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A polyhedral FE formulation using projected gradients and the dual basis with applications to nonlinear solid mechanics

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Outline

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

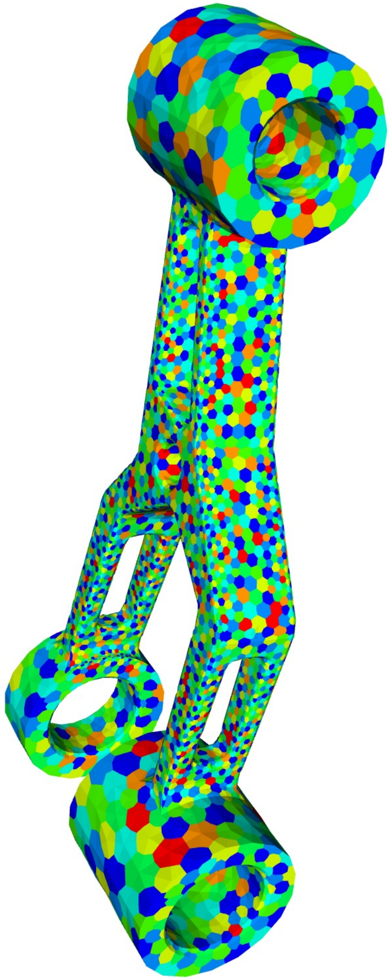
Applications of interest

- nonlinear solid mechanics
- large deformation, plasticity
- implicit and explicit dynamics
- For plasticity, need quadrature points to carry material history.
- For efficiency in explicit dynamics, need to minimize number of quadrature points
- Avoid artificial stabilization since, in engineering practice, discretizations are typically in pre-asymptotic regime.

Motivation for polyhedral discretizations

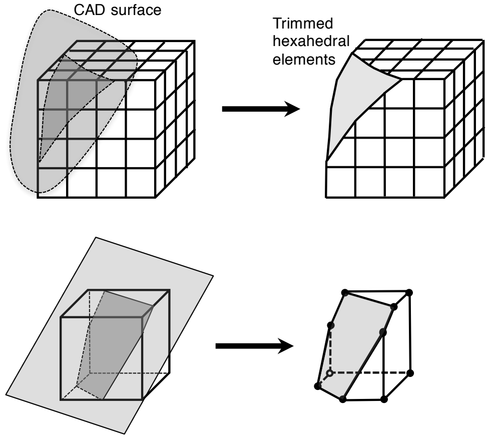
- more general discretizations
- hybrid meshing (tet-hex-poly)
- hex dominant meshing using frame fields
- cut-cell discretizations
- use of Voronoi tessellations
- tetrahedral dual cells discretizations

tetrahedral dual cell

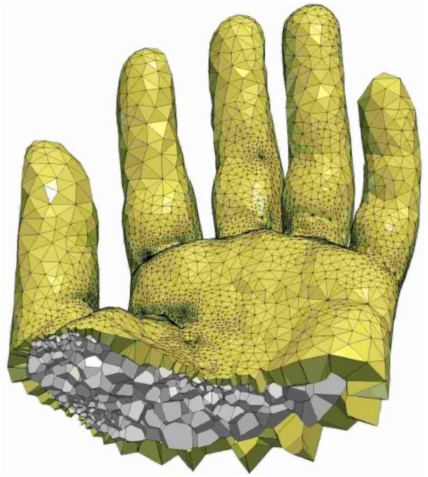


hex-dominant meshing using frame field

cut-cell



Voronoi



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”
- 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:

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

The minimizer of this functional satisfies the following variational problem:

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

$$\int_{\Omega_\mathrm{e}} \nabla\phi \cdot \nabla v \, d\Omega$$

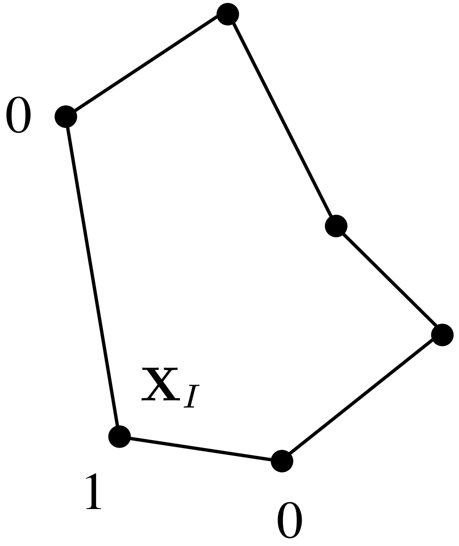
for all test functions $v \in H^1_0(\Omega_\mathrm{e})$

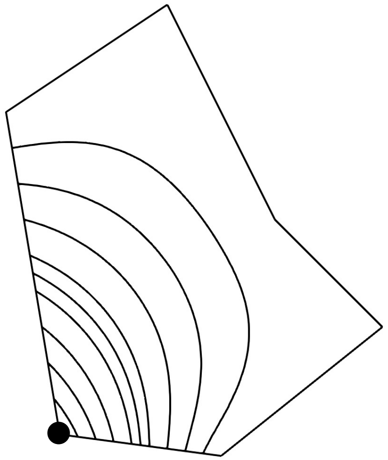
The strong form of this variational problem is given by:

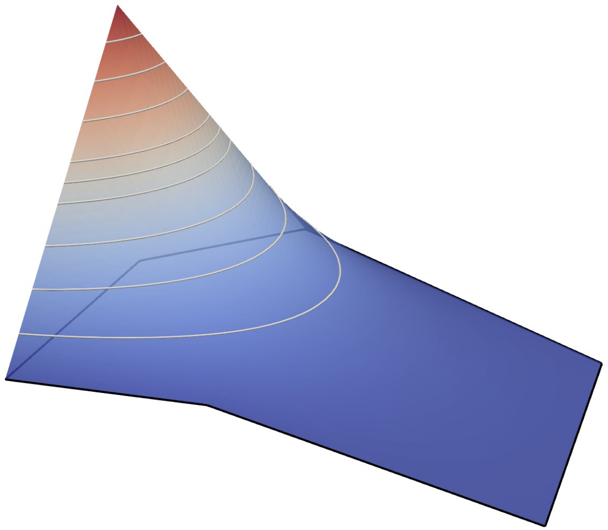
$$\nabla^2\phi = 0 \text{ in } \Omega_\mathrm{e} \text{ with } \phi = \overline{\phi} \text{ on } \Gamma_\mathrm{e}$$

