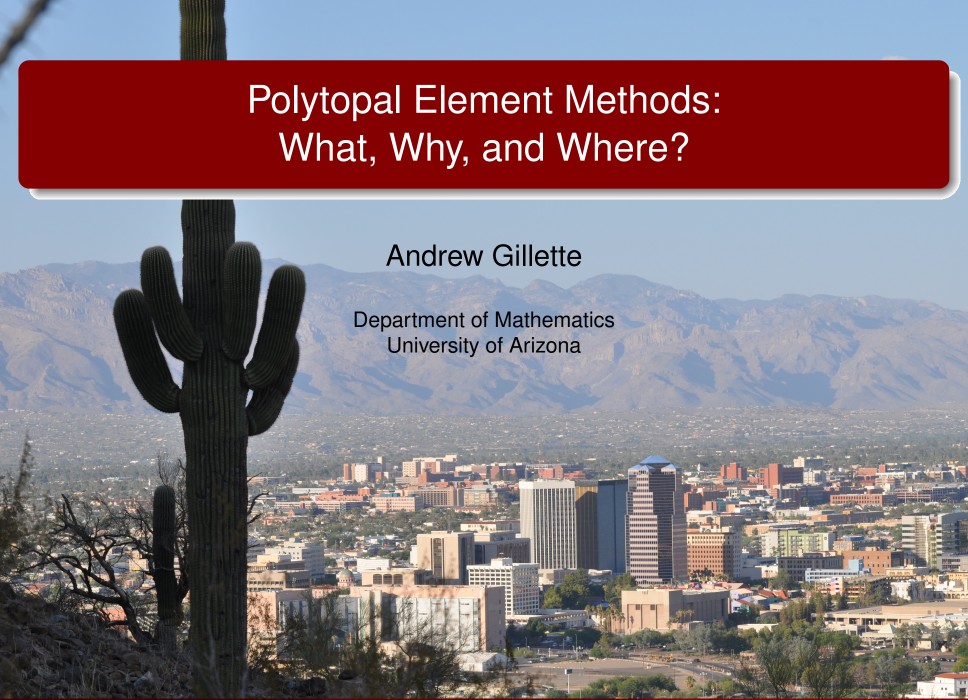


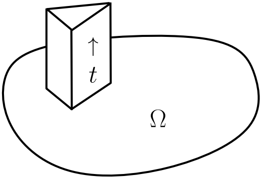
Polytopal Element Methods: What, Why, and Where?

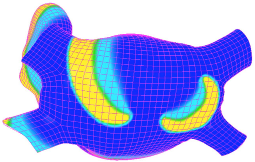
Andrew Gillette

Department of Mathematics
University of Arizona

What are finite element methods?

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





$$\left[\ \mathbb{A}\ \right]\left[\mathbf{x}\right] = \left[\mathbf{b}\right]$$

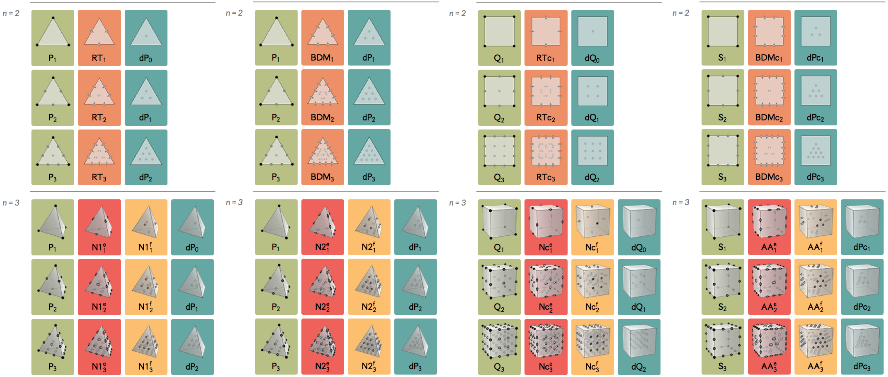
CHARACTERIZE	DISCRETIZE	SOLVE
Real analysis	Geometry & Topology	Linear algebra
PDEs	Combinatorics	Numerical analysis

Examples of research questions related to finite elements:

- Does the PDE have a unique (weak) solution, bounded in some norm?
- How does the discretization affect the quality of the approximate solution?
- Is the solution method optimally efficient?

Discretization with Simplices or Cubes

Domain meshing with simplices or cubes is now so well-understood that there is a **Periodic Table of Finite Elements:**



→ Viewable online at `femtable.org` (and on the wall of my office!)

