Sandia National Laboratories

A generalized derivative-projection methodology for assuring quadrature consistency in Bubnov-Galerkin polyhedral FEA

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Outline

1. motivation for polyhedral discretizations
2. challenges
3. gradient-correction approach for integration consistency
4. verification examples, linear elasticity
5. nonlinear solid mechanics, examples
6. summary

Application of interest is primarily nonlinear solid mechanics.
- large deformation
- plasticity, contact, implicit and explicit dynamics

# Motivation for polyhedral discretizations

- more general discretizations
- hybrid meshing (tet-hex-poly)
- hex dominant meshing using frame fields
- cut-cell discretizations
- use of Voronoi tessellations
- tetrahedral dual cells discretizations

tetrahedral dual cell

hex-dominant meshing
using frame field

cut-cell

Voronoi

CAD surface

Trimmed
hexahedral
elements
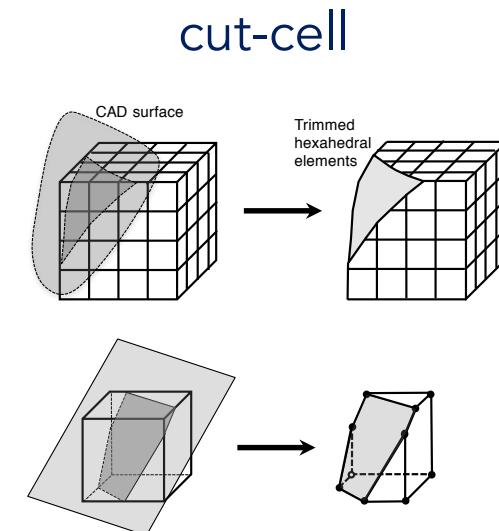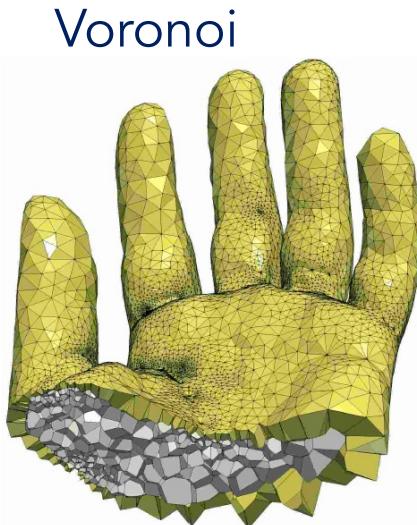
Abdelkader, A., et al. (2020). *ACM Trans. Graph.* **39,** Article 23.

Kim, H. and D. Sohn (2015). *IJNME,* **102,** 1527-1553.

Gao, X., et al. (2017). *ACM Trans. Graph.* **36,** 1-13.
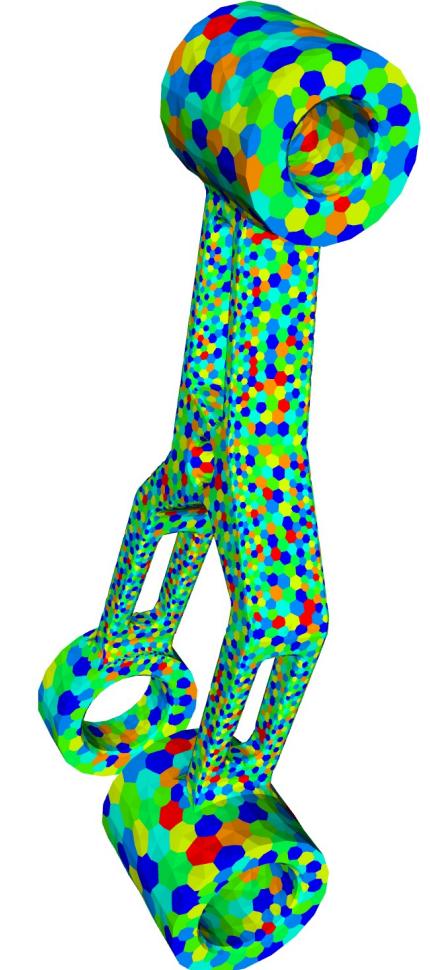
Bishop, J and N. Sukumar (2020). *Computer Aided Geometric Design*, **77,** 101812

Challenges

- ## meshing

  As poly elements become available in commercial software, meshing tools will follow.

  Vorocrust mesher (Ebeida, M. et al.)

- ## shape functions

  Many generalized barycentric coordinates (GBC) are now available, e.g. harmonic, maxent (Hormann and Sukumar, 2018)

- ## quadrature

  Several approaches for consistent and stable quadrature schemes, including VEM and other gradient projection methods.

- ## stability

  Depends on quadrature scheme; behavior in near-incompressibility regime (plasticity)

- Beirao da Veiga, et al., 2014, "Hitchhiker's Guide to VEM"
- J. Droniou, et al., 2018, The gradient discretisation method.
- Bishop, J. (2014). "A displacement-based finite element formulation for general polyhedra using harmonic shape functions." *IJNME* 97: 1-31.

Harmonic shape functions

Harmonic functions minimize the Dirichlet energy given by the following functional:

$$J(\phi) := \frac{1}{2} \int_{\Omega_e} \nabla\phi \cdot \nabla\phi \, d\Omega \qquad \text{with } \phi \in H^1(\Omega_e)$$

The minimizer of this functional satisfies the following variational problem:

find $\phi \in H^1(\Omega_e)$ with $\phi = \overline{\phi}$ on Γ_e such that

$$\int_{\Omega_e} \nabla\phi \cdot \nabla v \, d\Omega$$

for all test functions $v \in H_0^1(\Omega_e)$

The strong form of this variational problem is given by:

$$\nabla^2\phi = 0 \text{ in } \Omega_e \text{ with } \phi = \overline{\phi} \text{ on } \Gamma_e$$

Harmonic shape functions

$$\nabla^2 \phi_I = 0$$
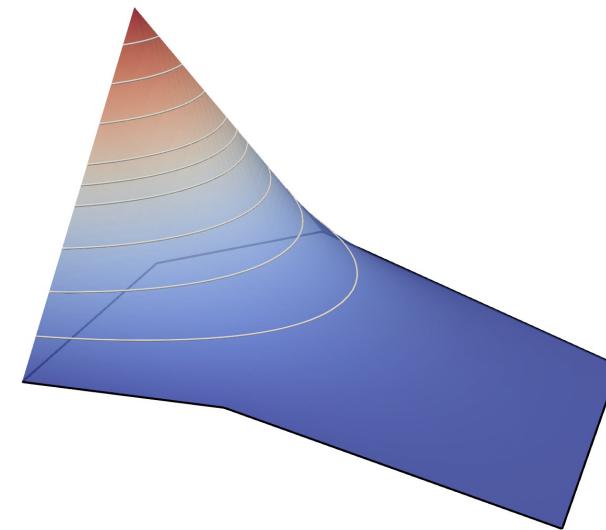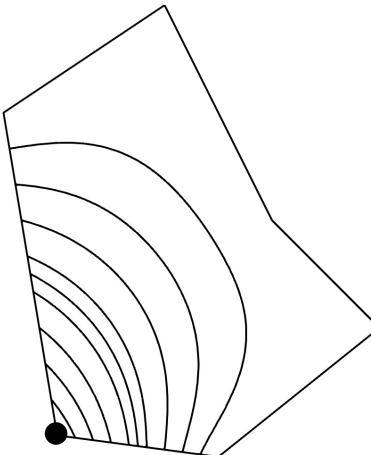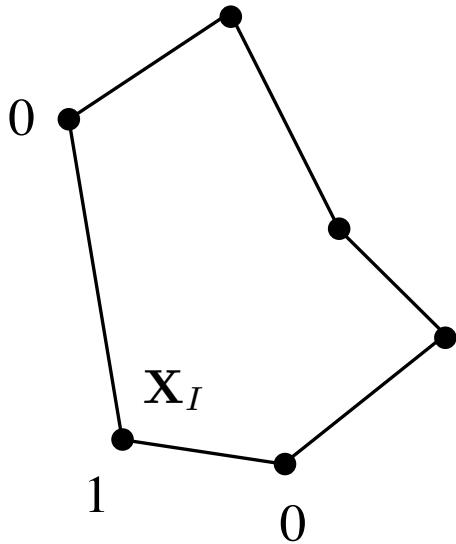
Harmonic shape functions
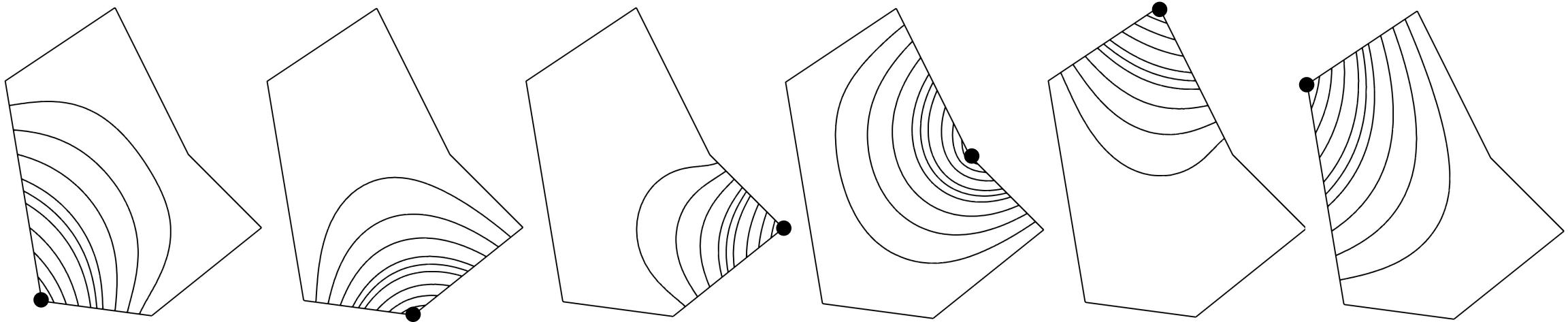
$$\sum_I \phi_I(\mathbf{x}) = 1 \qquad \text{partition of unity}$$

$$\sum_I \mathbf{x}_I \, \phi_I(\mathbf{x}) = \mathbf{x} \qquad \text{linear reproducibility}$$

Can also do higher-order reproducibility.