Harmonic shape functions

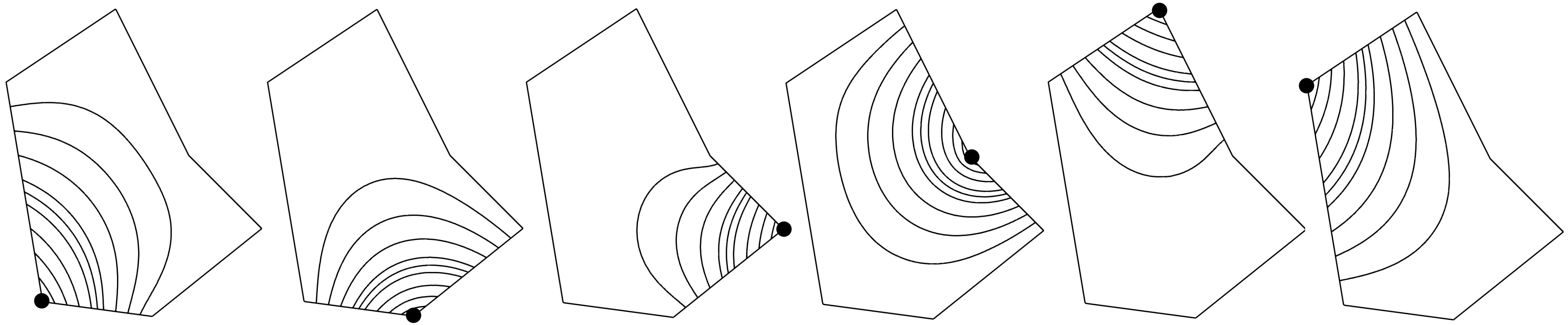
$$\nabla^2 \phi_I = 0$$







Harmonic shape functions



$$\sum_I \phi_I(\mathbf{x}) = 1$$ partition of unity

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

Can also do higher-order reproducibility.

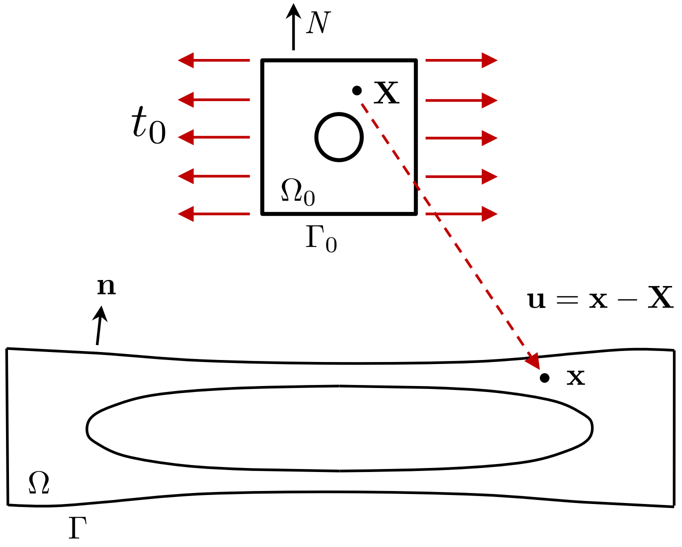
Governing equations (total-Lagrangian formulation)

strong form

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

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

$\boldsymbol{P}$ is first Piola-Kirchhoff stress tensor



weak form

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

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

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

Governing equations for small strain elasticity

strong form

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

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

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

weak form

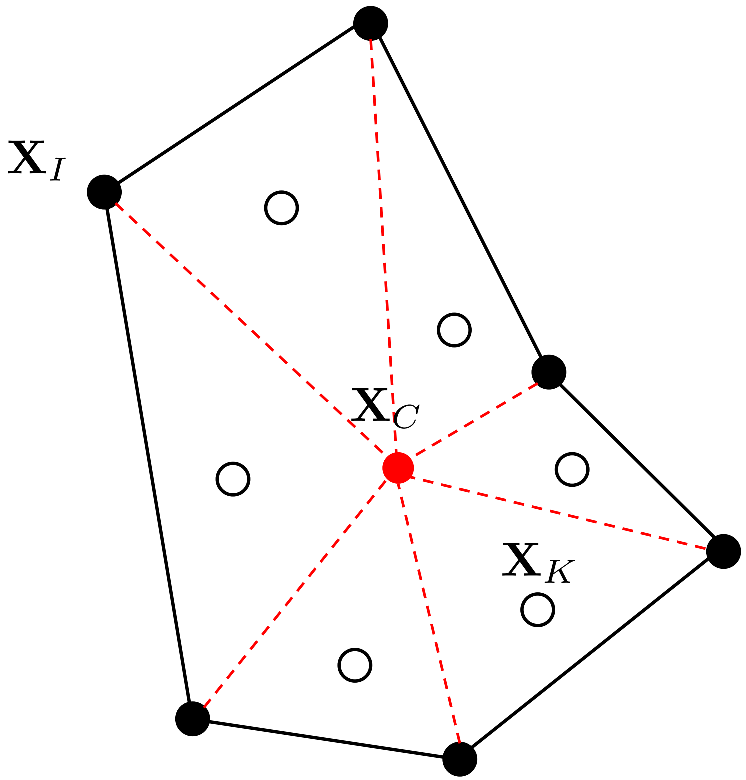
find the trial functions $\boldsymbol{u} \in \boldsymbol{H}^1(\Omega_0)$ such that

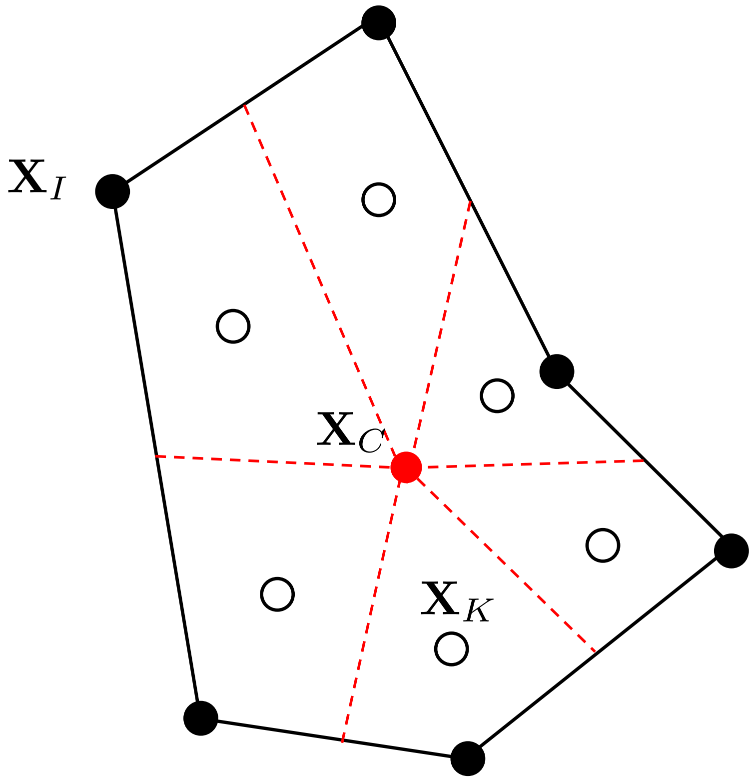
$$\int_{\Omega} \boldsymbol{\sigma} : (\partial \mathbf{v} / \partial \mathbf{x})\, d\Omega = \int_{\Omega} \mathbf{f} \cdot \mathbf{v}\, d\Omega + \int_{\Gamma_{\mathrm{t}}} \mathbf{t} \cdot \mathbf{v}\, d\Gamma$$