→ Scientific content prepared by Doug Arnold and Anders Logg

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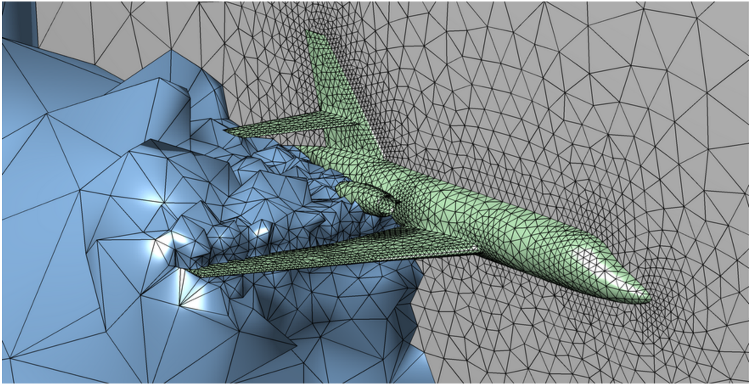
Outline

1. Why polytopal meshes?
2. Wait, what is the finite element method again?
3. What are some modern polytopal element methods?
4. Generalized barycentric coordinate methods

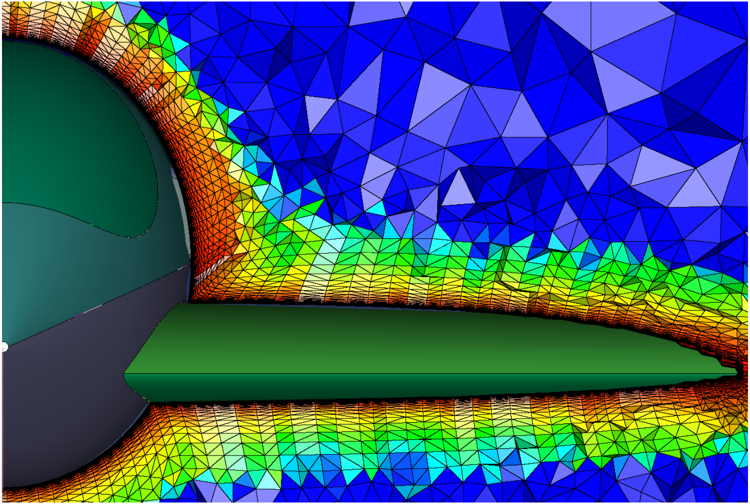
Volume meshing for Computational Fluid Dynamics



Tetrahedral volume mesh for CFD, using ***DistMesh*** *software.*

(courtesy of Per-Olof Persson)

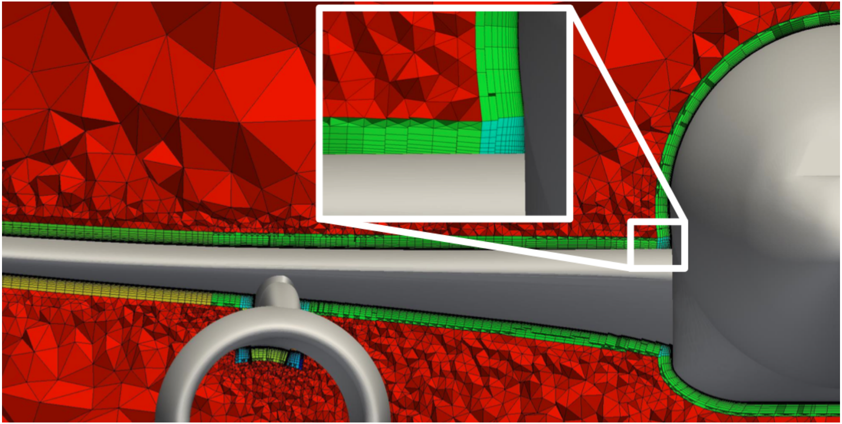
Volume meshing for Computational Fluid Dynamics



*Tetrahedral volume mesh for CFD, using **Pointwise** software.*

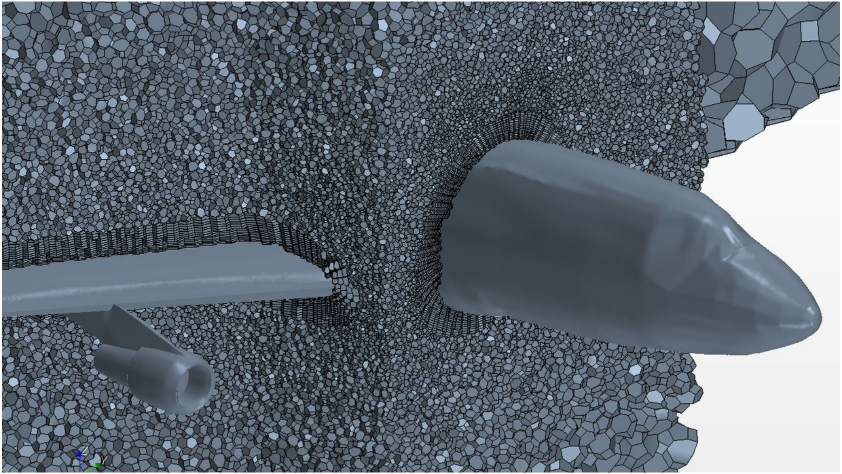
(from blog.pointwise.com)

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)