Governing equations (total-Lagrangian formulation)

strong form

$$\frac{\partial \boldsymbol{P}}{\partial \boldsymbol{X}} : \boldsymbol{I} = \rho_0 \, \ddot{\boldsymbol{u}}$$

$$\boldsymbol{u} = \overline{\boldsymbol{u}} \quad \text{on} \quad \Gamma_0^u \quad \text{and} \quad \boldsymbol{P} \cdot \boldsymbol{N} = \boldsymbol{t}_0 \quad \text{on} \quad \Gamma_0^t$$

P is first Piola-Kirchhoff stress tensor
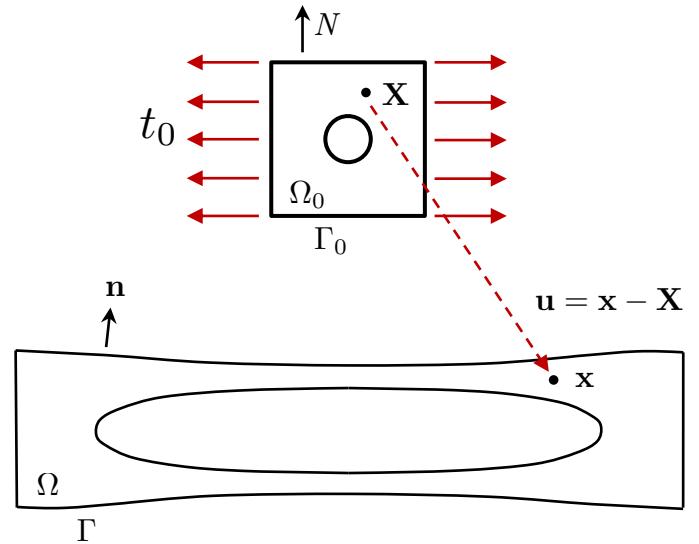
weak form

find the trial functions $\boldsymbol{u} \in \boldsymbol{H}^1(\Omega_0)$ such that

$$\int_{\Gamma_0^t} \boldsymbol{t}_0 \cdot \boldsymbol{v} \, dS - \int_{\Omega_0} \boldsymbol{P} : (\partial \boldsymbol{v}/\partial \boldsymbol{X}) \, d\boldsymbol{X} = \int_{\Omega_0} \rho_0 \, \ddot{\boldsymbol{u}} \cdot \boldsymbol{v} \, d\boldsymbol{X}$$

for all test functions $\boldsymbol{v} \in \boldsymbol{H}_0^1(\Omega_0)$

Governing equations for small strain elasticity

strong form

$$\frac{\partial \boldsymbol{\sigma}}{\partial \mathbf{x}} : \mathbf{I} + \mathbf{f} = \mathbf{0} \qquad \mathbf{u} = \bar{\mathbf{u}} \ \text{ on } \ \Gamma_{\mathrm{u}} \ \text{ and } \ \boldsymbol{\sigma}\,\mathbf{n} = \mathbf{t} \ \text{ on } \ \Gamma_{\mathrm{t}}$$

$$\boldsymbol{\sigma} = \mathbb{C}\,\boldsymbol{\epsilon}, \text{where } \boldsymbol{\epsilon} := \mathrm{sym}\,(\nabla \mathbf{u}) \qquad \text{(linear elastic)}$$

$$\exists\, \alpha_l\,,\ \alpha_u > 0 \ \text{ such that } \ \alpha_l\,\boldsymbol{\epsilon} : \boldsymbol{\epsilon} \ \leq \ \boldsymbol{\epsilon} : (\mathbb{C}(\mathbf{x})\,\boldsymbol{\epsilon}) \ \leq \ \alpha_u\,\boldsymbol{\epsilon} : \boldsymbol{\epsilon} \qquad \forall \boldsymbol{\epsilon} \qquad \text{(uniform ellipticity)}$$

weak form

find the trial functions $\boldsymbol{u} \in \boldsymbol{H}^1(\Omega_0)$ such that

$$\int_{\Omega} \boldsymbol{\sigma} : (\partial \mathbf{v}/\partial \mathbf{x})\,d\Omega = \int_{\Omega} \mathbf{f} \cdot \mathbf{v}\,d\Omega + \int_{\Gamma_{\mathrm{t}}} \mathbf{t} \cdot \mathbf{v}\,d\Gamma$$

for all test functions $\boldsymbol{v} \in \boldsymbol{H}_0^1(\Omega_0)$

Classical quadrature

If the polyhedron is "star convex", can use a simple sub-triangulation to create quadrature points.
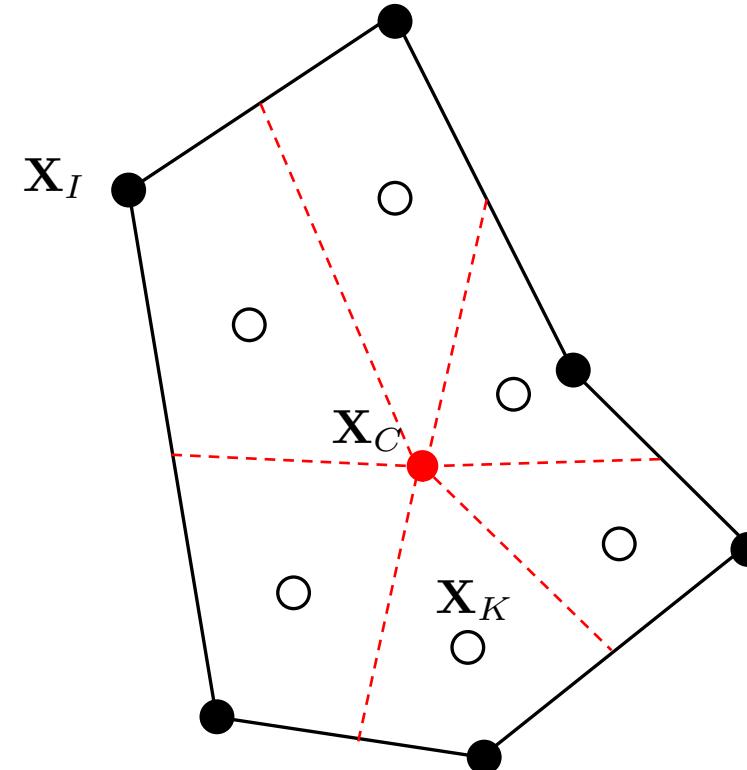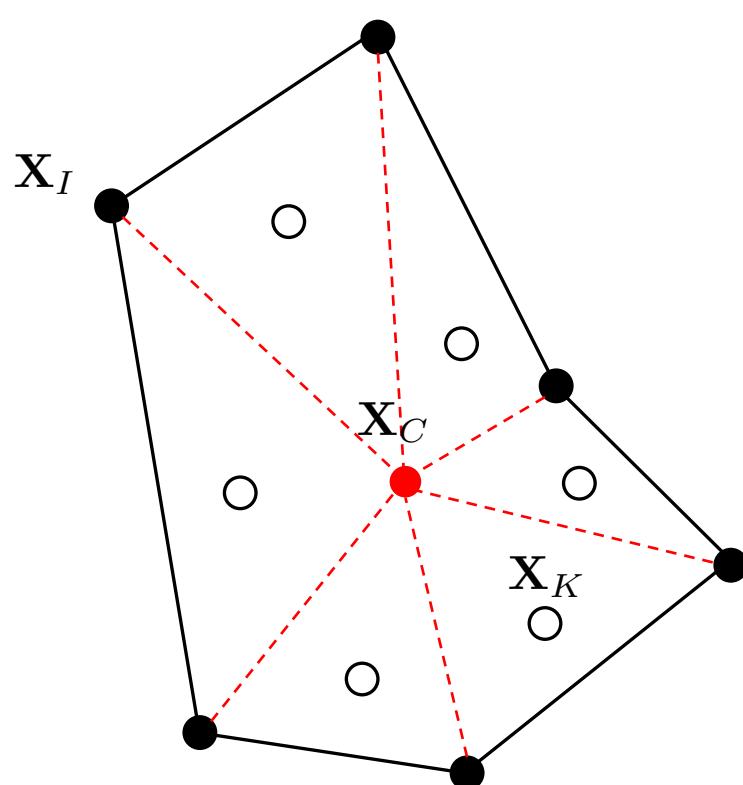
quadrature points $\mathbf{X}_K$

Integration consistency

Divergence theorem states that:

$$\int_{\Omega_e} \nabla \phi_I \, d\Omega = \int_{\Gamma_e} \phi_I \, \mathbf{N} \, d\Gamma$$

In discrete form:

$$\sum_K w_K \underbrace{\nabla \phi_I |_K} = \sum_L w_L^\Gamma \phi_I |_L \, \mathbf{N}_L \qquad I = 1, \dots, N_v$$

gradient value at
quadrature point K

- For non-polynomial shape functions, this will not be satisfied in general.
- This will result in a lack of consistency (failure of the engineering patch test).

