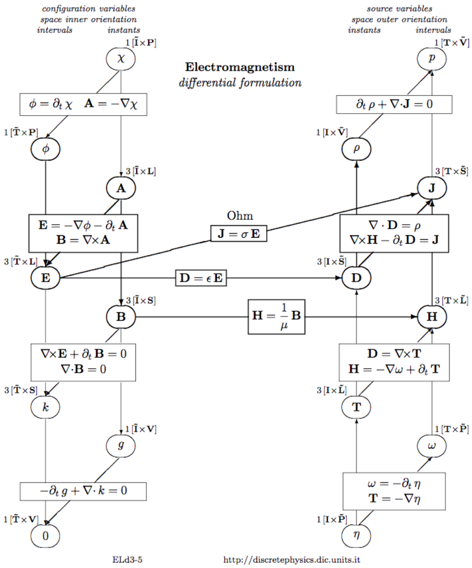




joint work with: Chandrajit Bajaj, Alex Rand

Snorre Christiansen, Tyler Kloefkorn

A brief story from graduate school. . .



from:

Enzo Tonti
“A classification diagram for physical variables”
2003

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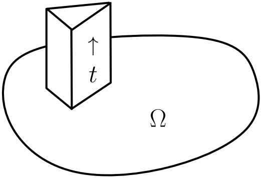
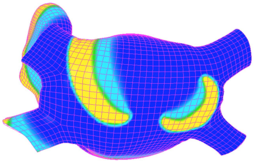
Outline

1. What are "old" serendipity elements?
2. New serendipity elements on polygons and cubes
3. Applications to "big data" and geometry

What are serendipity finite element methods?

The **finite element method** is a way to numerically approximate the solution to PDEs.





$$\begin{bmatrix} & \mathbb{A} & \end{bmatrix} \begin{bmatrix} \mathbf{x} \end{bmatrix} = \begin{bmatrix} \mathbf{b} \end{bmatrix}$$

CHARACTERIZE	DISCRETIZE	SOLVE
Real analysis	Geometry & Topology	Linear algebra
PDEs	Combinatorics	Numerical analysis

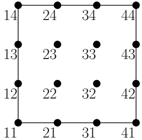
Order of accuracy of computed solution $\rightarrow$ depends on local “basis” functions on each element.

Size of the linear system $\rightarrow$ depends on the number of mesh elements and the number of degrees of freedom associated to each element.

Serendipity methods maximize order of accuracy while minimizing degrees of freedom.

Cubic order tensor product basis functions: 2D

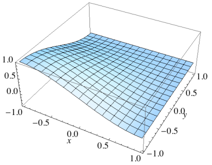
$$\underbrace{\left\{ \begin{array}{c} x^r y^s \\ 0 \le r, s \le 3 \end{array} \right\}}_{\mathcal{Q}_3([0,1]^2)} \longleftrightarrow \left\{ \begin{array}{c} \psi_{ij}(x,y) \\ 1 \le i,j \le 4 \end{array} \right\} \longleftrightarrow$$



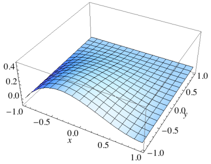
monomials $\longleftrightarrow$ **basis functions** $\longleftrightarrow$ **domain points**

Approximation: For $0 \le r, s \le 3$, the monomial $x^r y^s$ is a linear combination of the ψ_{ij}.

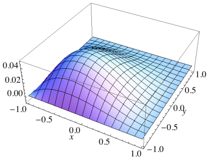
Geometry:



ψ_{11}



ψ_{21}



ψ_{22}

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

Which monomials do we really *need* for cubic order?

tensor product cubics (dim=16)

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

total degree cubics (dim=10)

superlinear cubics (dim=12)

$$\text{total degree}(x^r y^s) = r + s$$

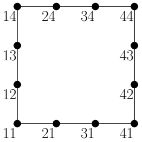
$$\text{superlinear degree}(x^r y^s) = r + s - \{\text{\# of linearly appearing variables}\}$$

	total degree	superlinear degree
xy^2	3	2
x^3y	4	3
xy^3	4	3
x^2y^2	4	4
x^3y^2	5	5

→ For cubic order accuracy, we only *need* all total degree cubics.
→ To ensure a "smooth enough" solution, we expand to the set of all superlinear degree cubics.
→ The notion of superlinear degree and its generalization for serendipity elements comes from ARNOLD, AWANOU Found. Comp Math 2011, Math. Comp. 2013.