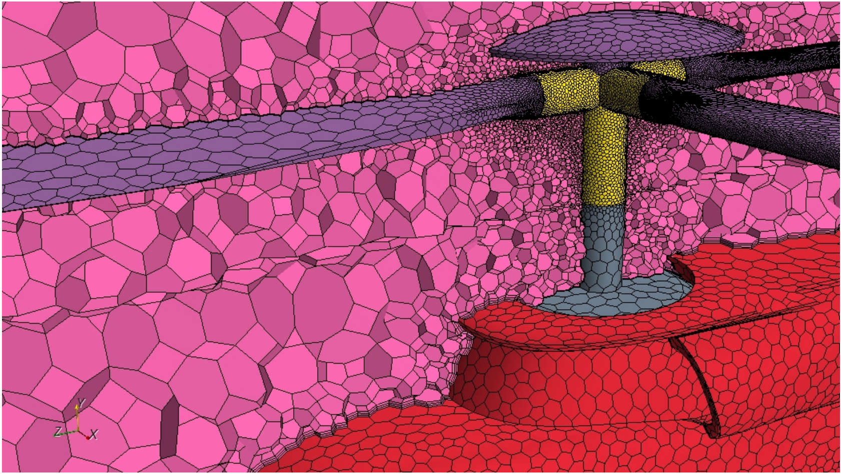
Volume meshing for Computational Fluid Dynamics



*Body-aligned prismatic polyhedral meshes for CFD, using **CD-adapco** software.*

(from cd-adapco.com image gallery)

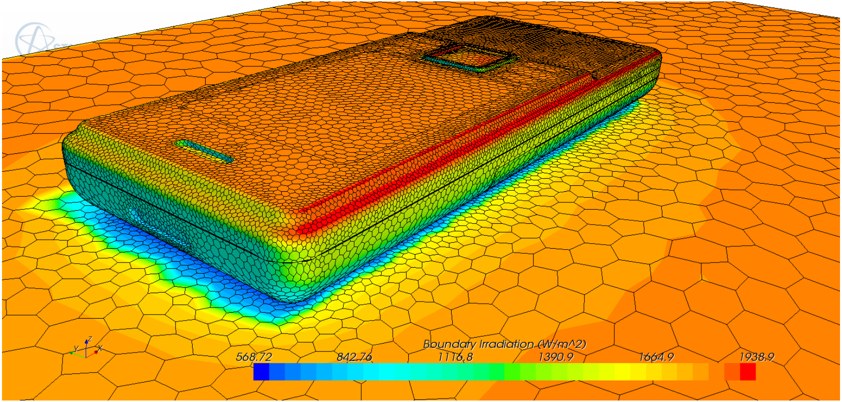
Volume meshing for Computational Fluid Dynamics



Polyhedral mesh of a Bell 407 helicopter and surrounding volume.

(from cd-adapco.com image gallery)

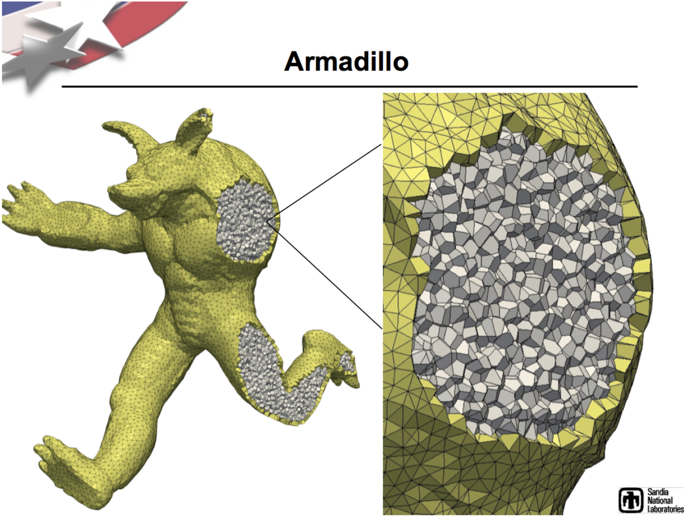
Volume meshing for. . . cel phone design!



A polyhedral mesh used to study heat transfer and cooling of a cell phone.

(from cd-adapco.com image gallery)

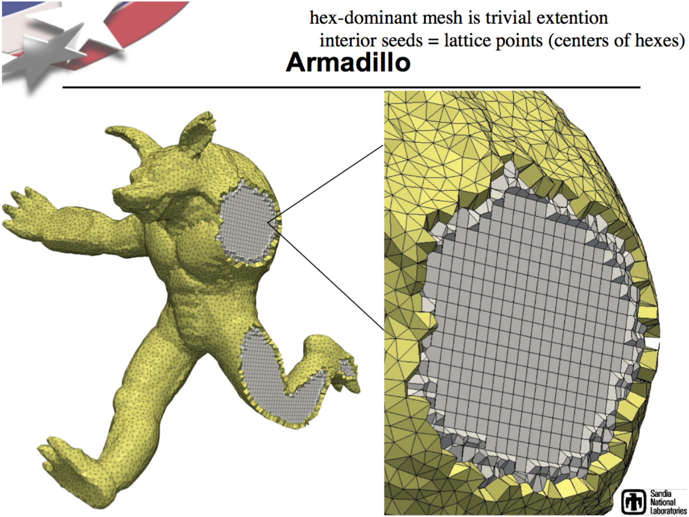
Volume meshing at Sandia National Labs



*A polyhedral mesh conforming to a surface triangulation using **VoroCrust** software.*