Shape function derivative correction

- Project the shape function derivatives to satisfy the integration consistency condition.
- Maintain the reproducing properties of the derivatives.
- Minimize the least-squares difference between the new derivatives and the old.
- Only performed once during simulation (pre-processing step).

$$\min_{\overline{\nabla}\phi_I|_K \in \mathbb{R}^3} \sum_K w_K \left(\overline{\nabla}\phi_I|_K - \nabla\phi_I|_K\right)^2 \quad \text{subject to the constraints} \quad \sum_K w_K \overline{\nabla}\phi_I|_K - \sum_L w_L^\Gamma \phi_I|_L \, \mathbf{N}_L = 0$$

This constrained optimization problem can be solved using the method of Lagrange multipliers:

$$\mathcal{L}(\overline{\nabla}\phi_I|_K, \boldsymbol{\lambda}) := \sum_K w_K \left(\overline{\nabla}\phi_I|_K - \nabla\phi_I|_K\right)^2 + \boldsymbol{\lambda} \cdot \left(\sum_K w_K \overline{\nabla}\phi_I|_K - \sum_L w_L^\Gamma \phi_I|_L \, \mathbf{N}_L\right)$$

Bishop, J. (2014). "A displacement-based finite element formulation for general polyhedra using harmonic shape functions." *IJNME* 97: 1-31.

# Shape function derivative correction

original bilinear form $\quad a(u,v) = \int_{\Omega^{\mathrm{e}}} \nabla u : \mathbb{C}\, \nabla v \, d\Omega$

discrete form $\quad a^h(u,v) := \sum_K w_K \nabla u|_K : \mathbb{C}\, \nabla v|_K$

replace with this modified bilinear form $\quad \overline{a}^h(u,v) := \sum_K w_K \overline{\nabla} u|_K : \mathbb{C}\, \overline{\nabla} v|_K$

Note: This modified bilinear form is still symmetric (Bubnov-Galerkin).

Verification: elasticity patch test
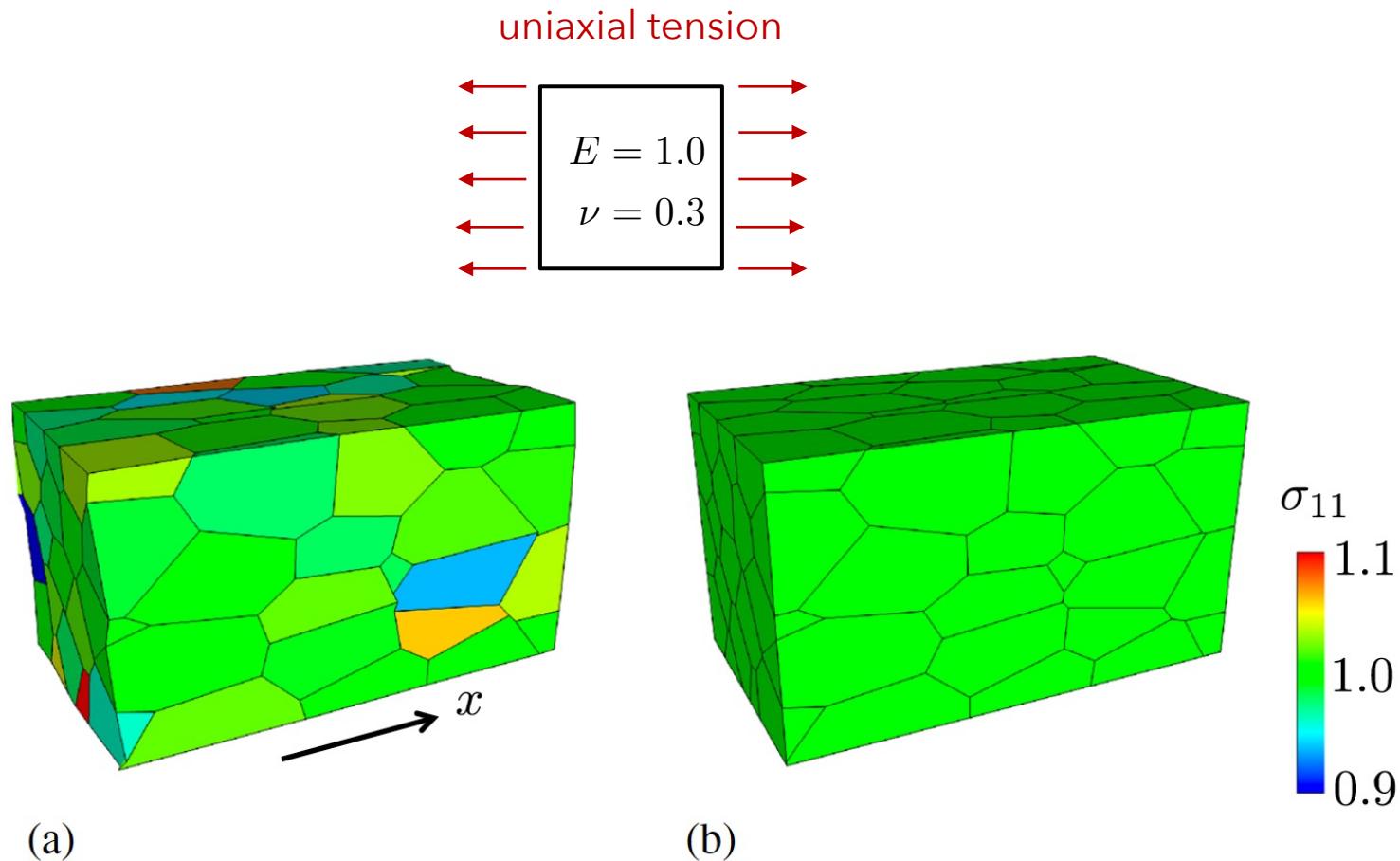
uniaxial tension

$E = 1.0$
$\nu = 0.3$

σ_{11}
1.1
1.0
0.9

(a)

(b)

x

Bishop, J. (2014). "A displacement-based finite element formulation for general polyhedra using harmonic shape functions." *IJNME* 97: 1-31.