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

Classical quadrature points

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:

$$\sum_K w_K \underbrace{\nabla \phi_I|_K}_{\text{gradient value at quadrature point K}} = \sum_L w_L^\Gamma \, \phi_I|_L \, \mathbf{N}_L \qquad I = 1, \ldots, N_v$$

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

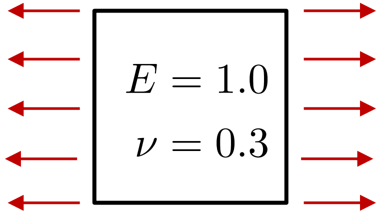
discrete form $$a^h(u,v) := \sum_K w_K \nabla u|_K : \mathbb{C}\, \nabla v|_K$$

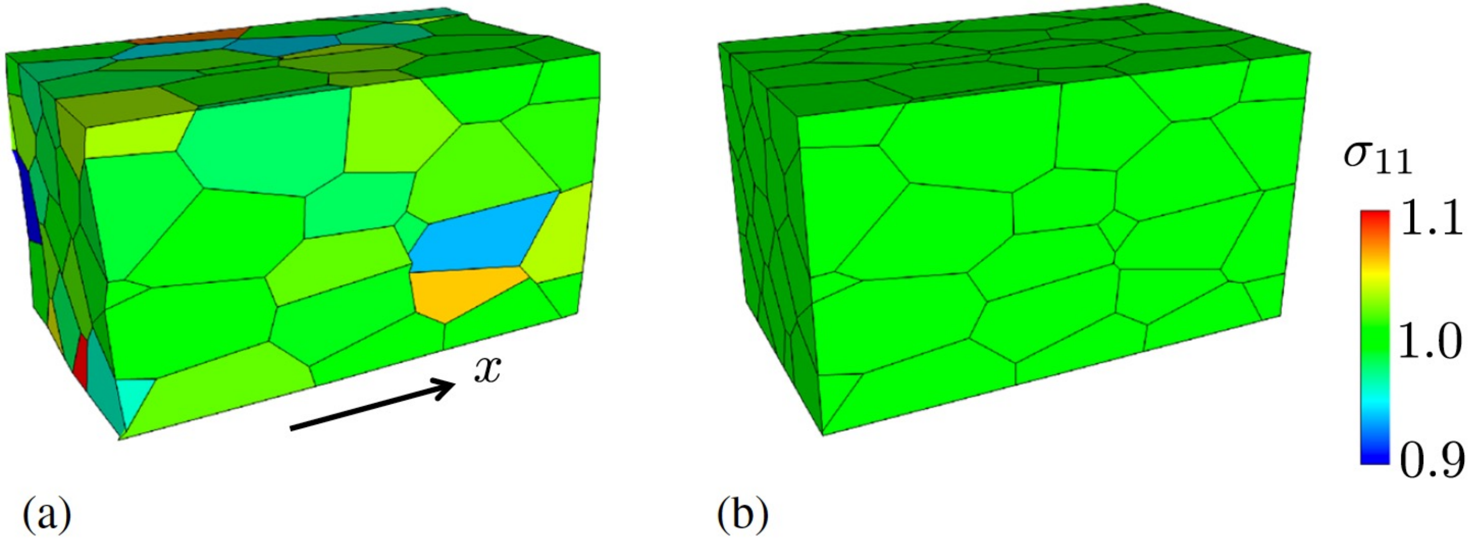
replace with this modified bilinear form $$\overline{a}^h(u,v) := \sum_K w_K \overline{\nabla} u|_K : \mathbb{C}\, \overline{\nabla} v|_K$$

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

Verification: elasticity patch test

uniaxial tension





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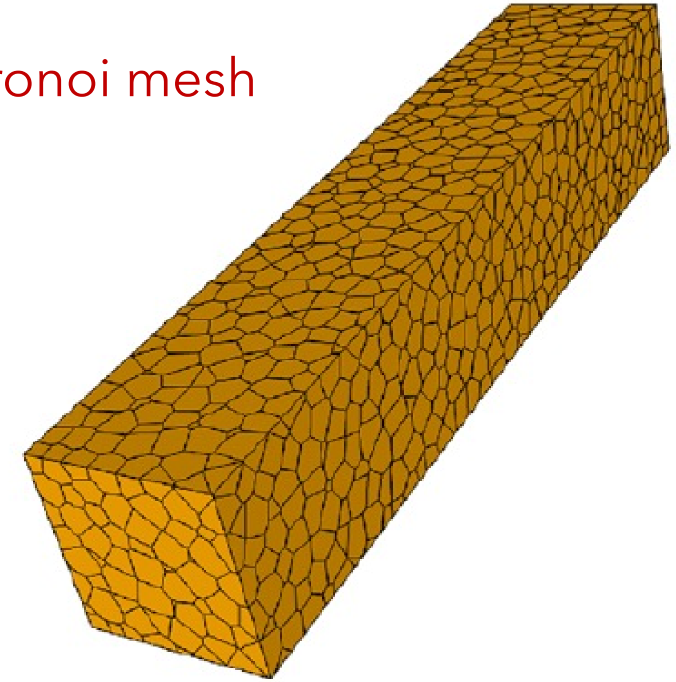
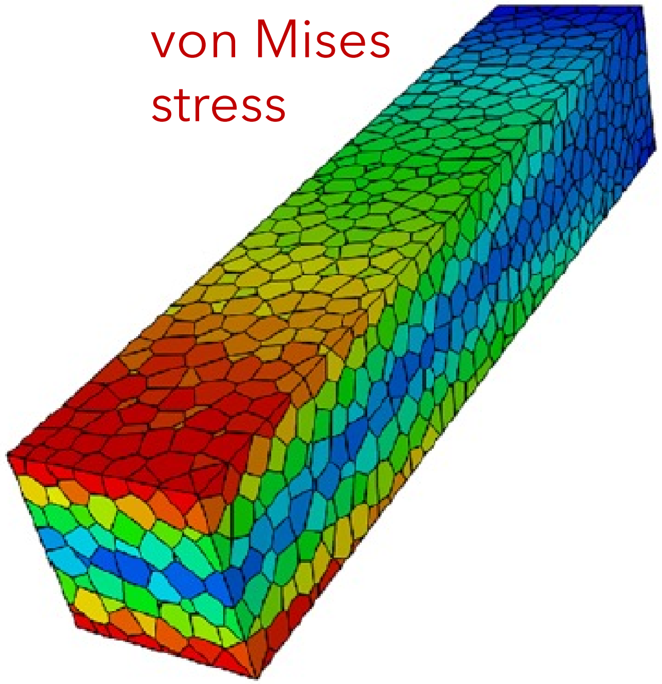
Verification: cantilever beam