(from Scott Mitchell, Sandia National Labs)

Volume meshing at Sandia National Labs



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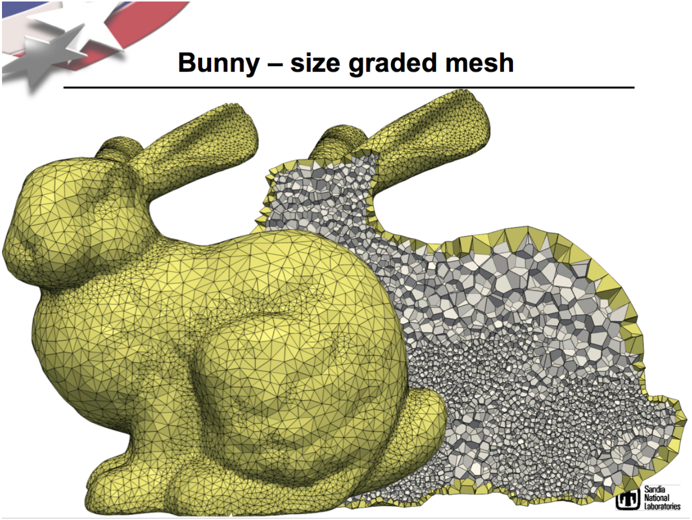
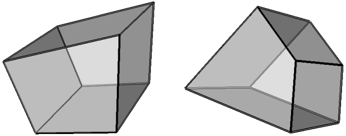


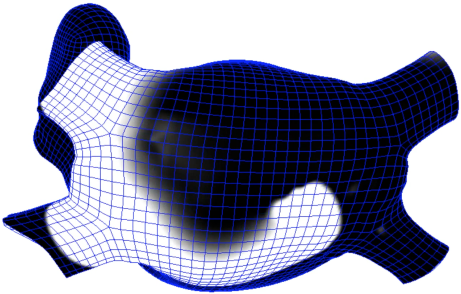
*The requisite Stanford Bunny example using **VoroCrust** software.*

(from Scott Mitchell, Sandia National Labs)

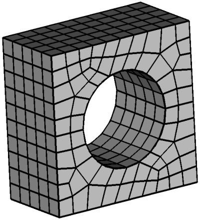
Hexahedral meshing is polyhedral meshing

Meshes of generic hexahedra require a generalized theory of polyhedral discretization, related to but distinct from the theory for perfect tensor product meshes.





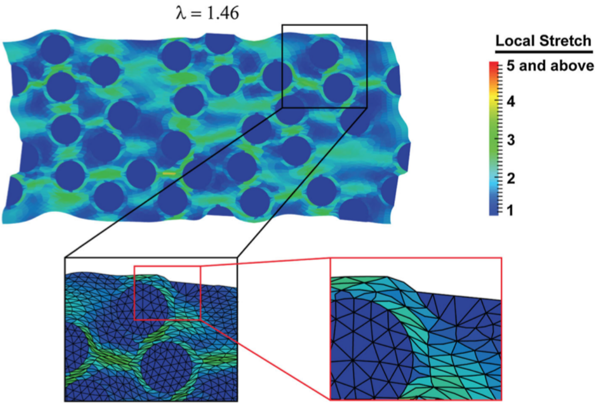
↑ *Heart mesh made using Continuity software, National Biomedical Computation Resource, UCSD*



← *Hole mesh made using CUBIT Geometry and Mesh Generation Toolkit, Sandia National Labs*

Elasticity modeling

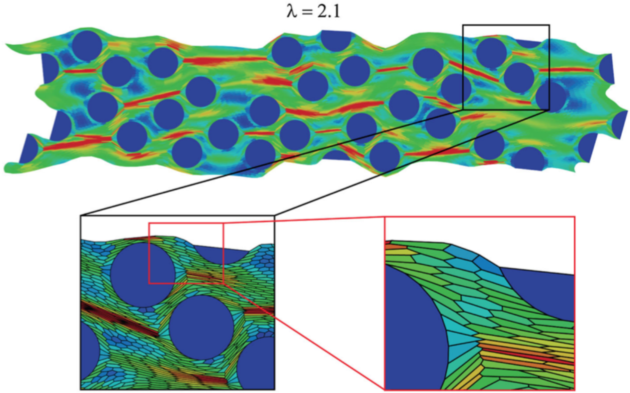
Standard triangular FEM cannot model maximal stretch factors due to numerical errors from the deformation.



(from Chi, Talischi, Lopez-Pamies, Paulino, "Polygonal finite elements for finite elasticity." International Journal for Numerical Methods in Engineering, 2015)

Elasticity modeling

The flexibility of polyhedral meshes allows greater shape deformation and more realistic stretch factors.



Chi et al. "Polygonal finite elements for finite elasticity."
Talischi et al. "Gradient correction for polygonal and polyhedral finite elements."
International Journal for Numerical Methods in Engineering, 2015

Outline

The Finite Element Method: 1D

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

Ex: The 1D Laplace equation: find $u(x) \in U$ s.t.

$$\begin{cases} -u''(x) = f(x) & \text{on } [a,b] \\ u(a) = 0, \\ u(b) = 0 \end{cases}$$

Make the problem easier by making it (seemingly) harder . . .