Verification: cantilever beam


Voronoi mesh

von Mises stress

energy norm

$\|\mathbf{u}^h - \mathbf{u}\|_E / \|\mathbf{u}\|_E$

1.00
1

N_x

L$_2$ norm

$\|\mathbf{u}^h - \mathbf{u}\|_2 / \|\mathbf{u}\|_2$

1
2.01

polyhedral formulation
trilinear hex formulation

N_x
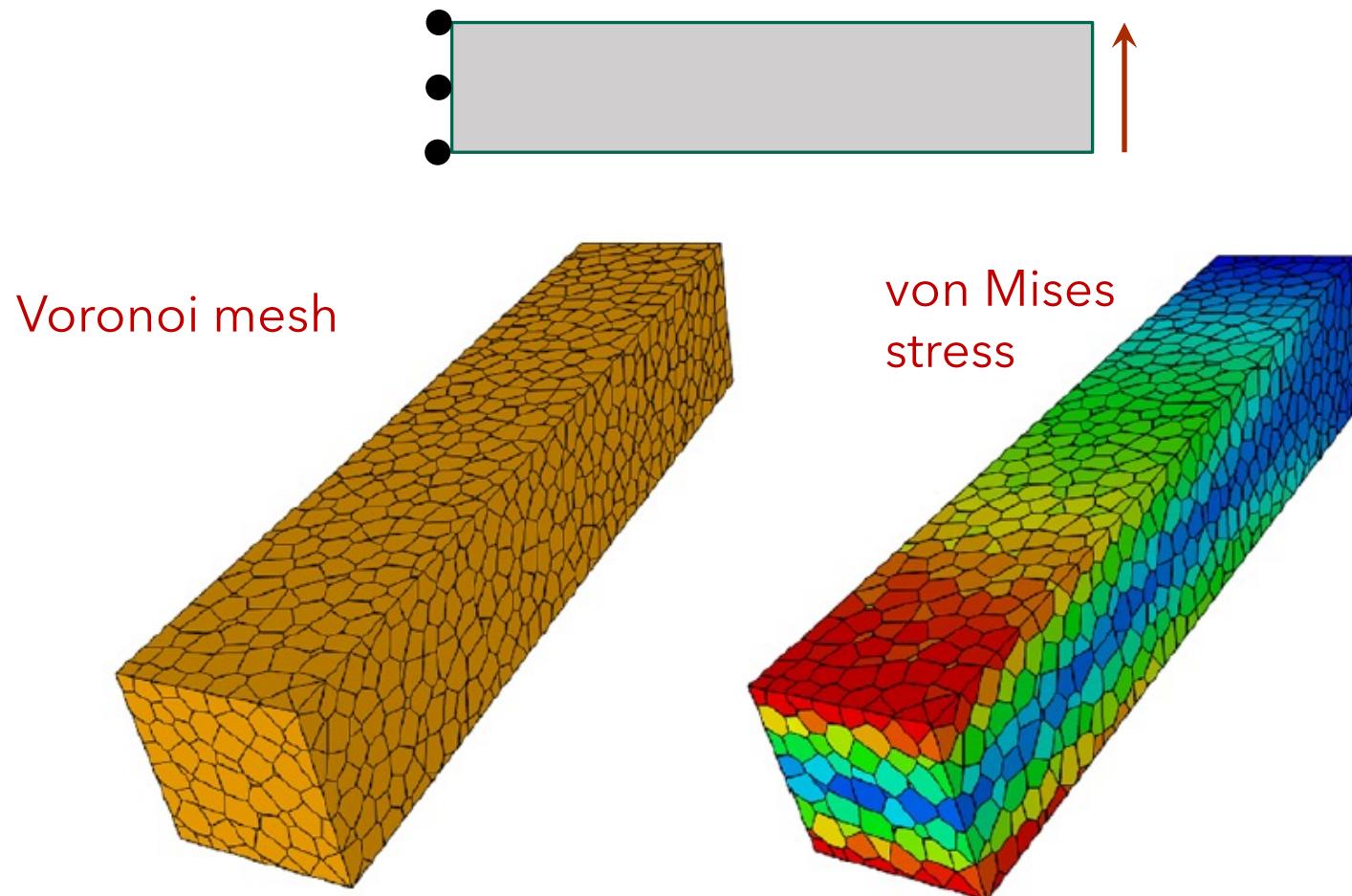
Bishop, J. (2014). *IJNME* 97: 1-31.
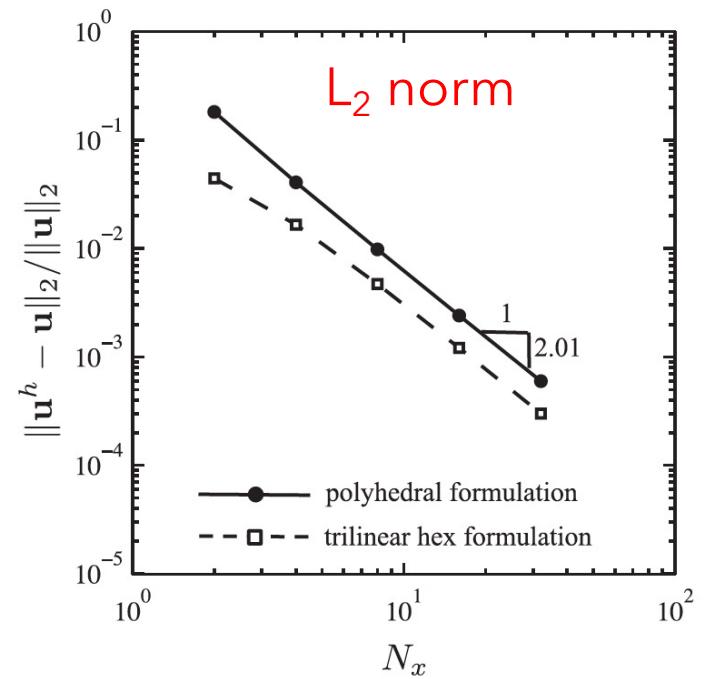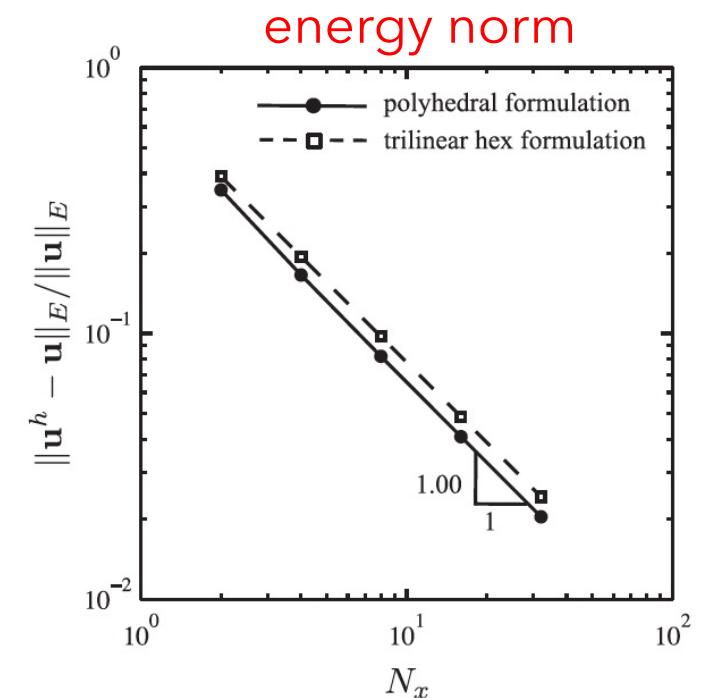
Nonlinear example

compressible neo-Hookean material
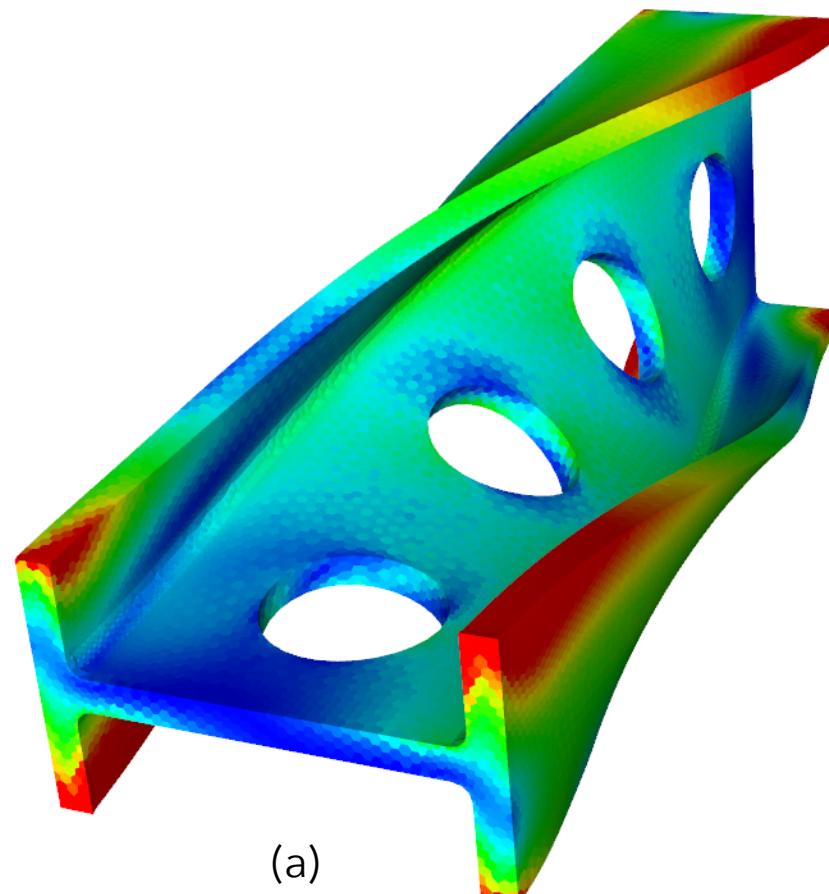
polyhedral mesh

conventional hexahedral mesh

$$\boldsymbol{\sigma} = \frac{\mu}{J}(\mathbf{F}\mathbf{F}^T - \mathbf{I}) + \frac{\lambda}{\ln J}\mathbf{I}$$

$$J = \det \mathbf{F} \qquad \mathbf{F} = \frac{\partial \mathbf{x}}{\partial \mathbf{X}}$$

10,000
5,000
0

von Mises stress

(a)

(b)

Bishop, J. and N. Sukumar (2020). "Polyhedral finite elements for nonlinear solid mechanics using tetrahedral subdivisions and dual-cell aggregation." Computer Aided Geometric Design 77: 101812
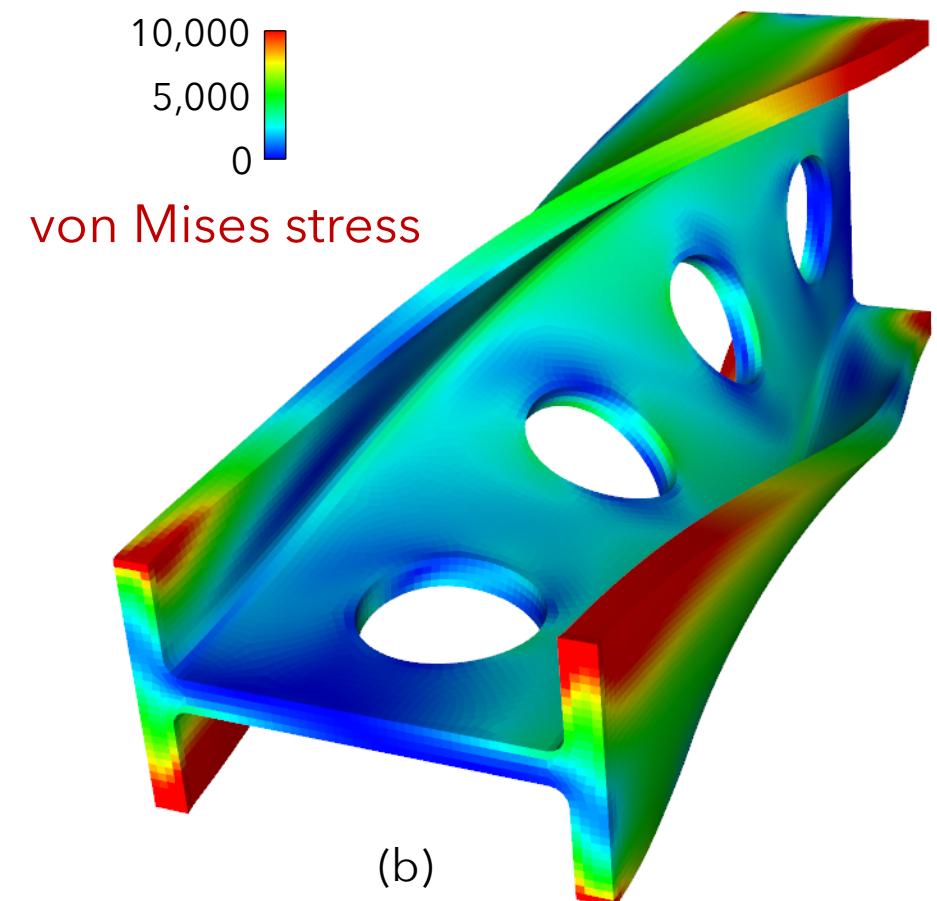
Point of departure: integration consistency

Try projecting shape function gradients before integrating.

