The State of the Art in Polytopal Finite Element Methods

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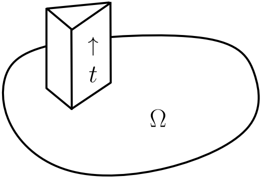
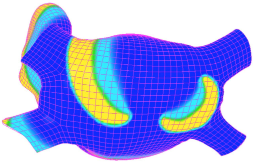
What are finite element methods?

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

In this talk:

- Why use meshes of polygons / polyhedra for discretization?
- What are some finite element methods that allow such meshes?
- Where is this line of research headed?

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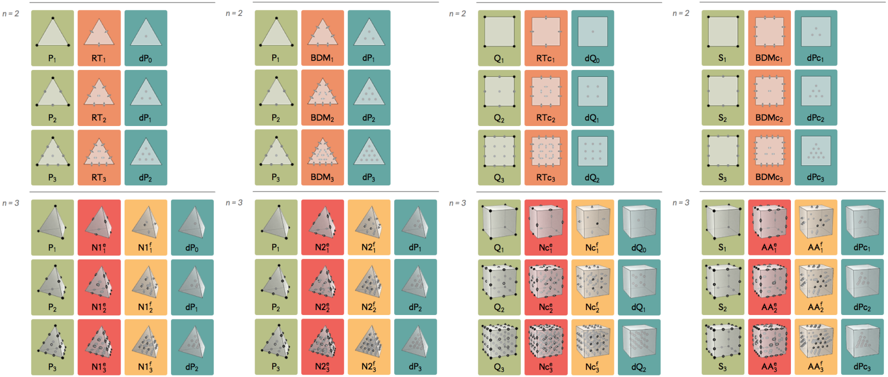
1. Why use polytopal meshes?
2. What are some polyhedral finite element methods?
3. Where is this line of research headed?

Discretization with Simplices or Cubes

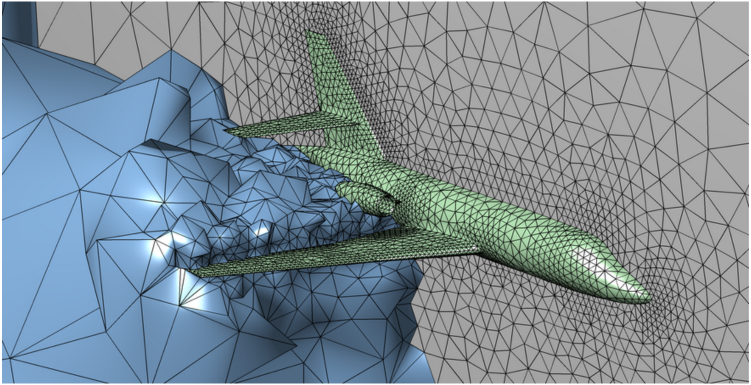
Domain meshing with simplices or cubes is now so well-understood that there is a **Periodic Table of Finite Elements:**



→ Viewable online at `femtable.org`

→ Scientific content prepared by Doug Arnold and Anders Logg

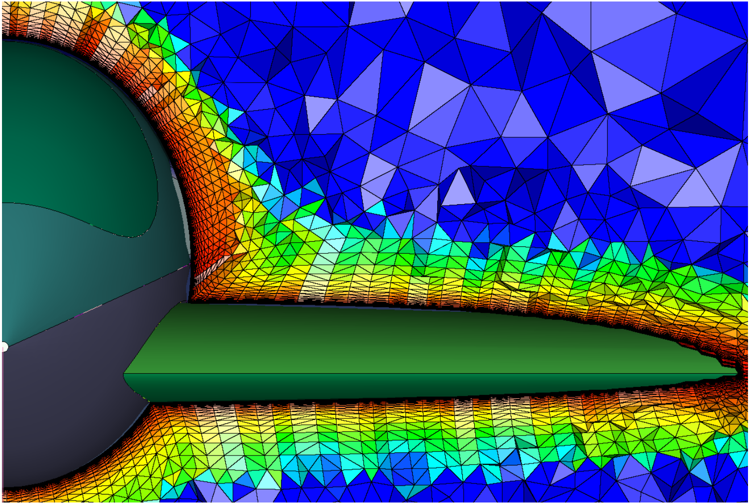
Volume meshing for Computational Fluid Dynamics