Cubic *serendipity* basis functions in 2D and 3D

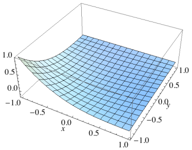
$$\underbrace{\left\{ \begin{array}{c} x^r y^s \\ \text{sldeg} \leq 3 \end{array} \right\}}_{\mathcal{S}_3([0,1]^2)} \longleftrightarrow \left\{ \begin{array}{c} \vartheta_{\ell m}(x,y) \\ \text{(limited indices)} \end{array} \right\} \longleftrightarrow$$



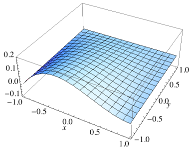
monomials $\longleftrightarrow$ **basis functions** $\longleftrightarrow$ **domain points**

Approximation: For sldeg$(x^r y^s) \leq 3$, $x^r y^s$ is a linear combination of the $\vartheta_{\ell m}$.

Geometry:



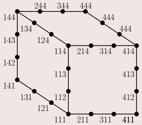
ϑ_{11}



ϑ_{21}

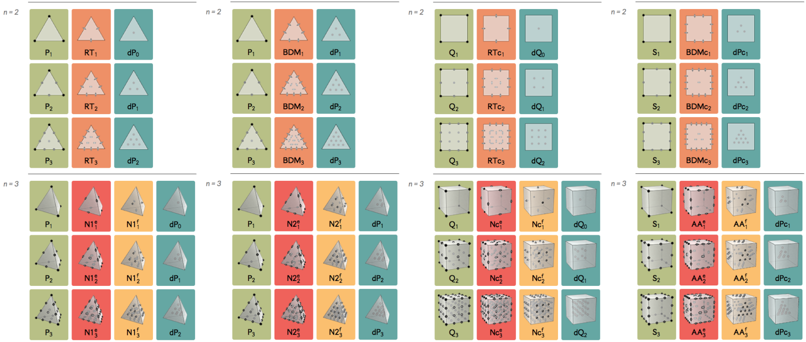
$$\begin{aligned} a(x,y) &= a|_{(0,0)}\vartheta_{11} \\ &+ \partial_x a|_{(0,0)}\vartheta_{21} \\ &+ \partial_y a|_{(0,0)}\vartheta_{12} \\ &+ \cdots \end{aligned}$$

in 3D: $\left\{ \begin{array}{c} x^r y^s z^t \\ \text{sldeg} \leq 3 \end{array} \right\} \longleftrightarrow \left\{ \begin{array}{c} \vartheta_{\ell mn} \\ \text{(limited indices)} \end{array} \right\} \longleftrightarrow$



The ‘Periodic Table of the Finite Elements’

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



Classification of many conforming finite elements on simplices (left) & cubes (right).

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

Prior to 2011, serendipity elements were restricted to squares/cubes & to $k = 0$.

Outline

The generalized barycentric coordinate technique

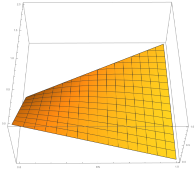
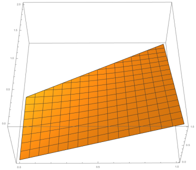
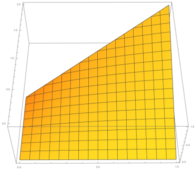
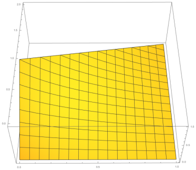
Let P be a convex polytope with vertex set V. We say that

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

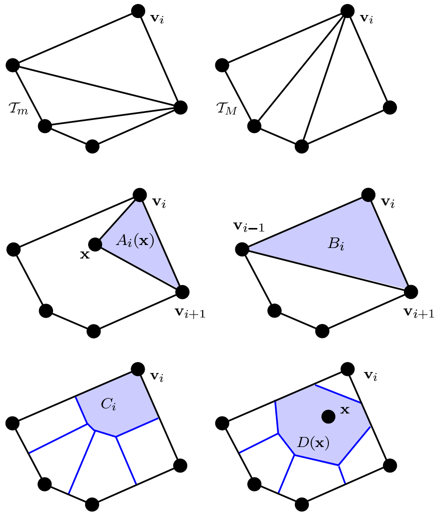
if they satisfy $\lambda_{\mathbf{v}} \geq 0$ on P and $L = \sum_{\mathbf{v} \in V} L(\mathbf{v}_{\mathbf{v}}) \lambda_{\mathbf{v}}, \quad \forall\, L : P \to \mathbb{R}$ linear.