Point of departure: integration consistency

- Project shape-function gradients to a space that is "easy" to integrate.
- VEM projects shape-function gradients to polynomial space.
- Instead here, project gradients to space of shape functions: $\{\phi_I, I = 1, \ldots, N_v\}$

$$\overline{\nabla}\phi_I := \arg\min \int_{\Omega_e} \left(\nabla\phi_I - \sum_J a^J \phi_J \right)^2 d\Omega \qquad (L_2 \text{ projection})$$

Note: Could also project to any other convenient basis, e.g. piecewise constant.

The solution can be written in terms of the dual basis $\{\phi^J\}$

$$(\phi_I, \phi^J) = \delta_I^J \qquad \text{bi-orthogonal}$$

$$\overline{\nabla}\phi_I = \sum_J \underbrace{(\nabla\phi_I, \phi_J)}\, \phi^J = \sum_J \underbrace{(\nabla\phi_I, \phi^J)}\, \phi_J$$

covariant   contravariant
components   components

Can prove polynomial consistency up to the order of the precision of $\{\phi_J\}$

Theorem: $\displaystyle\int_{\Omega_e} \mathbf{p}\,\overline{\nabla}\phi_I\,d\Omega = \int_{\Omega_e} \mathbf{p}\,\nabla\phi_I\,d\Omega$ for all $\mathbf{p} \in \mathbb{P}_k(\Omega_e)$ This ensures satisfaction of the patch test.

Replace the original bilinear form $\quad a(u,v) = \displaystyle\int_{\Omega_e} \nabla u : \mathbb{C}\,\nabla v\, d\Omega$

with this modified bilinear form $\quad \overline{a}(u,v) = \displaystyle\int_{\Omega_e} \overline{\nabla} u : \mathbb{C}\,\overline{\nabla} v\, d\Omega$

Note: This modified bilinear form is still symmetric (Bubnov-Galerkin).

$$\overline{a}(u,v) = \int_{\Omega_e} \left[\sum_I (\nabla u, \phi_I)\phi^I\right] \mathbb{C} \left[\sum_J (\nabla v, \phi_J)\phi^J\right] d\Omega$$
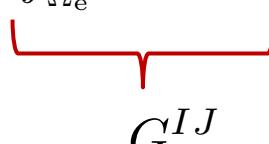
$$\overline{a}(u,v) = \sum_{I,J} (\nabla u, \phi_I)\,\mathbb{C}\,(\nabla v, \phi_J) \underbrace{\int_{\Omega_e} \phi^I \phi^J\, d\Omega}_{G^{IJ}}$$

Can show that $G^{IJ} = (G_{IJ})^{-1}$

where $G_{IJ} = \displaystyle\int_{\Omega_e} \phi_I \phi_J \, d\Omega$ is the Gram matrix of the element of category 0.

$$\bar{a}(u,v) = \sum_{I,J} G_{IJ}^{-1} (\nabla u, \phi_I) \, \mathbb{C} \, (\nabla v, \phi_J)$$

Still need to show that $\bar{a}(u,v)$ is coercive.

Also, for nonlinear problems, need to "lump" G_{IJ} to quadrature points.

What are the quadrature points?

Going to replace G_{IJ} with row-sum lumped version:

$$G_{IJ}^L := \sum_J G_{IJ} = \mathrm{diag}\{w_I\} \qquad \text{where} \qquad \boxed{w_I = \int_{\Omega_e} \phi_I(\mathbf{x})\, d\Omega}$$

Then $\quad \overline{a}(u,v) \to \overline{a}^L(u,v) = \sum_K \frac{1}{w_K} (\nabla u, \phi_K)\, \mathbb{C}\, (\nabla v, \phi_K)$

Can write $\overline{a}^L(u,v)$ as $\quad \overline{a}^L(u,v) = \sum_K w_K\, (\overline{\nabla} u)_K : \mathbb{C}\, (\overline{\nabla} v)_K$

where $\quad (\overline{\nabla} u)_K := \frac{1}{w_K} \int_{\Omega_e} (\nabla u)\phi_K\, d\Omega \qquad$ which now has the form of a discrete derivative at a quadrature point K.

Can prove that these discrete/projected derivatives have the same reproducing and polynomial consistency properties as the original derivatives.
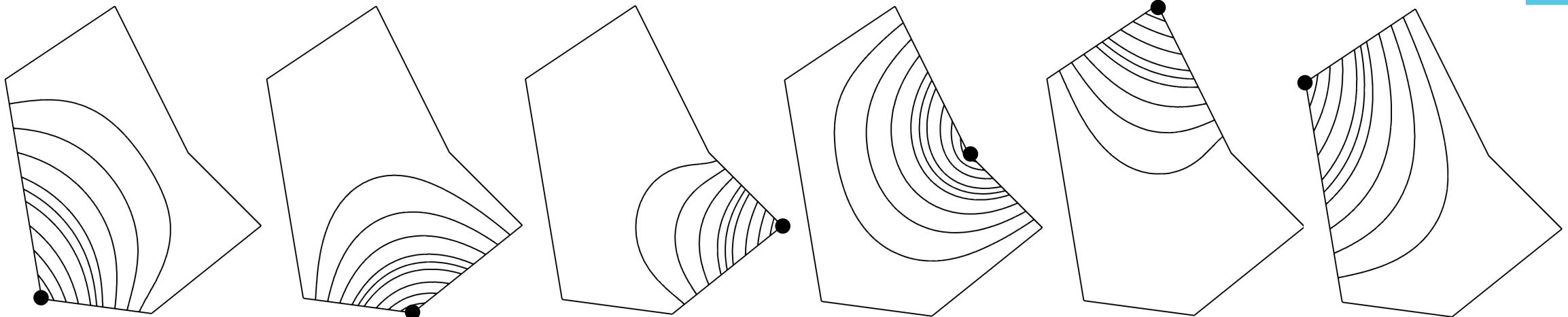
$$\frac{w_1}{A} = 0.201 \qquad \frac{w_2}{A} = 0.147 \qquad \frac{w_3}{A} = 0.110 \qquad \frac{w_4}{A} = 0.196 \qquad \frac{w_5}{A} = 0.138 \qquad \frac{w_6}{A} = 0.209$$

A = area

quadrature weights $\qquad \sum_K w_K = A \qquad\qquad \boxed{w_K = \int_{\Omega_e} \phi_K(\mathbf{x})\, d\Omega}$

max error in discrete derivative reproducibility $\qquad \max_K \sum_I (\overline{\nabla}\phi_I)_K = 9 \times 10^{-15}$

$$\max_K \sum_I (\overline{\nabla}\phi_I)_K \mathbf{x}_I - \mathbf{I} = 5 \times 10^{-15}$$

max error in integration consistency $= 8 \times 10^{-16}$

Quadrature-revisited

Start with reproducing conditions
$$\sum_K \mathbf{x}_K \, \phi_K(\mathbf{x}) = \mathbf{x}$$
linear consistency

Integrate both sides

(1) $$\int_{\Omega_e} \sum_K \mathbf{x}_K \, \phi_K(\mathbf{x}) \, d\Omega = \int_{\Omega_e} \mathbf{x} \, d\Omega$$

(2) $$\sum_K \mathbf{x}_K \int_{\Omega_e} \phi_K(\mathbf{x}) \, d\Omega = \int_{\Omega_e} \mathbf{x} \, d\Omega$$

Define quadrature weight as
$$\boxed{w_K = \int_{\Omega_e} \phi_K(\mathbf{x}) \, d\Omega}$$
then $$\sum_K w_K \, \mathbf{x}_K = \int_{\Omega^e} \mathbf{x}$$

Quadrature points are just $\mathbf{x}_K$

$\mathbf{x}_K$

Ω_e
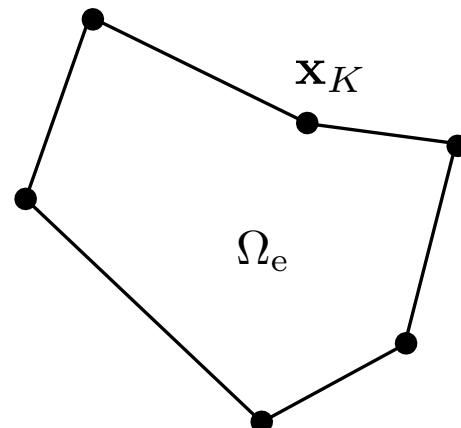
Quadrature points are now just the vertices.