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

(courtesy of Per-Olof Persson)

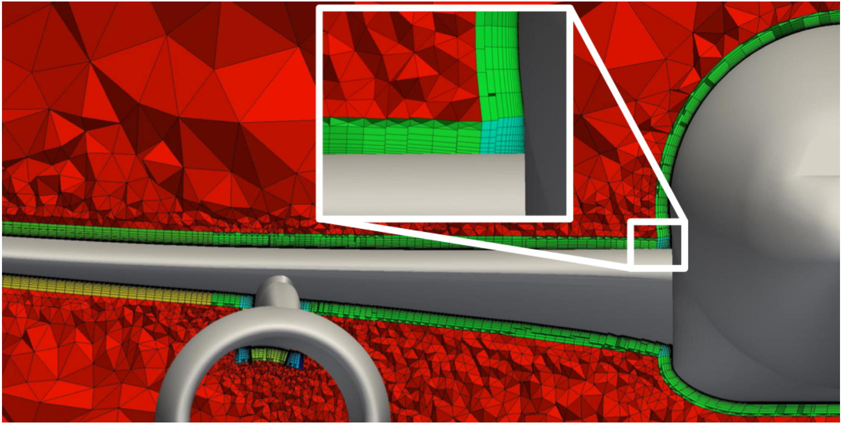
Volume meshing for Computational Fluid Dynamics



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

(from blog.pointwise.com)

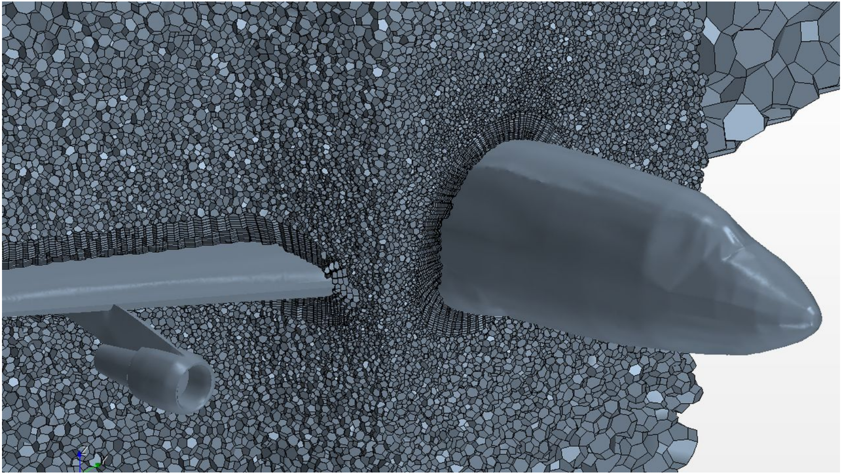
Volume meshing for Computational Fluid Dynamics



*Hyrbid hex / pyramid / prism / tet mesh for CFD, using **ITI Transcendata** software.*

(from a keynote address at Geometric Modeling and Processing 2015)

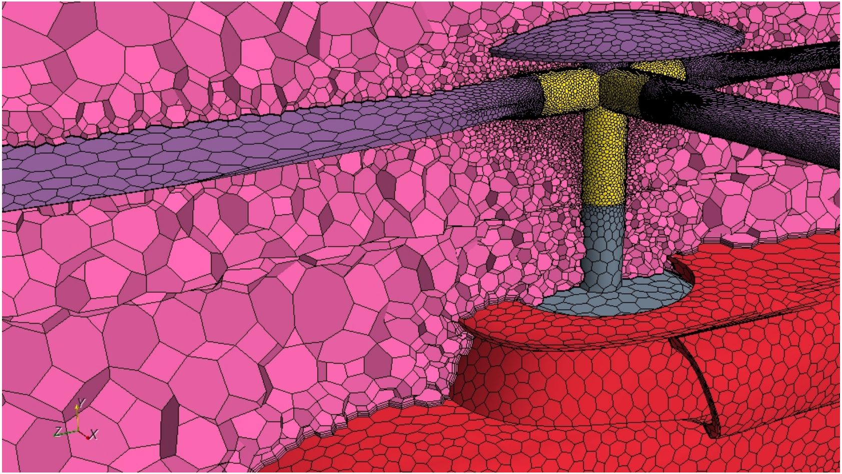
Volume meshing for Computational Fluid Dynamics