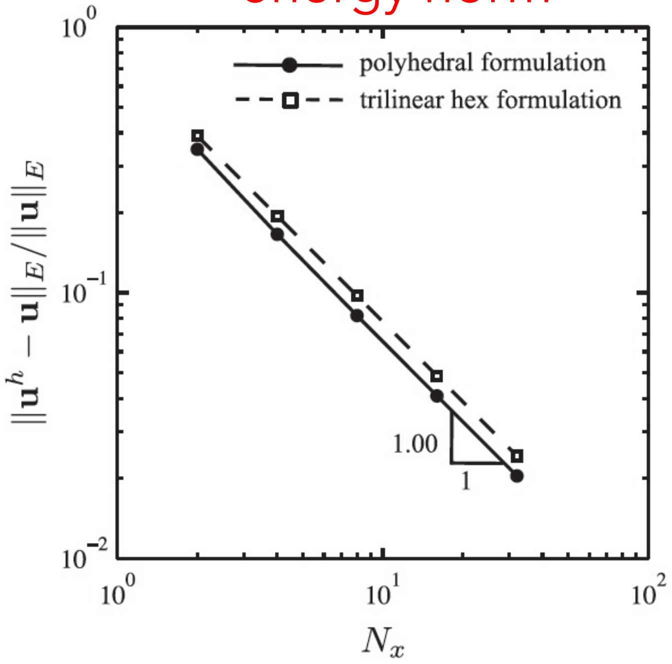
Voronoi mesh



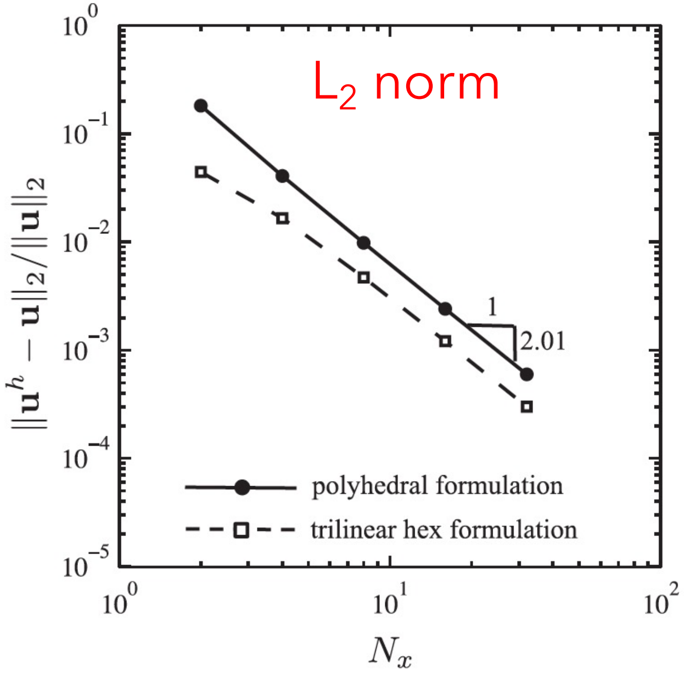
von Mises stress



energy norm



L_2 norm



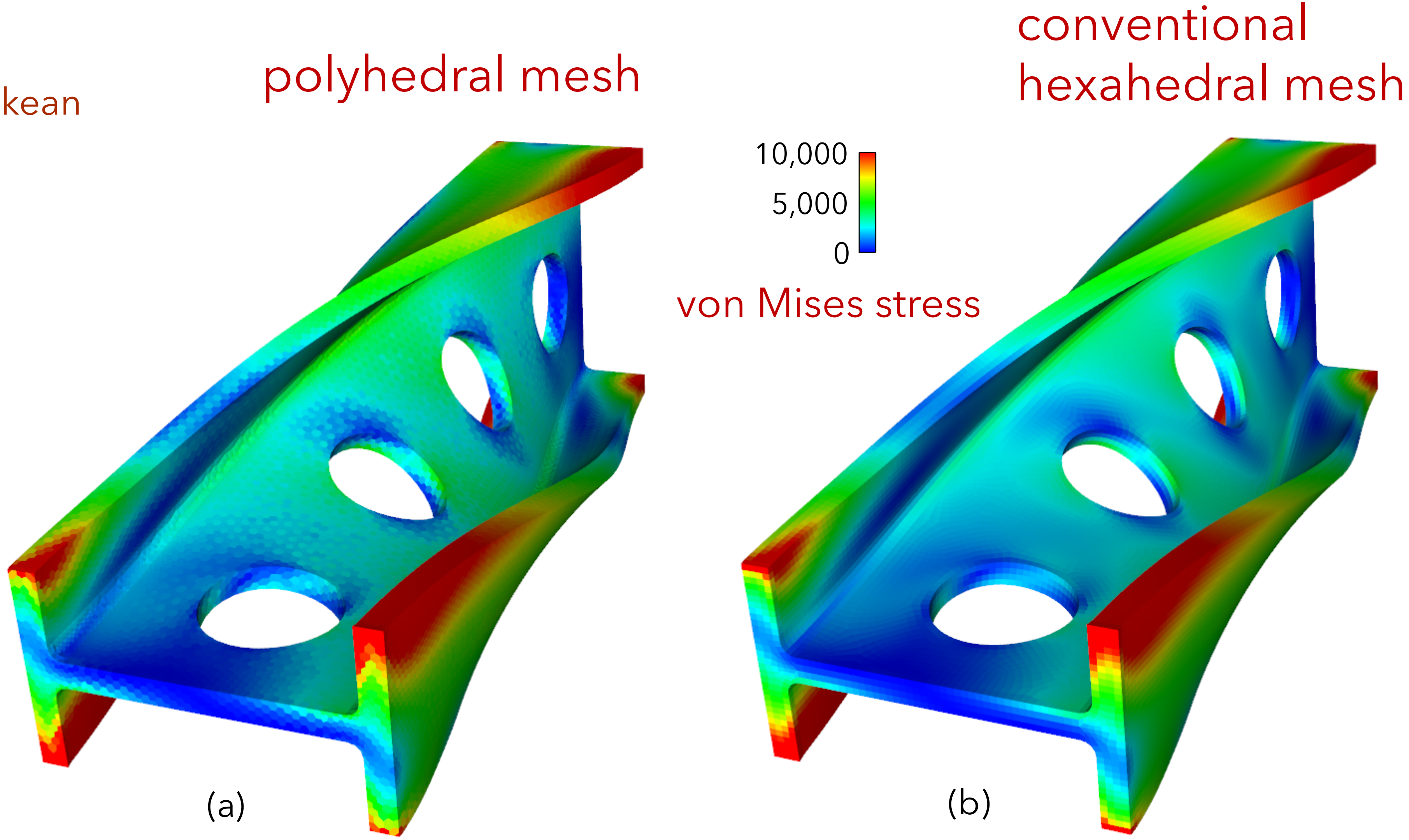
Bishop, J. (2014). *IJNME* 97: 1-31.