Quadrature

Also, note that

$$\sum_K w_K = \sum_K \int_{\Omega_e} \phi_K(\mathbf{x}) \, d\Omega = \int_{\Omega_e} \sum_K \phi_K(\mathbf{x}) \, d\Omega = \int_{\Omega_e} 1 \, d\Omega = V$$

Now have a second-order integration scheme that can integrate linear functions exactly.

$$\sum_K w_K = V \quad \text{and} \quad \sum_K w_K \mathbf{x}_K = \int_{\Omega_e} \mathbf{x} \, d\Omega$$

Can extend to higher-order integration using higher-order reproducing conditions.

Verification: quadrature

$$\text{error} = \left| \int f - \sum_i w_i f_i \right|$$

$$f(x,y) = \left[1 - \left(\frac{2x}{L_x} \right)^2 \right] \left[1 - \left(\frac{2y}{L_y} \right)^2 \right]$$

quadrature error

error

element size, h
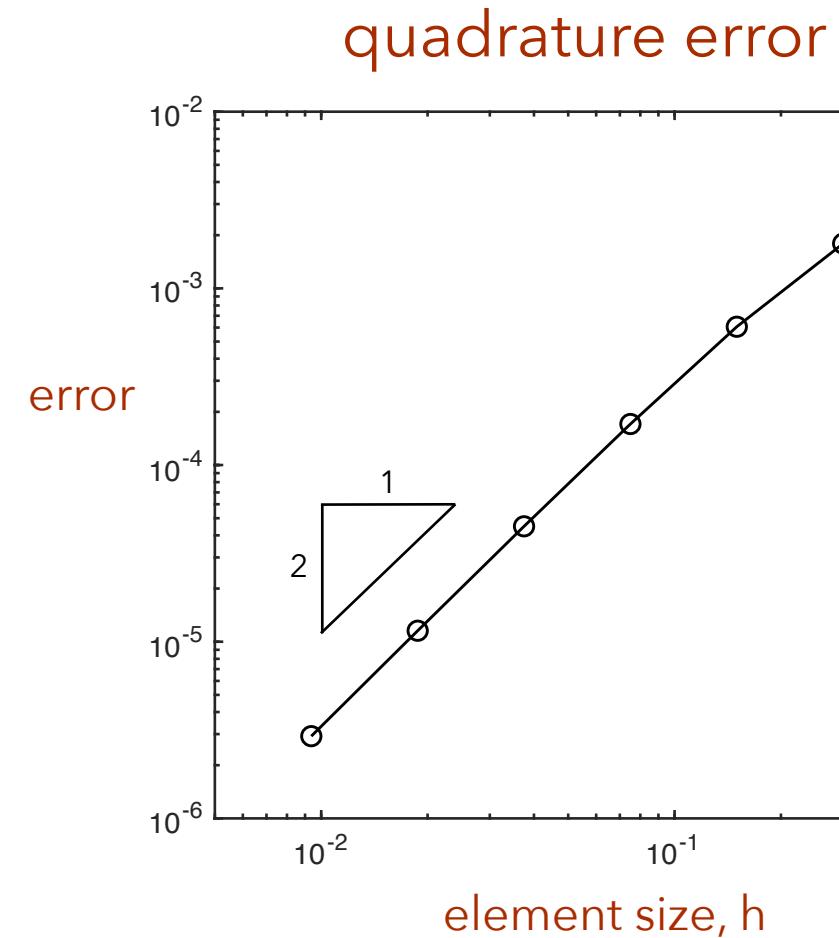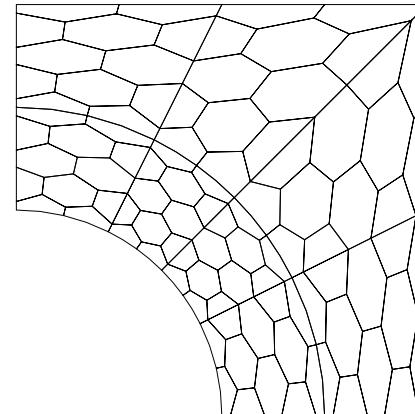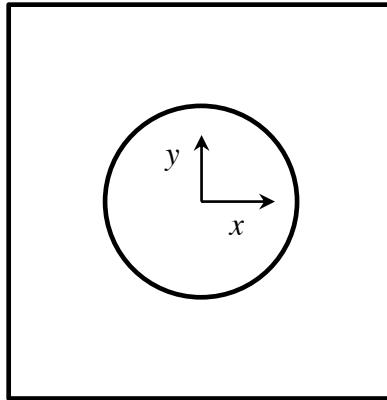
Verification examples: linear elasticity

Verification: elasticity patch test

uniaxial tension

$$E = 1.0$$
$$\nu = 0.3$$
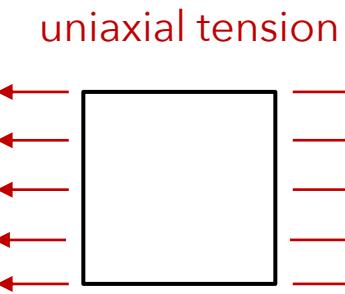
hexagon mesh

subtriangle quadrature
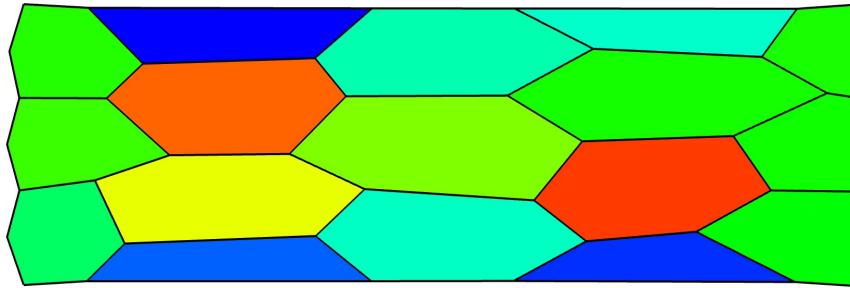
max stress error = 2%
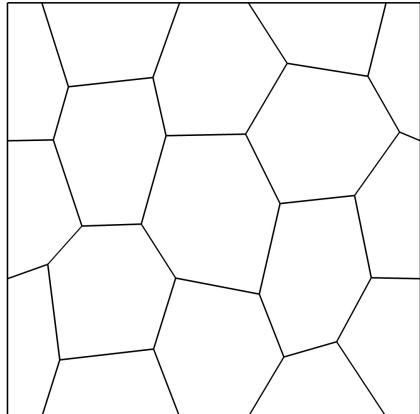
projection based quadrature
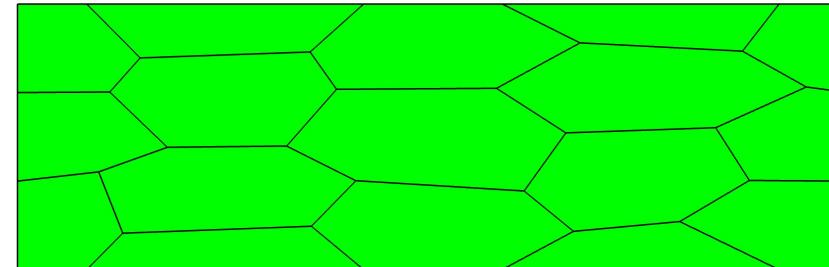
max stress error = 3×10^{-15}

Verification: elasticity, hole-in-plate tension

uniaxial tension

mapped hexagon mesh

von Mises stress invariant

- exact tension prescribed corresponding to infinite plate
- plane strain
- quarter symmetry model used