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

(from cd-adapco.com image gallery)

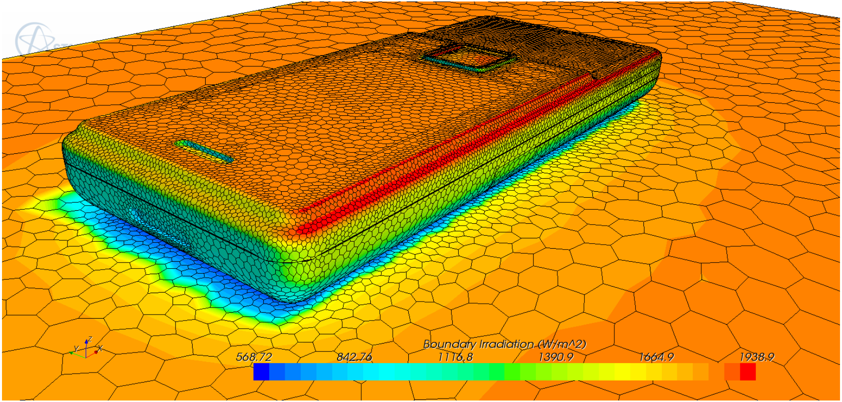
Volume meshing for Computational Fluid Dynamics



Polyhedral mesh of a Bell 407 helicopter and surrounding volume.

(from cd-adapco.com image gallery)

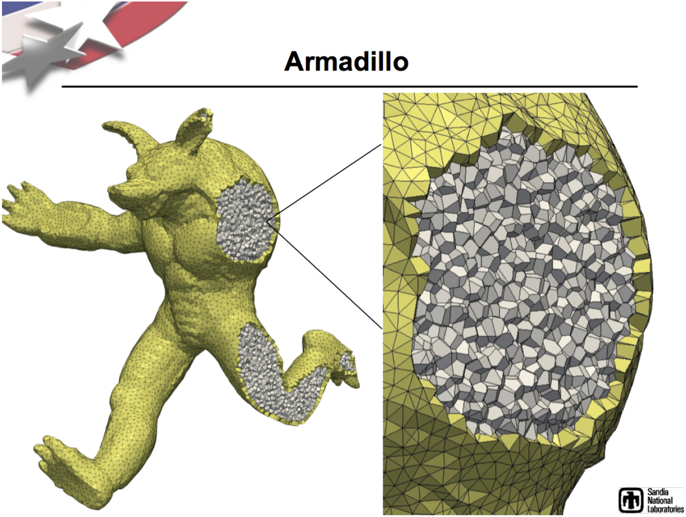
Volume meshing for. . . cel phone design!



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)

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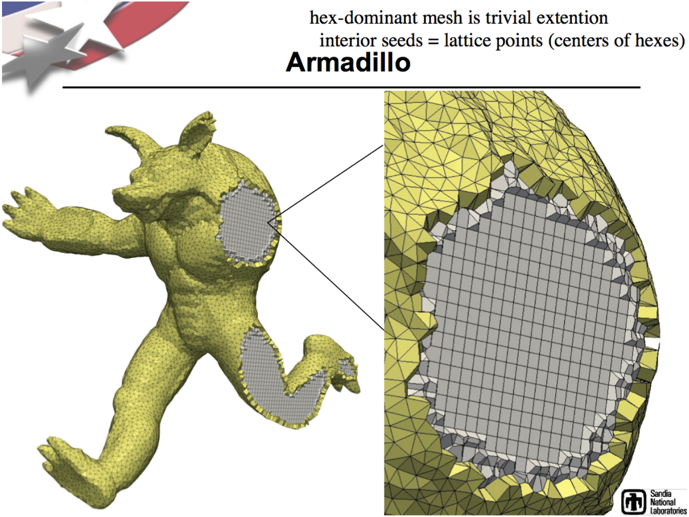