Weak form: find $u(x) \in U$ ($\dim U = \infty$) s.t.

$$\int_a^b u'(x)v'(x)\,dx = \int_a^b f(x)v(x)\,dx, \quad \forall v \in V \quad (\dim V = \infty)$$

. . . but we can now search a finite-dimensional space. . .

Discrete form: find $u_h(x) \in U_h$ ($\dim U_h < \infty$) s.t.

$$\int_a^b u_h'(x)v_h'(x)\,dx = \int_a^b f(x)v_h(x)\,dx, \quad \forall v_h \in V_h \quad (\dim V_h < \infty)$$

The Finite Element Method: 1D

Suppose $u_h(x)$ can be written as linear combination of V_h elements:

$$u_h(x) = \sum_{v_i \in V_h} u_i v_i(x)$$

The discrete form becomes: find coefficients $u_i \in \mathbb{R}$ such that

$$\sum_i \int_a^b u_i v_i'(x) v_j'(x)\ dx = \int_a^b f(x) v_j(x)\ \ dx, \quad \forall v_j \in \text{basis for } V_h \quad (\dim V_h < \infty)$$

Written as a linear system:

$$[\ \mathbb{K}\ ]_{ji}\ [\ u\ ]_i = [\ f\ ]_j\,, \quad \forall v_j \in \text{basis for } V_h$$

With some functional analysis we can prove: $\exists\ C > 0$, independent of h, s.t.

$$\underbrace{||u - u_h||_{H^1(\Omega)}}_{\substack{\text{error between cnts}\\ \text{and discrete solution}}} \leq \underbrace{C\,h\,|u|_{H^2(\Omega)}}_{\substack{\text{bound in terms of}\\ \text{2nd order osc. of } u}}, \quad \underbrace{\forall u \in H^2(\Omega)}_{\substack{\text{holds for any } u \text{ with}\\ \text{bounded 2nd derivs.}}}.$$

where h = maximum width of elements use in discretization.

The Finite Element Method: 2D and 3D

The discrete form becomes: find coefficients $u_i \in \mathbb{R}$ such that

$$\int_E u_i \nabla v_i \cdot \nabla v_j = \int_E f\ v_j, \quad \forall v_j \in \text{basis for } V_h \quad (\dim V_h < \infty)$$

We still have a linear system, $[\ \mathbb{K}\ ]_{ji}\ [\ u\ ]_i = [\ f\ ]_j$, but the key question is:

How do we compute the entries of the "stiffness matrix" $\mathbb{K}$?

$$[\ \mathbb{K}\ ]_{ji} = \int_E \nabla v_i \cdot \nabla v_j, \quad \forall v_j \in \text{basis for } V_h$$

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Two basic approaches:

1. Choose the basis functions $\{v_i\}$ wisely.

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Two basic approaches:

1. Choose the basis functions $\{v_i\}$ wisely.
2. Don't. That is, don't choose *any* basis functions.

The first two polytopal element methods

Mimetic finite differences — 1960s-present

(The "don't choose basis functions" approach.)

→ Idea is to mimic key properties like conservation laws, symmetry of solutions, duality of variables, etc.
→ 'Straightforward' to implement.
→ Popular at Los Alamos & other national labs.
→ Difficult to analyze error.

Generalized barycentric coordinates — 1970s-present

(The "choose basis functions wisely" approach.)

→ Idea is to generalize basis functions for simple shapes to general polygons and polyhedra.
→ More obstacles to implementation.
→ Popular with mathematicians and computer graphics researchers.
→ Easier to analyze error.

How to not choose basis functions

Choose a solution space V_h that contains some polynomial space $\mathcal{P}_r$.

Let $\Pi : V_h \to \mathcal{P}_r$ denote the (L^2)-projection to $\mathcal{P}_r$.

Let I be the identity operator.

Write:

$$\int_E \nabla\phi_i \nabla\phi_j = \underbrace{\int_E \nabla\Pi\phi_i \cdot \nabla\Pi\phi_j}_{A} + \underbrace{\int_E \nabla(I-\Pi)\phi_i \cdot \nabla(I-\Pi)\phi_j}_{B}$$

To compute A: an integral of two polynomials $\implies$ can compute exactly.

To compute B: if $\phi_i \in \mathcal{P}_r$, then $(I-\Pi)\phi_i = 0 \implies$ integral is 0

if $\phi_j \in \mathcal{P}_r$, then $(I-\Pi)\phi_j = 0 \implies$ integral is 0

if $\phi_i, \phi_j \notin \mathcal{P}_r \implies$ use some kind of trick to approximate.

This idea is very popular for polytopal element methods because *you never have to specify what the* ϕ_i *are*!

Outline

1. Why polytopal meshes?
2. Wait, what is the finite element method again?
3. What are some modern polytopal element methods?
4. Generalized barycentric coordinate methods

A few kinds of polytopal element methods...

CDO = Compatible discrete operator schemes

A few kinds of polytopal element methods. . .

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Moreover, some kinds of $* * *$ methods are the same as $\star \star \star$ methods. . .