$$E = 1.0$$

$$\nu = 0.3$$

# Verification: elasticity, hole-in-plate tension

L₂ norm

energy norm
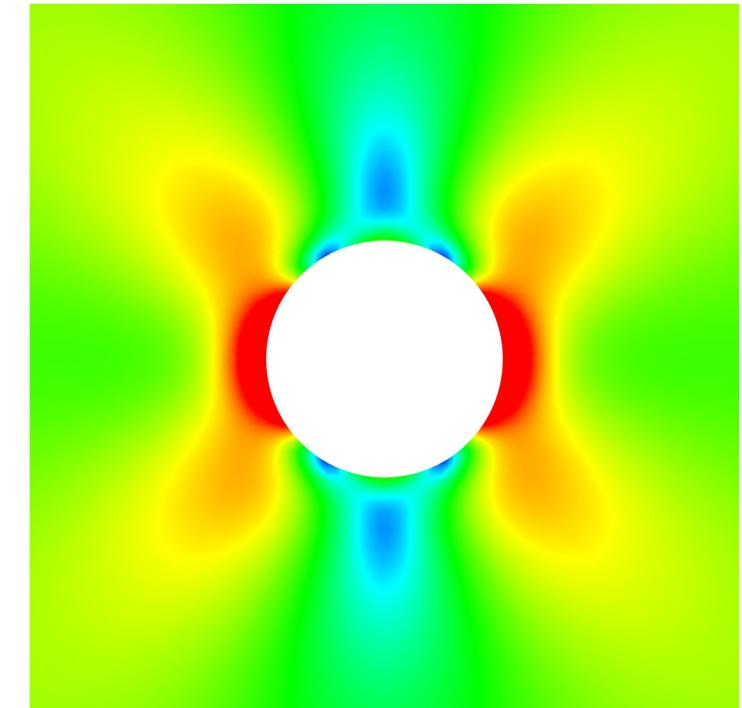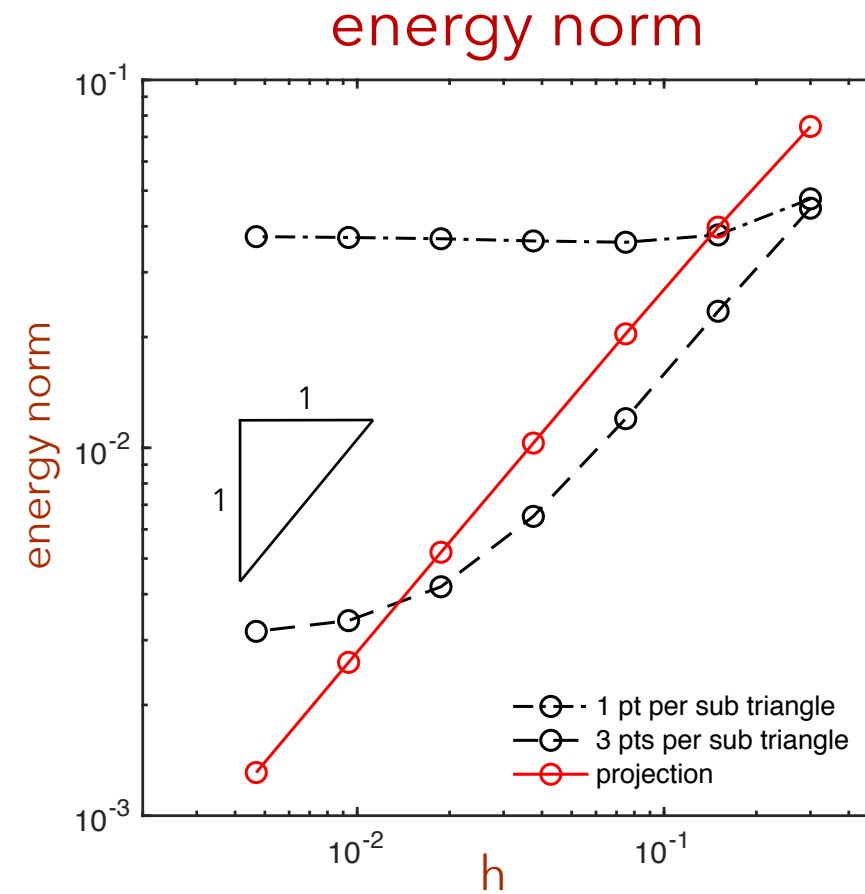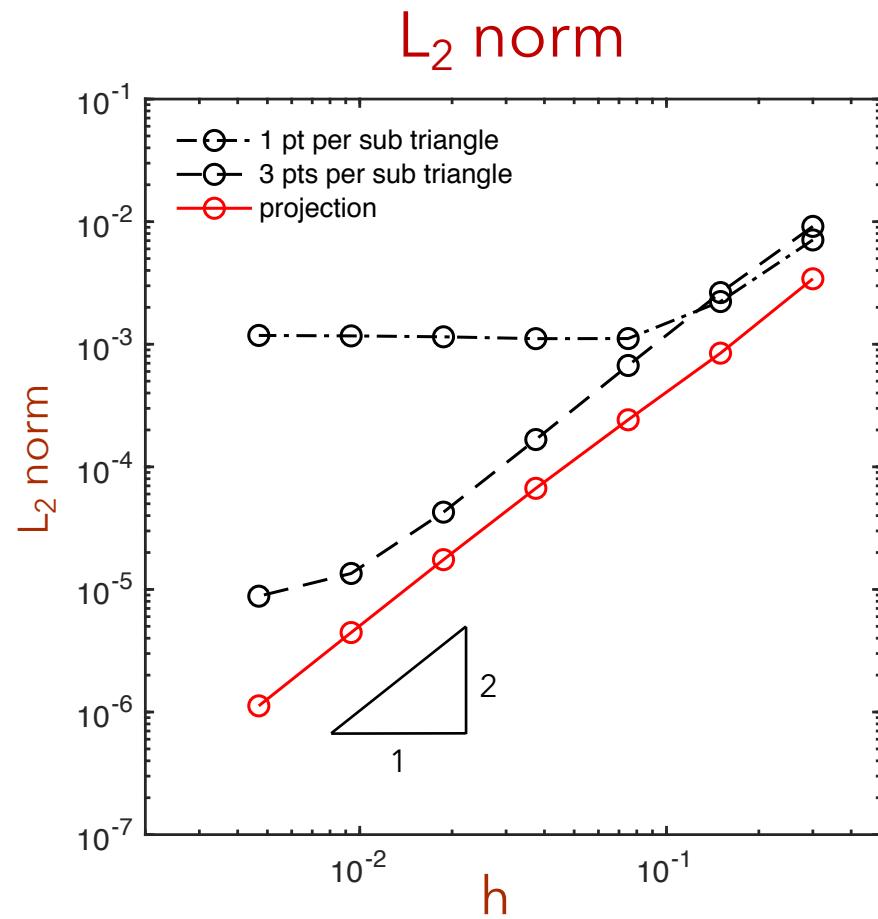
Optimal rates of convergence

Nonlinear solid mechanics, examples

Application example: hyperelastic, hole-in-plate

uniaxial extension


quad mesh

mapped hexagon mesh
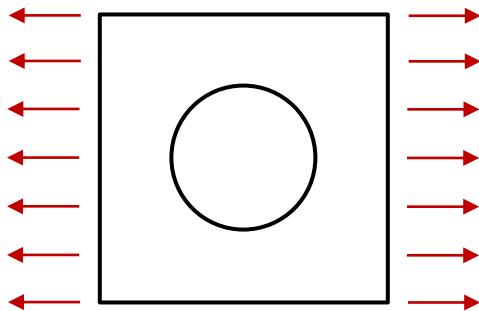
- plane strain
- quarter symmetry model used

compressible neo-Hookean material

$$\boldsymbol{\sigma} = \frac{\mu}{J}(\mathbf{F}\mathbf{F}^T - \mathbf{I}) + \frac{\lambda}{\ln J}\mathbf{I}$$