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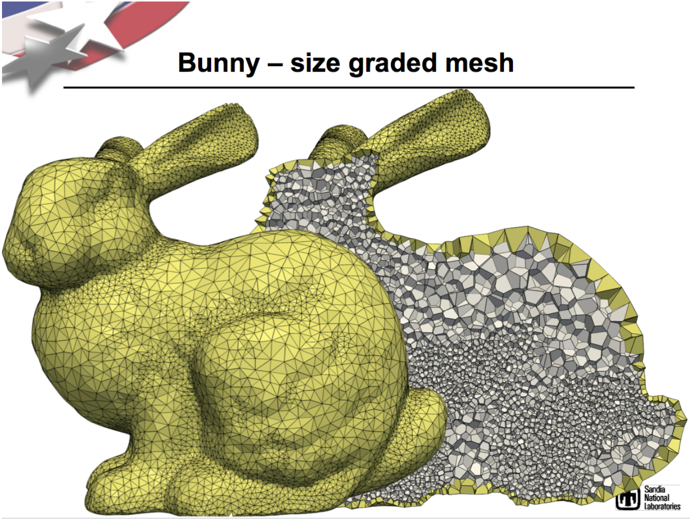
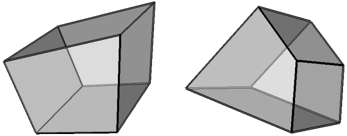


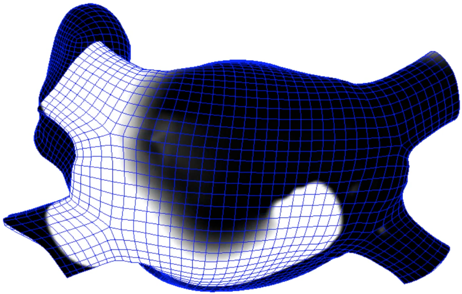
*The requisite Stanford Bunny example using **VoroCrust** software.*

(from Scott Mitchell, Sandia National Labs)

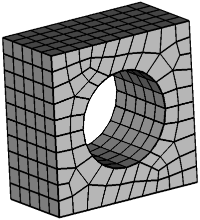
Hexahedral meshing is polyhedral meshing

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





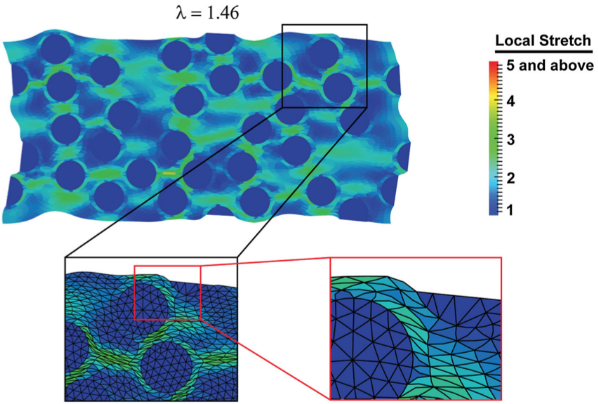
↑ *Heart mesh made using Continuity software, National Biomedical Computation Resource, UCSD*



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

Elasticity modeling

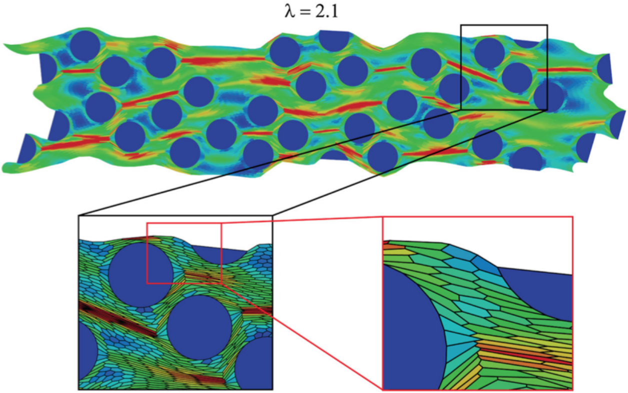
Standard triangular FEM cannot model maximal stretch factors due to numerical errors from the deformation.