A few kinds of polytopal element methods...

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Moreover, some kinds of $* * *$ methods are the same as $\star \star \star$ methods...

"Polytopal Element Methods in Mathematics and Engineering"

$\rightarrow$ Special NSF-funded workshop held at Georgia Tech in Oct 2015

$\rightarrow$ Slides from talks: `http://www.poems15.gatech.edu/`

Outline

The generalized barycentric coordinate approach

Choose specific ϕ_i related to polygonal / polyhedral geometries, and then compute

$$\int_E \nabla\phi_i \nabla\phi_j$$

What properties should the ϕ_i have?

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

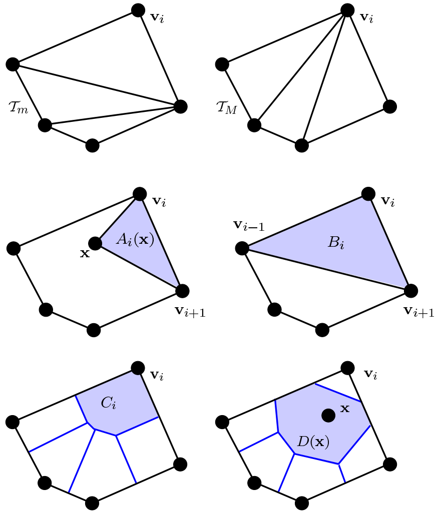
$$\lambda_{\mathbf{v}} : P \to \mathbb{R} \quad \text{are} \quad \textbf{generalized barycentric coordinates (GBCs)} \text{ on } P$$

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



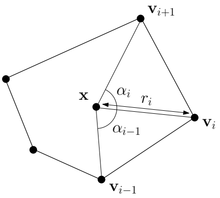
- **Triangulation**
  ⇒ FLOATER, HORMANN, KÓS, *A general construction of barycentric coordinates over convex polygons*, 2006

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

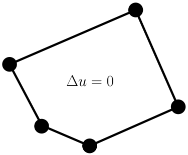
- **Wachspress**
  ⇒ WACHSPRESS, *A Rational Finite Element Basis*, 1975.

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

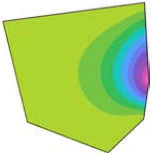
Many generalizations to choose from ...



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



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



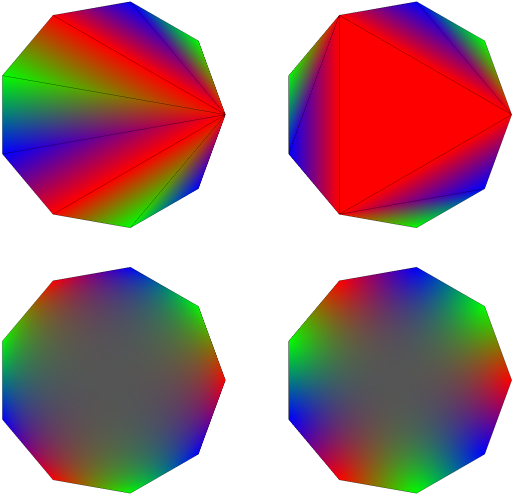
- **Maximum Entropy** ⇒ HORMANN, SUKUMAR, *Maximum Entropy Coordinates for Arbitrary Polytopes*, 2008.

← (this figure is from the above paper)

Also: moving least squares coordinates, barycentric coordinates on surfaces, ...

Comparison via ‘eyeball’ norm

Triangulated | Triangulated



Wachspress | Mean Value

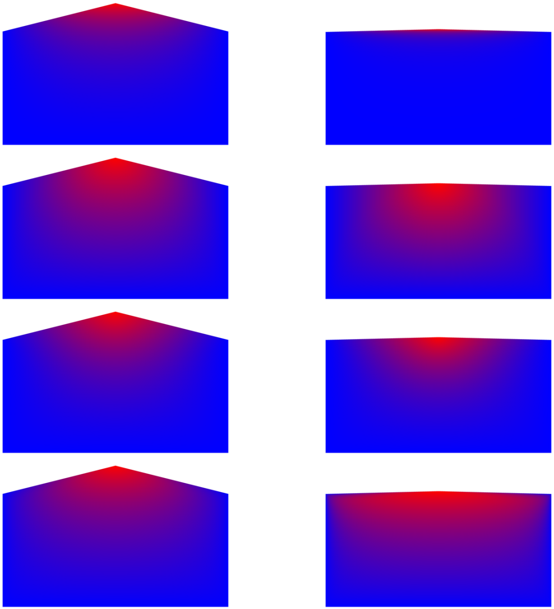
Comparison via 'eyeball' norm

Wachspress

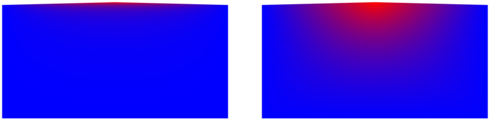
Sibson

Mean Value

Discrete Harmonic



Interplay of gradients and geometry



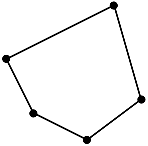
Wachspress   Mean Value

Choice of $\{\phi_i\}$ + control of geometry

$\Rightarrow$ bounds on $|\nabla \phi_i|$

$\Rightarrow$ robust computation of $\displaystyle\int_E \nabla \phi_i \nabla \phi_j$

Revisiting ***a priori* error estimates** for finite element methods.