Nonlinear example

compressible neo-Hookean material

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

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



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

Project shape function gradients to span of shape function basis.

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: $\{\phi_I, I = 1, \ldots, N_v\}$

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

(L_2 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 $\{\phi^J\}$

$$(\phi_I, \phi^J) = \delta_I^J$$ bi-orthogonal

$$\overline{\nabla}\phi_I = \sum_J \underbrace{(\nabla\phi_I, \phi_J)}_{\text{covariant components}}\, \phi^J = \sum_J \underbrace{(\nabla\phi_I, \phi^J)}_{\text{contravariant components}}\, \phi_J$$

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

Theorem: $\int_{\Omega_e} \mathbf{p}\,\overline{\nabla}\phi_I \, d\Omega = \int_{\Omega_e} \mathbf{p}\,\nabla\phi_I \, d\Omega$ for all $\mathbf{p} \in \mathbb{P}_k(\Omega_e)$

This ensures satisfaction of the patch test.

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

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

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

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

Still need to show that $\overline{a}(u,v)$ 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:

$$G_{IJ}^{L} := \sum_{J} G_{IJ} = \mathrm{diag}\{w_I\}$$

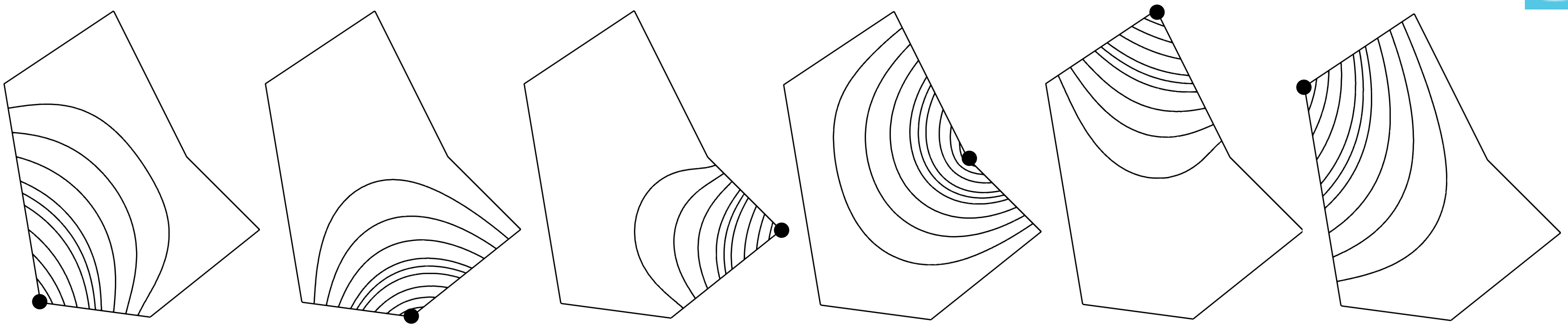
where $w_I = \int_{\Omega_\mathrm{e}} \phi_I(\mathbf{x})\, d\Omega$

Then $\overline{a}(u,v) \rightarrow \overline{a}^{L}(u,v) = \sum_{K} \frac{1}{w_K} (\nabla u, \phi_K)\, \mathbb{C}\, (\nabla v, \phi_K)$

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

where $(\overline{\nabla} u)_K := \frac{1}{w_K} \int_{\Omega_\mathrm{e}} (\nabla u) \phi_K \, d\Omega$ 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.



$\frac{w_1}{A} = 0.201$ $\frac{w_2}{A} = 0.147$ $\frac{w_3}{A} = 0.110$ $\frac{w_4}{A} = 0.196$ $\frac{w_5}{A} = 0.138$ $\frac{w_6}{A} = 0.209$

A = area

quadrature weights $\sum_K w_K = A$

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

max error in discrete derivative reproducibility

$$\max_K \sum_I (\overline{\nabla}\phi_I)_K = 9 \times 10^{-15}$$

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

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

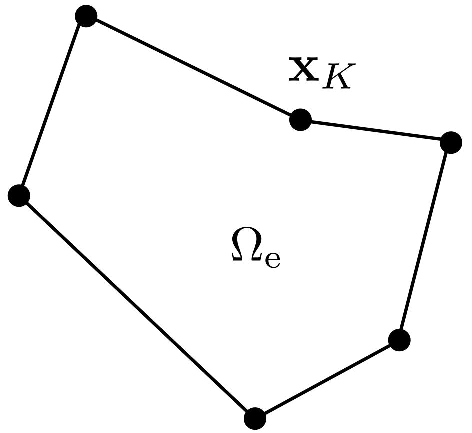
Integrate both sides

(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 $$w_K = \int_{\Omega_e} \phi_K(\mathbf{x}) \, d\Omega$$ then $$\sum_K \mathrm{w}_K \, \mathbf{x}_K = \int_{\Omega^e} \mathbf{x}$$

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



Quadrature points are now just the vertices.