(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

1. Why use polytopal meshes?
2. What are some polyhedral finite element methods?
3. Where is this line of research headed?

The Finite Element Method for Poisson's Problem

Continuous problem: find $u \in U$ s.t.

$$\Delta u = f \ \text{ on } \Omega \subset \mathbb{R}^n$$

Weak form: find $u \in U$ s.t.

$$\int_\Omega \nabla u \cdot \nabla v = \int_\Omega f\ v, \quad \forall v \in V \quad (\text{dim } V = \infty)$$

Discrete form: find $u_h \in U_h$ s.t.

$$\int_\Omega \nabla u_h \cdot \nabla v_h = \int_\Omega f\ v_h, \quad \forall v_h \in V_h \quad (\text{dim } V_h < \infty)$$

Linear system: Set $U_h := V_h$ (Galerkin method). Find $u \in \mathbb{R}^{\text{dim } V_h}$ solving

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

where

$$[\,\mathbb{K}\,]_{ji} = \int_E \nabla v_i \cdot \nabla v_j \quad \text{and} \quad [\,f\,]_j = \int_E f(x) v_j(x)$$

A key challenge for polyhedral FEM

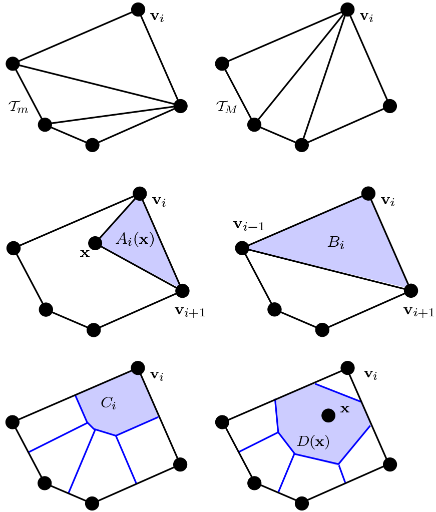
How do we compute the entries of the "stiffness matrix" $\mathbb{K}$?

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

Two basic approaches:

1. Choose the basis functions $\{v_i\}$ wisely.
   - $\rightarrow$ Generalize basis functions for simple shapes to polygons / polyhedra.
   - $\rightarrow$ Various obstacles to implementation.
   - $\rightarrow$ **Key method:** Generalized barycentric coordinates (1970s-present)
2. Don't choose *any* basis functions.
   - $\rightarrow$ Mimic key properties like conservation laws, symmetry of solutions, duality of variables, etc.
   - $\rightarrow$ Easier to implement; can be difficult to visualize solutions.
   - $\rightarrow$ **Key method:** Mimetic finite differences (1960s-present)

How to choose basis functions



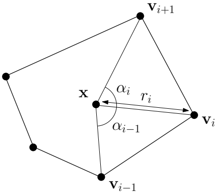
- **Triangulation**
  ⇒ FLOATER, HORMANN, KÓS, *A general construction of barycentric coordinates over convex polygons*, 2006

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

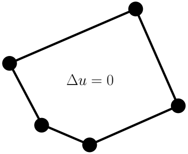
- **Wachspress**
  ⇒ WACHSPRESS, *A Rational Finite Element Basis*, 1975.
  ⇒ WACHSPRESS, *Rational Bases and Generalized Barycentrics*, 2016.

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

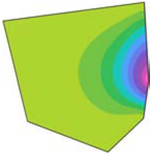
How to choose basis functions



- **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.

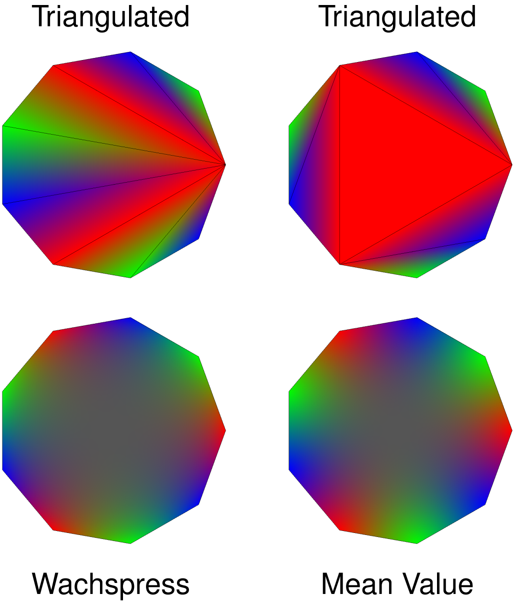


- **Maximum Entropy**
  ⇒ HORMANN, SUKUMAR, *Maximum Entropy Coordinates for Arbitrary Polytopes*, 2008.