P,	a polygon or polytope geometry.
u,	a function from P to $\mathbb{R}$, known only at the vertices of P.
$\mathcal{I}u$,	an interpolant for u over P.
C,	a constant depending on the geometry of P

$$\underbrace{|u - \mathcal{I}u|_{H^1(P)}}_{\text{error between function and its interpolation}} \leq \underbrace{C \cdot \operatorname{diam}(P)\ |u|_{H^2(P)}}_{\text{bound depends on size and geometry of } P}, \quad \underbrace{\forall u \in H^2(P)}_{\text{estimate holds for any } u \text{ with bounded 2nd derivatives}}$$

The 40 year history of the triangular case

$$|u - \mathcal{I}u|_{H^1(P)} \leq C \cdot \text{diam}(P)\ |u|_{H^2(P)}, \quad \forall u \in H^2(P)$$

If P is a triangle, the **maximum angle condition** refers to the fact that C can be large when P has a large interior angle.

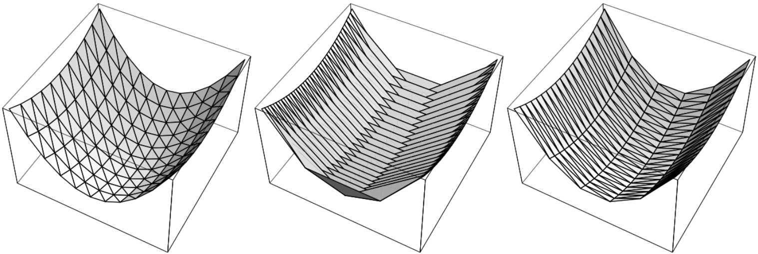


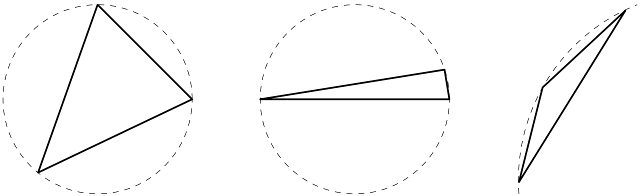
Figure from: Shewchuk: What is a good linear element? *Int'l Meshing Roundtable*, 2002.

Babuška, Aziz: On the angle condition in the finite element method, *SINUM*, 1976.
Jamet: Estimations d'erreur pour des éléments finis... *RAIRO Analyse Numérique.*, 1976.
Rippa, Schiff: Minimum energy triangulations for elliptic problems, *CMAME*, 1990.
Shenk: Uniform error estimates for certain narrow Lagrange finite elements, *Math. Comp.*, 1994.
Warren et al: Barycentric coordinates for convex sets, *Adv. Comp. Math.*, 2007.

The triangular case, revisited

The **aspect ratio** of a polygon P is $\dfrac{\text{diam}(P)}{\text{max radius of an inscribed circle}}$.

The **circumradius** of a triangle T is $R_T :=$ radius of circle through the vertices of T.



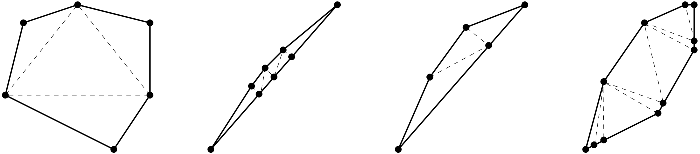
aspect ratio	small	**large**	large
circumradius	small	**small**	large
C	small	**small**	large

On triangles, a large aspect ratio does not necessarily imply that C is large. . .
. . . but a large circumradius always does.

Polygonal shape quality measures

The **aspect ratio** of a polygon P is $\dfrac{\text{diam}(P)}{\text{max radius of an inscribed circle}}$.

The **circumradius** of a triangle T is $R_T :=$ radius of circle through the vertices of T.



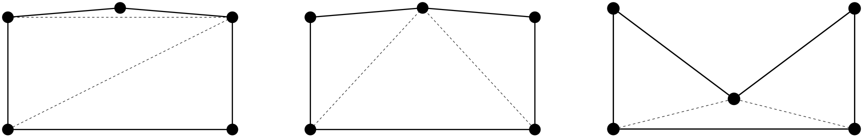
polygon aspect ratio	good	**bad**	bad	okay?
quality of trian-gulation	good	**good**	bad	okay?

On polygons, a large aspect ratio does not correlate in a clear way with the circumradii of triangulations of its vertices

Polygonal shape quality measures

The **aspect ratio** of a polygon P is $\dfrac{\text{diam}(P)}{\text{max radius of an inscribed circle}}$.

The **circumradius** of a triangle T is $R_T :=$ radius of circle through the vertices of T.



not Delaunay

max R_T large

Delaunay

max R_T small

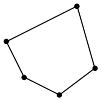
(constrained) Delaunay

max R_T large
(and no alternative triangulation possible!)