Quadrature

Also, note that $$\sum_K \mathrm{w}_K = \sum_K \int_{\Omega_\mathrm{e}} \phi_K(\mathbf{x})\, d\Omega = \int_{\Omega_\mathrm{e}} \sum_K \phi_K(\mathbf{x})\, d\Omega = \int_{\Omega_\mathrm{e}} 1\, d\Omega = V$$

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

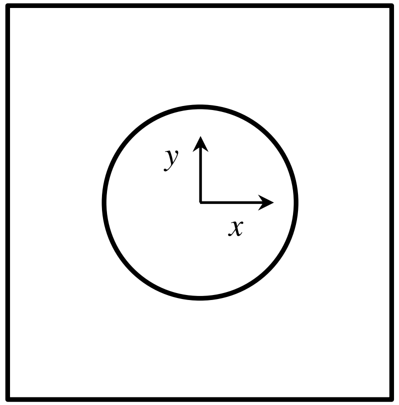
$$\sum_K \mathrm{w}_K = V \quad \text{and} \quad \sum_K \mathrm{w}_K\, \mathbf{x}_K = \int_{\Omega_\mathrm{e}} \mathbf{x}\, d\Omega$$

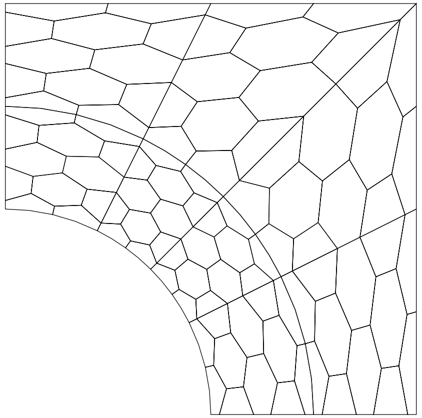
Can extend to higher-order integration using higher-order reproducing conditions.