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 . . .

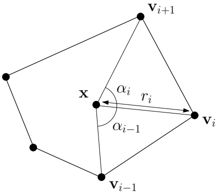


- Triangulation
  ⇒ FLOATER, HORMANN, KÓS, *A general construction of barycentric coordinates over convex polygons*, 2006

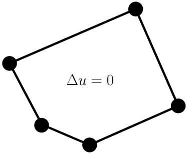
  $$0 \leq \lambda_i^{\mathcal{T}_m}(\mathbf{x}) \leq \lambda_i(\mathbf{x}) \leq \lambda_i^{\mathcal{T}_M}(\mathbf{x}) \leq 1$$

- 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.

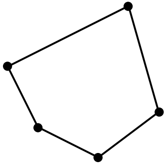


- Harmonic
  ⇒ WARREN, SCHAEFER, HIRANI, DESBRUN, *Barycentric coordinates for convex sets*, 2007.
  ⇒ CHRISTIANSEN, *A construction of spaces of compatible differential forms on cellular complexes*, 2008.
  ⇒ Similar to virtual elements

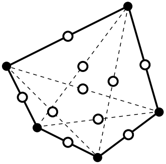
Many more papers could be cited (maximum entropy coordinates, moving least squares coordinates, surface barycentric coordinates, etc...)

From linear to quadratic elements

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



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



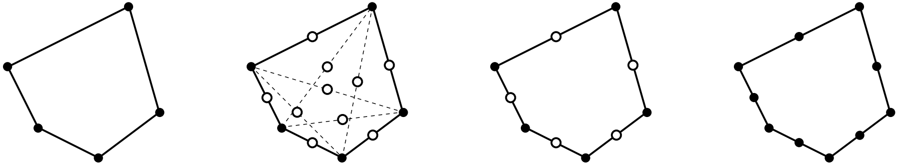
Why is this naïve?

- For a k-gon, this construction gives $k + \binom{k}{2}$ basis functions $\lambda_a\lambda_b$
- The space of quadratic polynomials is only dimension 6: $\{1, x, y, xy, x^2, y^2\}$
- Conforming to a linear function on the boundary requires 2 degrees of freedom per edge $\Rightarrow$ *only $2k$ functions needed!*

Problem Statement

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

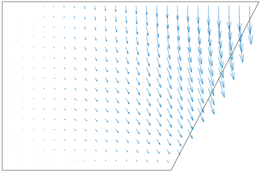
Quadratic and vector-valued GBC elements

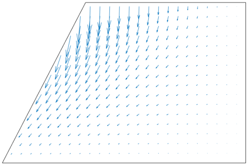


$$\{\lambda_i\} \xrightarrow[\text{products}]{\text{pairwise}} \{\lambda_a\lambda_b\} \xrightarrow{\mathbb{A}} \{\xi_{ij}\} \xrightarrow{\mathbb{B}} \{\psi_{ij}\}$$

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

RAND, G, BAJAJ, "Quadratic Serendipity Finite Element on Polygons Using Generalized Barycentric Coordinates," *Math. Comp.*, 2014.



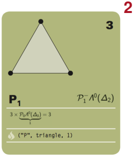


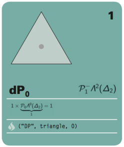
Generalized techniques for vector-valued elements: $\{\lambda_i \nabla \lambda_j\}$

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

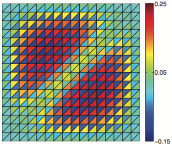
Stable pairs of elements for mixed methods

Picking vector/scalar element pairs for a mixed method for the Poisson problem:



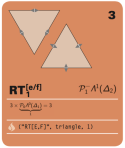


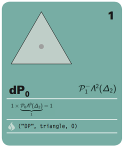
$\Rightarrow$



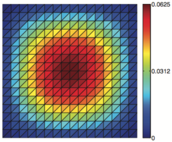
Unstable method

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





$\Rightarrow$



Provably stable method

converges to

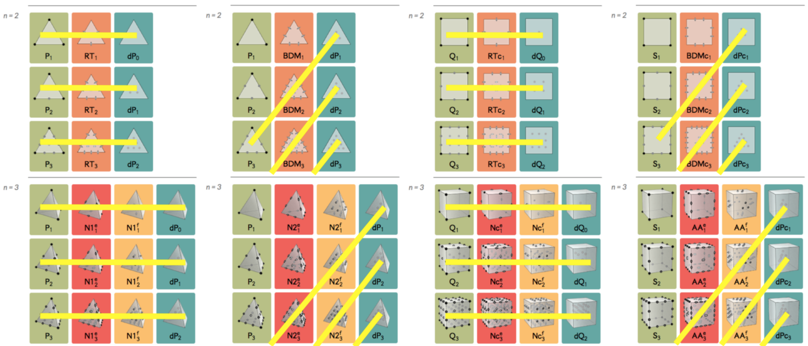
u = $x(1-x)y(1-y)$

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

Example and images on right from:

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

Hidden sequences in the Periodic Table

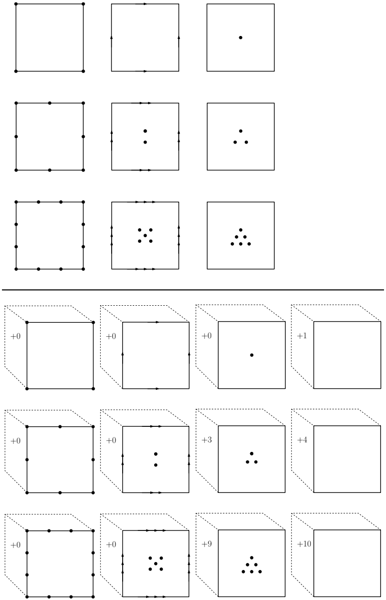


- *Sequences* of elements are used to design stable mixed methods for problems like Darcy flow, Maxwell's equations, vector Poisson, etc.
- The sequences occur either horizontally or diagonally in the table as shown.

Problem Statement

Find a family of serendipity-like elements on squares and cubes with horizontal rather than diagonal sequences.

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`

Outline

1. What are "old" serendipity elements?
2. New serendipity elements on polygons and cubes
3. Applications to "big data" and geometry

Mixed Method dimension comparison 1

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

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

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:

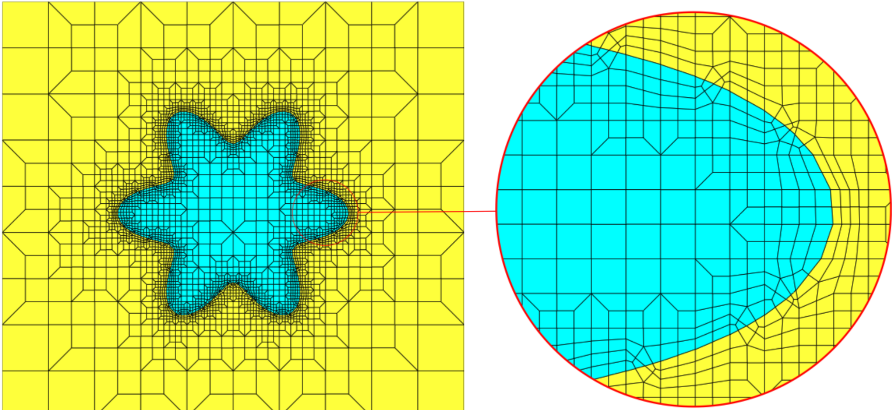
\# of **interface** (edge) degrees of freedom on a square ($n = 2$):

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

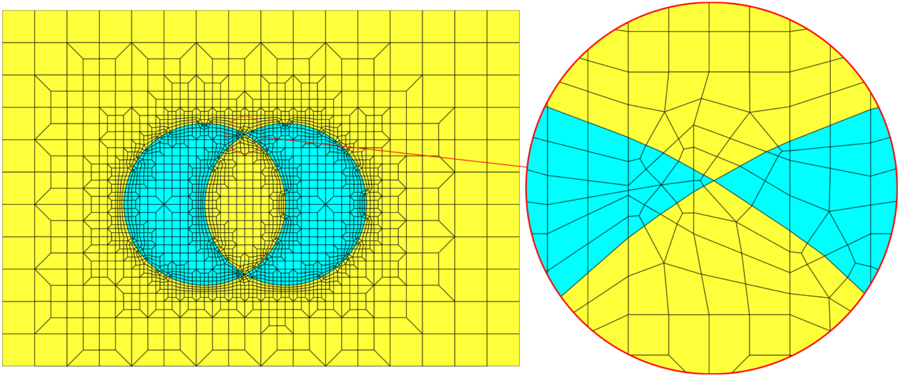
Recent advances in quad meshing



An all-quad mesh conforming to a given curve.