← (this figure is from the above paper)

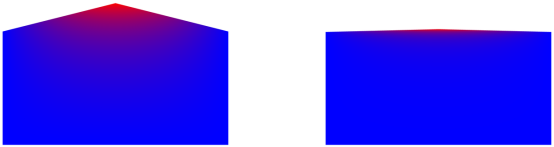
Also: moving least squares coordinates, barycentric coordinates on surfaces, . . .

Comparison via ‘eyeball’ norm

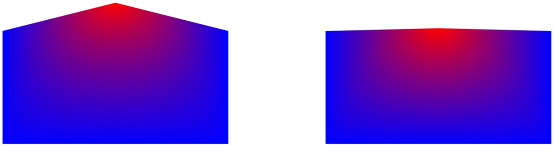


Comparison via ‘eyeball’ norm

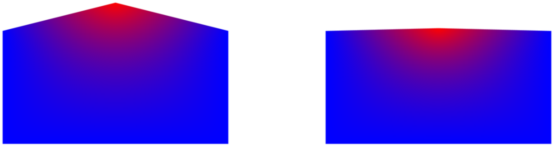
Wachspress



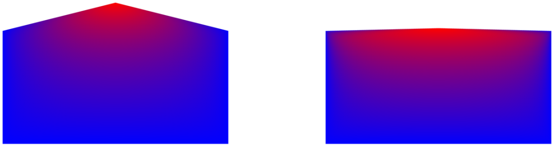
Sibson



Mean Value



Discrete Harmonic



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 a projection to $\mathcal{P}_r$ satisfying

$$(\nabla p, \nabla(\mathbb{I} - \Pi)v_h) = 0, \quad \forall\, p \in \mathcal{P}_r, \;\; v_h \in V_h, \;\; (\mathbb{I} = \text{identity operator})$$

Then for any (unchosen) basis functions $\{\phi_i\}$:

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

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

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

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

A few kinds of polytopal element methods. . .

CDO = Compatible discrete operator schemes

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CDO	=	Compatible discrete operator schemes
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Moreover, some kinds of $* * *$ methods are the same as $\star \star \star$ methods. . .

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"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/`

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Conclusions from the Atlanta workshop

- Robust **polygonal meshing** is available.

  (e.g. “Polymesher” from Glaucio Paulino’s group at Georgia Tech,
  “Poisson-Disk Sampling” from Sandia Labs)

- Robust and ‘standardized’ **polyhedral meshing** is needed, including mesh quality metrics.
- Increased **communication with industry** will be crucial for the widespread adoption of new methods.
- **Quadrature rules** for polyhedral methods are not obvious, but not impossible!

  (e.g. for homogeneous functions, work from N. Sukumar’s group at UC Davis)

- *There is no ‘silver bullet’ method!*

Upcoming publications and events

- "Discretization of PDEs on Polyhedral Meshes"
  ESAIM:M2AN **special issue**, to appear in early 2016.
- "Mathematical Analysis of Polygonal and Polyhedral Finite Element Methods"
  book to be published by AK Peters in 2016/2017.
- "High-order methods for polygonal and polyhedral meshes"
  mini-symposium at European Congress on Computational Methods in Applied Sciences and Engineering, Greece, June 2016.
- "PDE Discretization Methods for Polygonal and Polyhedral Meshes"
  mini-symposium at Mathematics Of Finite Elements And Applications conference, London, June 2016.
- Another focused workshop to be planned for 2017. . .

Acknowledgments

THE UNIVERSITY OF ARIZONA

Thanks to Harbir and Lise-Marie
for the invitation to speak!

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