$$J = \det \mathbf{F} \qquad \mathbf{F} = \frac{\partial \mathbf{x}}{\partial \mathbf{X}}$$
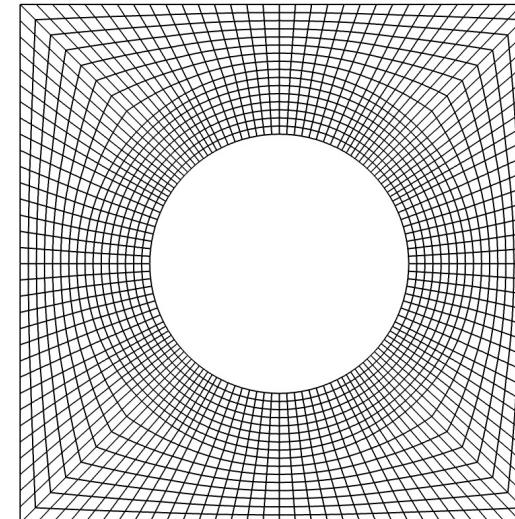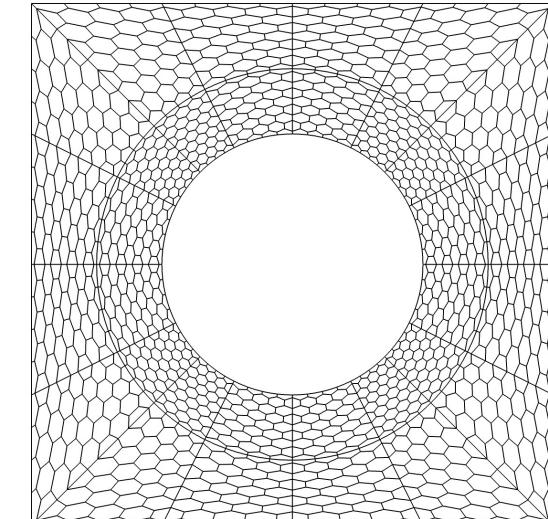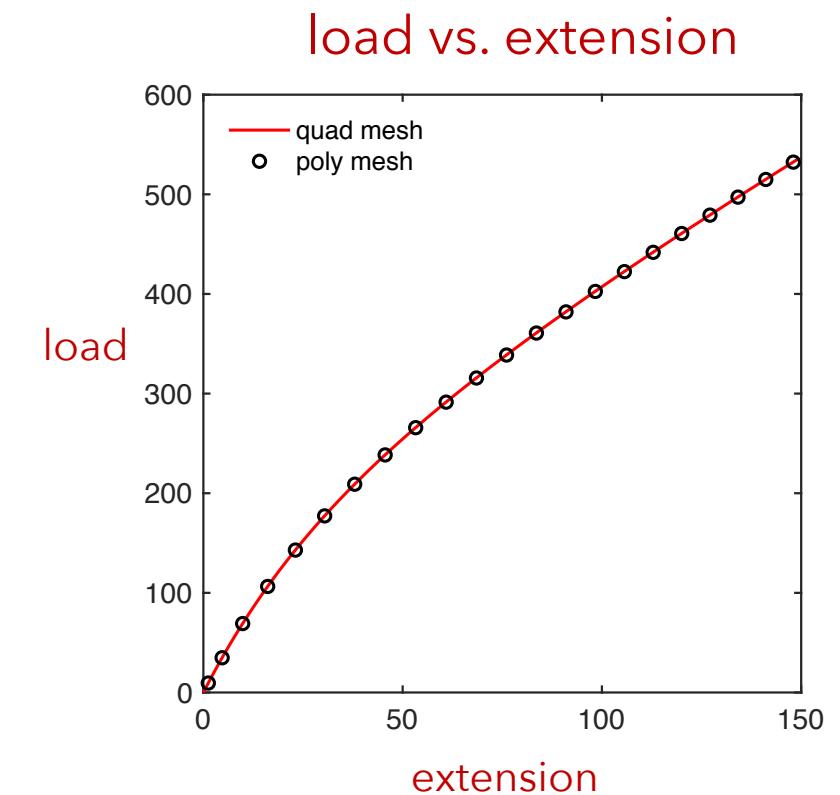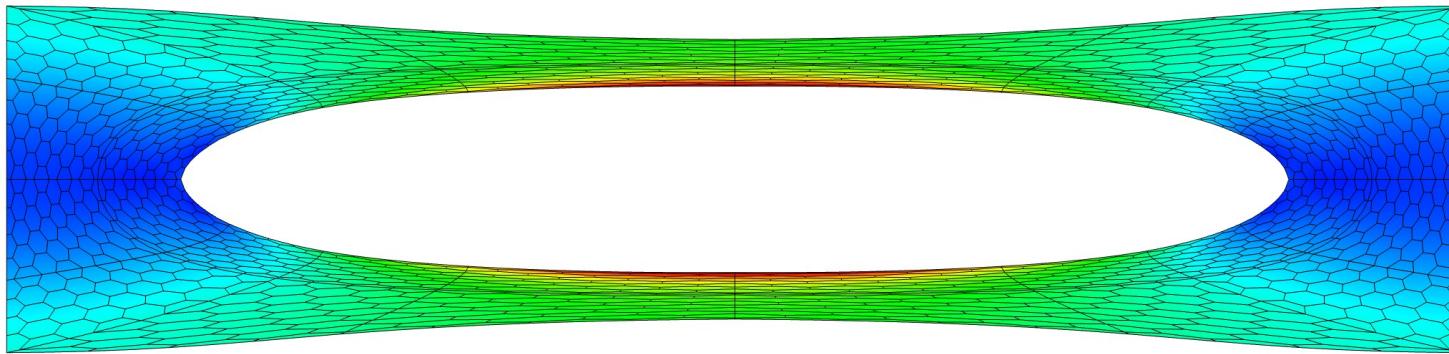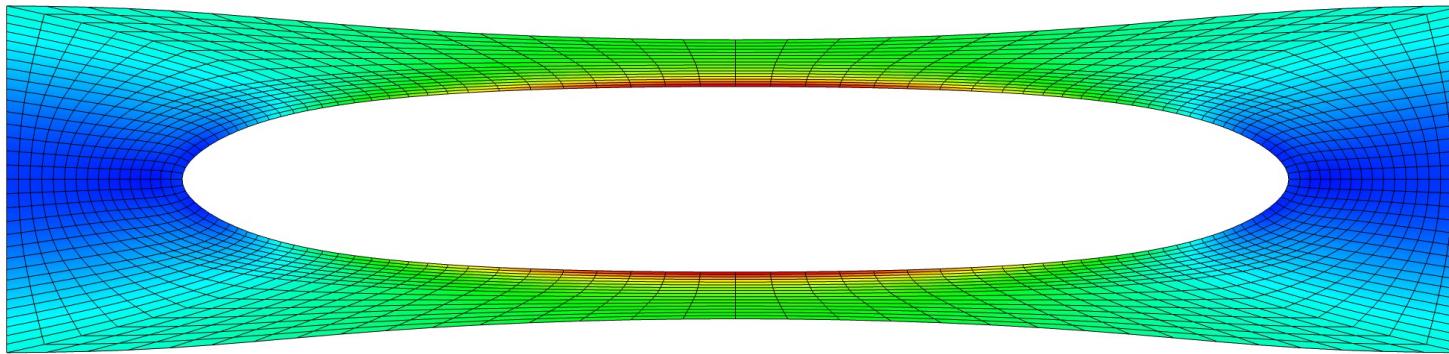
load vs. extension

# Application example: elastic-plastic, hole-in-plate

yield surface
$$f(\sigma, \bar{\varepsilon}^p) = \phi(\sigma) - \sigma_y(\bar{\varepsilon}^p) = 0$$

$$\phi(\sigma) = \left\{ \frac{1}{2} \left(|\sigma_1 - \sigma_2|^2 + |\sigma_1 - \sigma_3|^2 + |\sigma_2 - \sigma_3|^2 \right) \right\}^{1/2}$$

plastic strain field
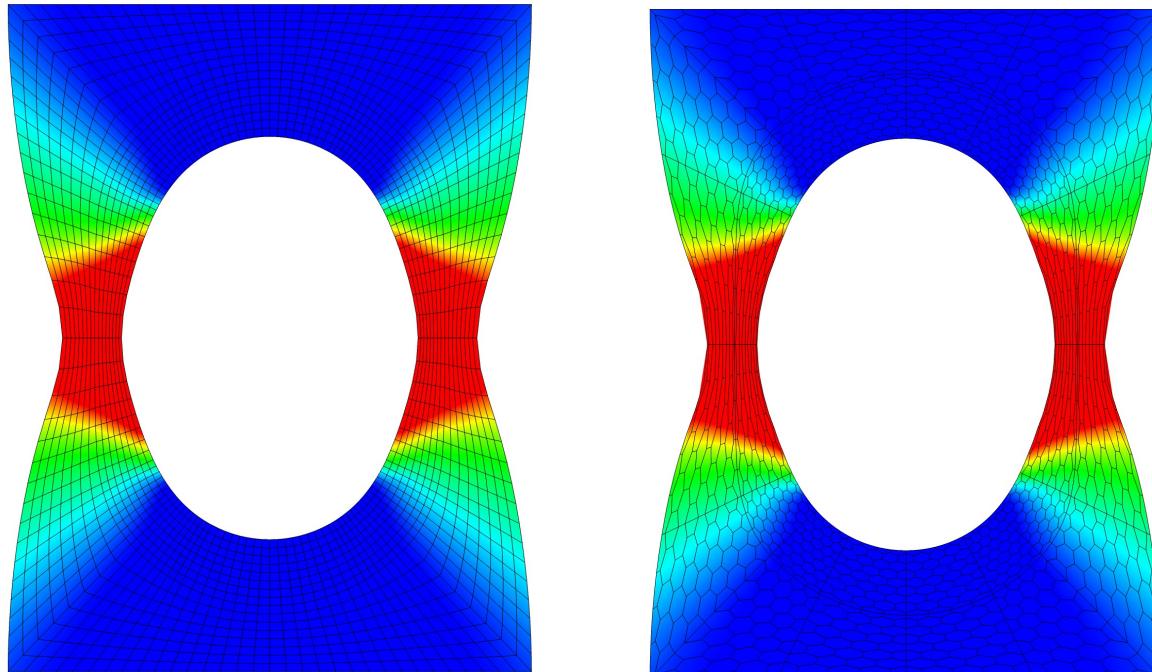
load vs. extension

load

extension
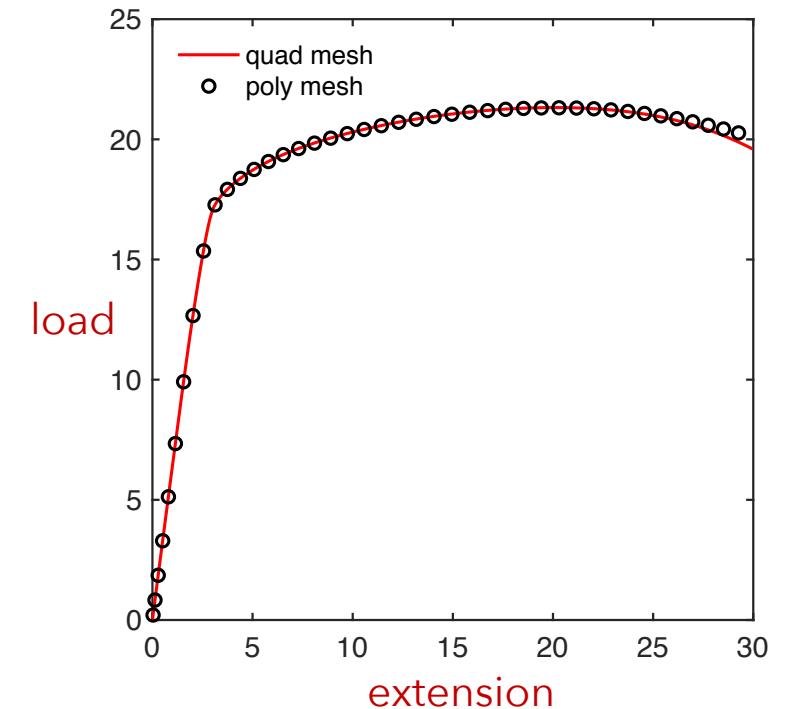
Calculation of ϕ_I and $(\nabla\phi_I, \phi_K)$

- Currently solving for harmonic shape functions and derivative projection using a sub-triangulation and FEA.
- Can also use boundary element techniques to solve for both the shape functions and their projection since shape function is harmonic.

Summary

1. Presented a generalized method for "correcting" shape function derivatives to satisfy integration consistency.
2. Observed optimal convergence rates for verification tests in 2D elasticity.
3. Presented nonlinear examples in solid mechanics
4. Exploring use of BEM to calculate shape function gradient projections.