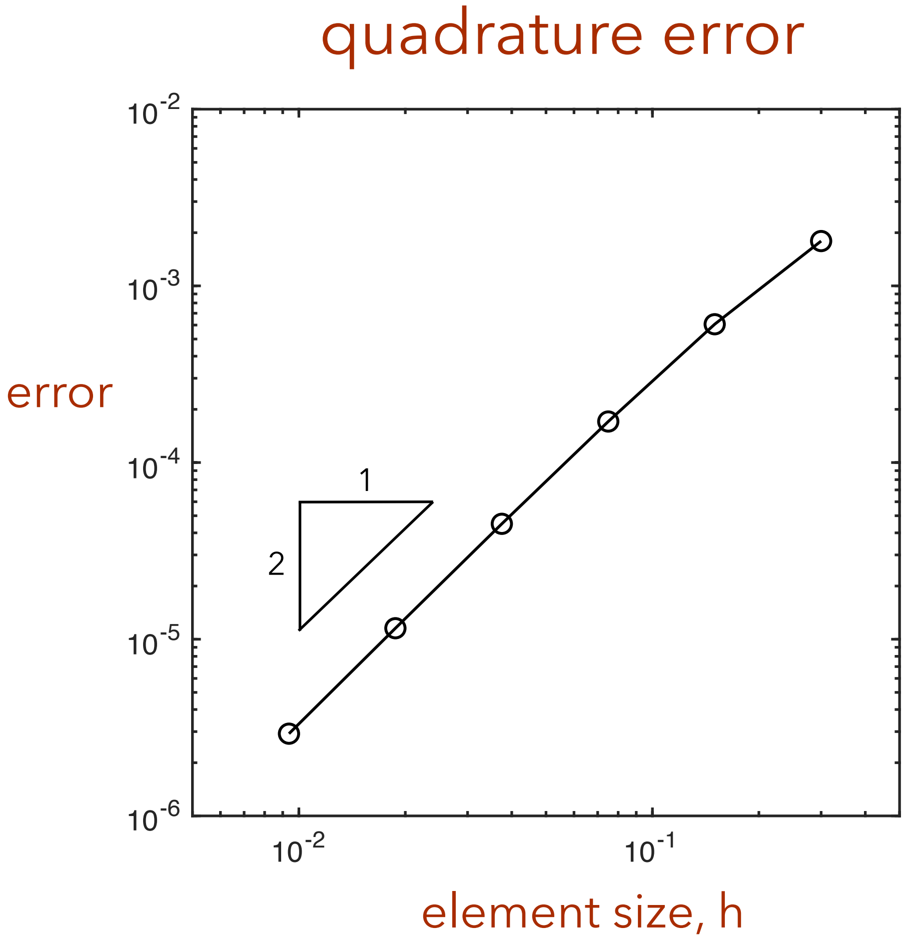
Verification: quadrature

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

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



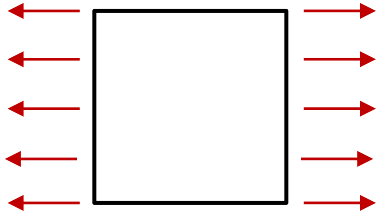




Verification examples: linear elasticity

Verification: elasticity patch test

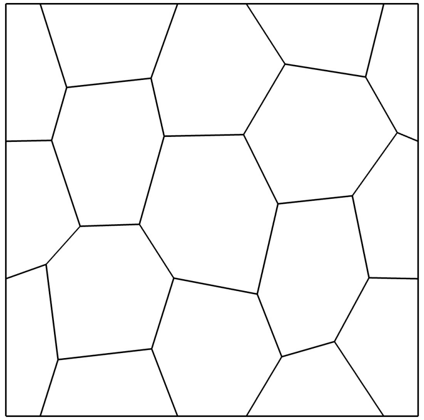
uniaxial tension



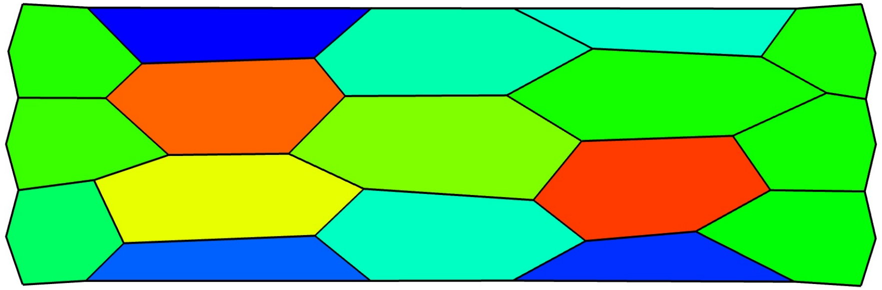
$E = 1.0$

$\nu = 0.3$

hexagon mesh

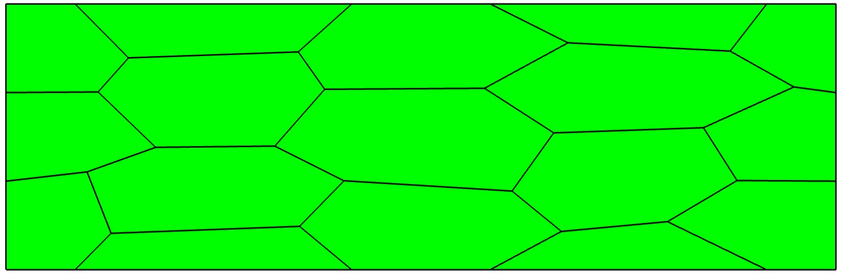


subtriangle quadrature



max stress error = 2%

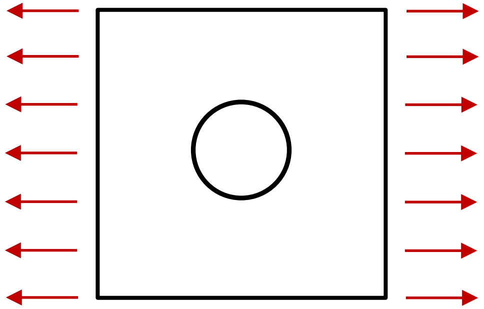
projection based quadrature



max stress error = 3×10^{-15}

Verification: elasticity, hole-in-plate tension

uniaxial tension

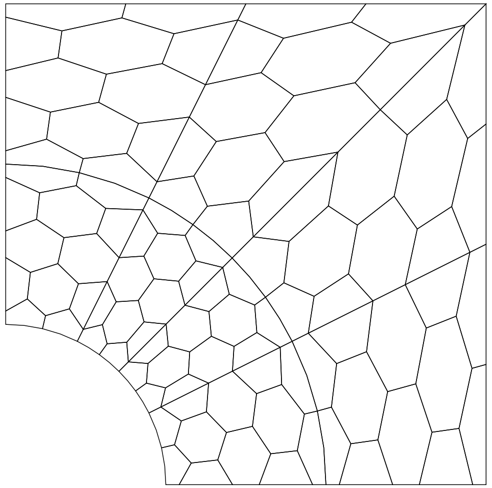


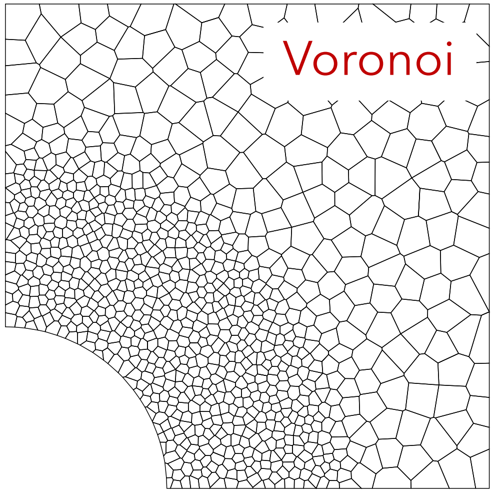
- exact tension prescribed corresponding to infinite plate
- plane strain
- quarter symmetry model used