RUSHDI, MITCHELL, MAHMOOUD, BAJAJ, EBEIDA
"All-quad meshing without cleanup," *Computer-Aided Design*, 2017

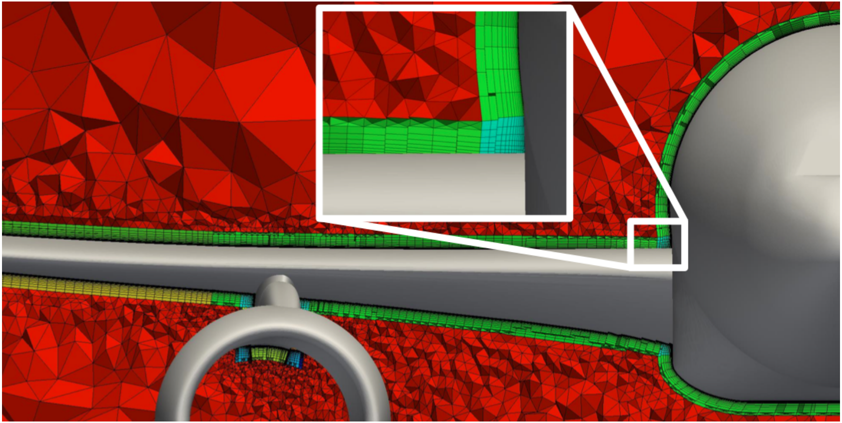
Recent advances in quad meshing



An all-quad mesh conforming to a given curve.

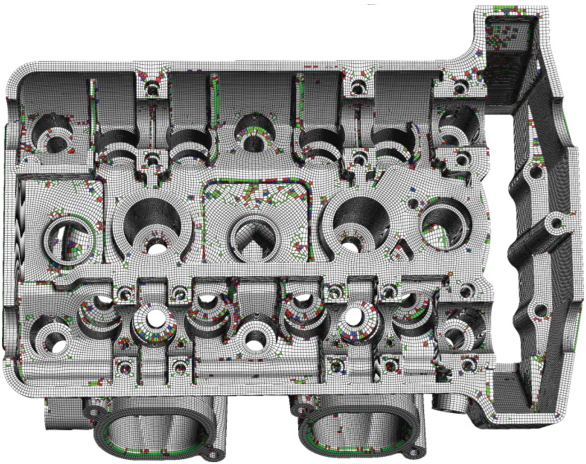
Rushdi, Mitchell, Mahmooud, Bajaj, Ebeida
"All-quad meshing without cleanup," *Computer-Aided Design*, 2017

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



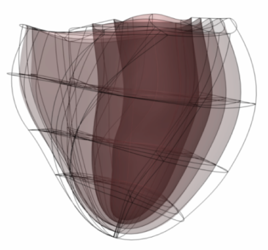
→ A hex-dominant mesh with ≈1.3 million cells, including ≈1 million hexahedra.

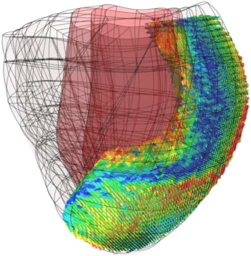
→ Re-meshed from a mesh of ≈ 10 million tetrahedra.

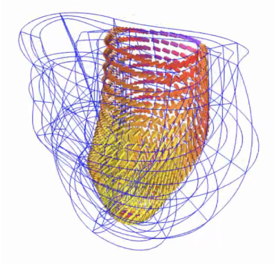
SOKOLOV ET AL. "Hexahedral-Dominant Meshing," *ACM Trans. Graphics*, 2016

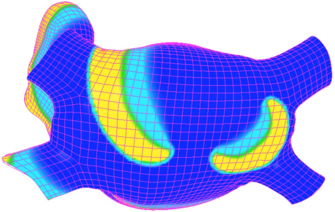
Established models use hexahedral meshes

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. . . yet!

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Slides and Pre-prints

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