Over all possible triangulations of the vertices of a polygon, the **constrained Delaunay triangulation** will have the minimal maximum circumradius.

Two related interpolants on polygons

The **harmonic interpolant** is the solution to



$$\begin{cases} \Delta(\mathcal{I}_P u) = 0, & \text{on } P, \\ \mathcal{I}_P u = g_u. & \text{on } \partial P. \end{cases}$$

where $g_u : \partial\Omega \to \mathbb{R}$ is the piecewise linear function equal to u at the vertices of P.

By **Dirichlet's principle**, $\mathcal{I}_P u$ is also the minimizer of H^1 semi-norm:

$$\mathcal{I}_P u = \text{argmin} \left\{ |v|_{H^1(P)} \ : \ v = g_u \text{ on } \partial P \right\}$$

The **triangulation interpolant**, denoted $\mathcal{I}_\mathcal{T} u$, is the piecewise linear interpolation of g_u with respect to a triangulation $\mathcal{T}$ of the vertices of P.

Theorem: There exists a constant $C > 0$ such that for any polygon P, and all triangulations $\mathcal{T}$ of P,

$$|u - \mathcal{I}_P u|_{H^1(P)} \leq C \left(\max_{T \in \mathcal{T}} R_T \right) |u|_{H^2(P)}, \qquad \forall u \in H^2(P),$$

where R_T denotes the circumradius of triangle T.

G., RAND Interpolation Error Estimates for Harmonic Coordinates On Polytopes, arXiv:1504.00599 2015.

Sharpness of the theorem

Theorem: $\exists\, C > 0,\ \forall\, P,\ \forall\, u \in H^2(P),\ \forall\, \mathcal{T}$ of P,

$$|u - \mathcal{I}_P u|_{H^1(P)} \leq C \left(\max_{T \in \mathcal{T}} R_T \right) |u|_{H^2(P)}\,.$$

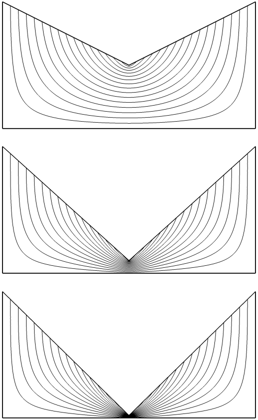
Lemma: Set $u(x,y) := x^2$.

Consider a sequence of polygon-vertex-edge tuples $(P_i, \mathbf{v}_i, e_i)_{i=1}^{\infty}$, such that $\operatorname{dist}(\mathbf{v}_i, e_i) \to 0$ as $i \to \infty$ and there exists $K > 0$ independent of i, s.t. $d(\mathbf{v}_i, \partial e_i) > K$.

Then regardless of the **convexity** of the P_i,

$$\lim_{i \to \infty} \frac{|u - \mathcal{I}_{P_i} u|_{H^1(P_i)}}{|u|_{H^2(P_i)}} = \infty.$$

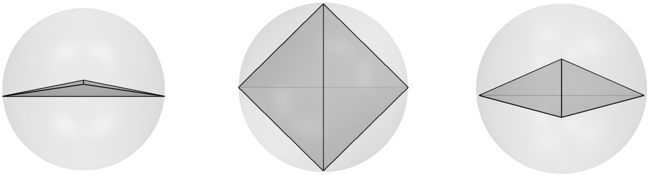
Thus, the harmonic interpolant, in general, has no sharper *a priori* estimate than estimates derived by triangulation of the domain!



Polyhedral shape quality measures

The **aspect ratio** of a polyhedron P is $\dfrac{\text{diam}(P)}{\text{max radius of an inscribed sphere}}$.

The **circumradius** of a tetrahedron T is $R_T :=$ radius of sphere through vertices of T.



Sliver tetrahedra have poor interpolation properties (C is large), but their circumradii are not necessarily large. Thus, a direct analogue of the theorem to 3D is not possible.

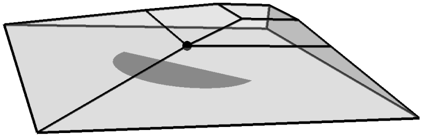
Conclusions for polyhedra

Theorem: Fix $\gamma > 2$. There exists a constant $C > 0$ depending only on γ such that for any polyhedron P with aspect ratio less than γ,

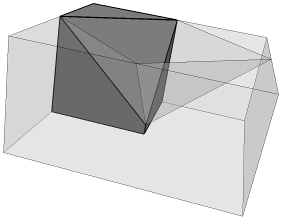
$$|u - \mathcal{I}_P u|_{H^1(P)} \leq C \operatorname{diam}(P) \ |u|_{H^2(P)}, \qquad \forall u \in H^2(P).$$

Convex element: The H^1-error in the harmonic interpolant cannot be bounded if a vertex can be arbitrarily close to a non-adjacent face.

Non-convex element: The H^1-error in the harmonic interpolant can remain bounded, even when a vertex and non-adjacent face are close.



convex



non-convex

Acknowledgments

THE UNIVERSITY OF ARIZONA

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Thanks for the invitation to speak!

Slides and pre-prints: `http://math.arizona.edu/~agillette/`