$$E = 1.0$$

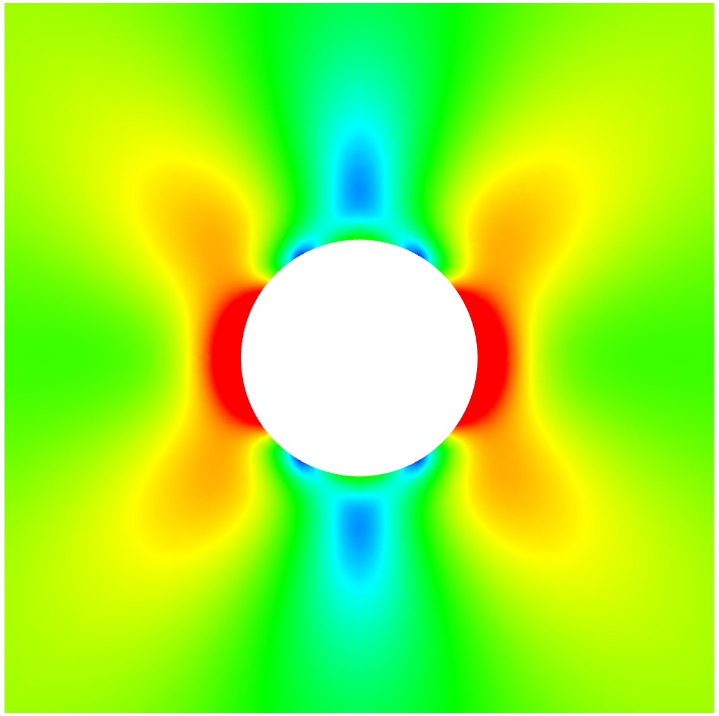
$$\nu = 0.3$$

mapped hexagon mesh

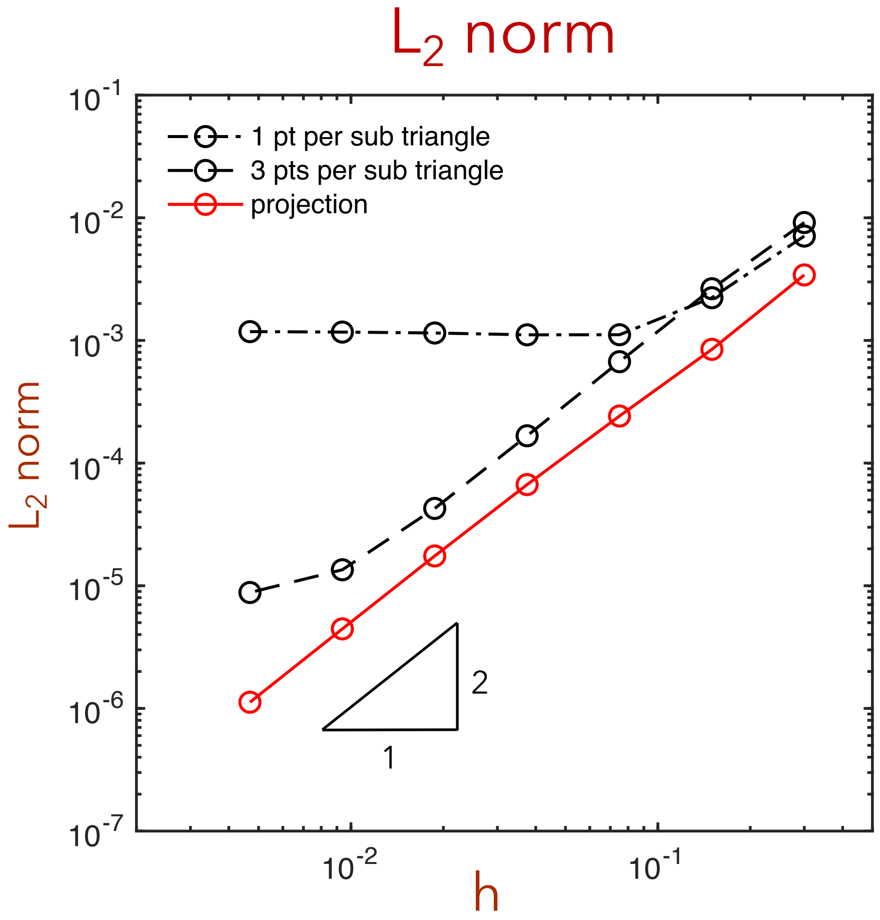


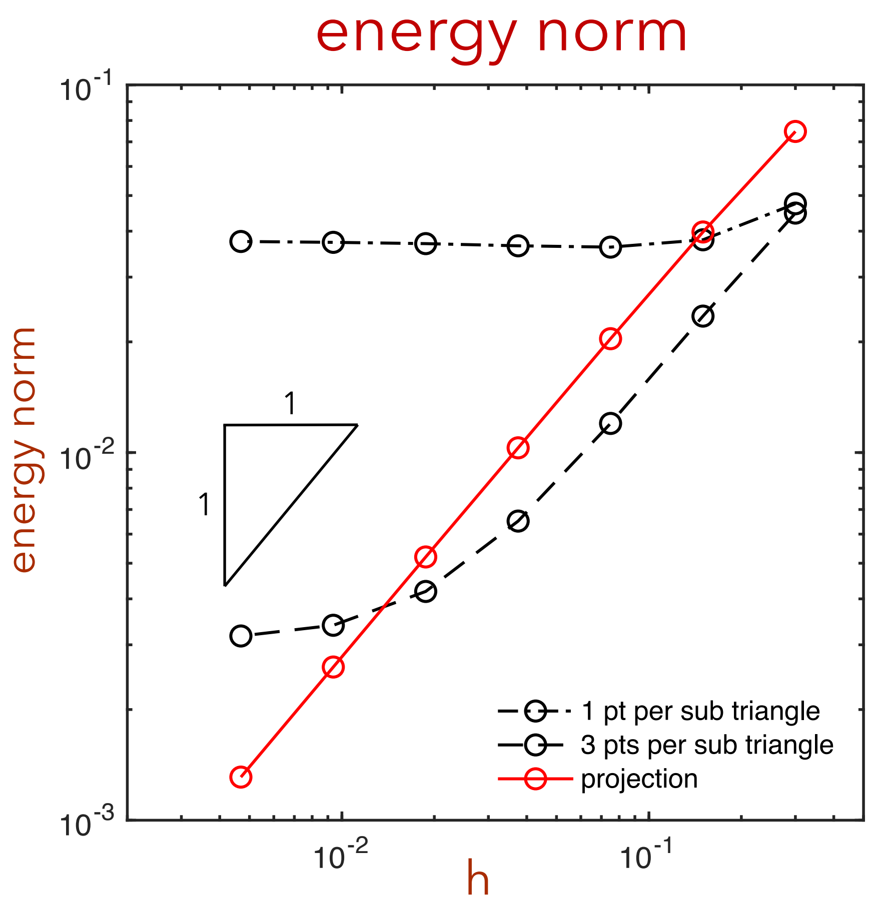


von Mises stress invariant



Verification: elasticity, hole-in-plate tension



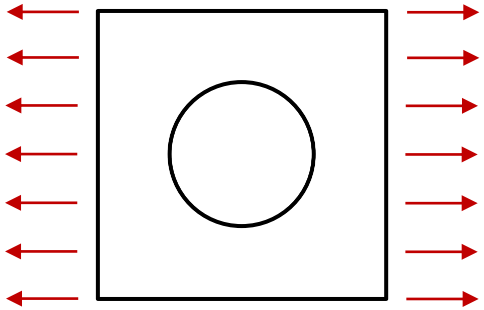


Optimal rates of convergence

Nonlinear solid mechanics, examples

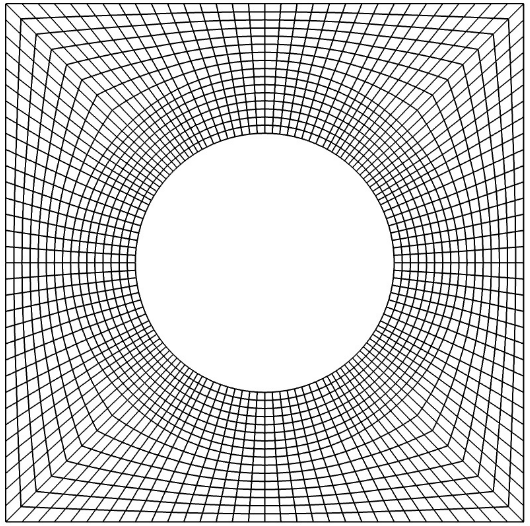
Application example: hyperelastic, hole-in-plate

uniaxial extension

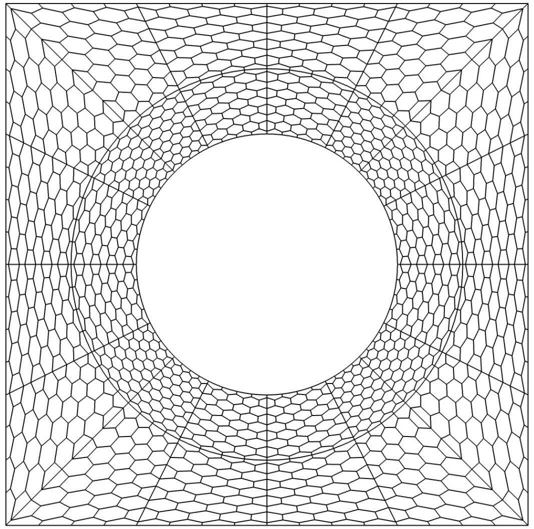


- plane strain
- quarter symmetry model used

quad mesh



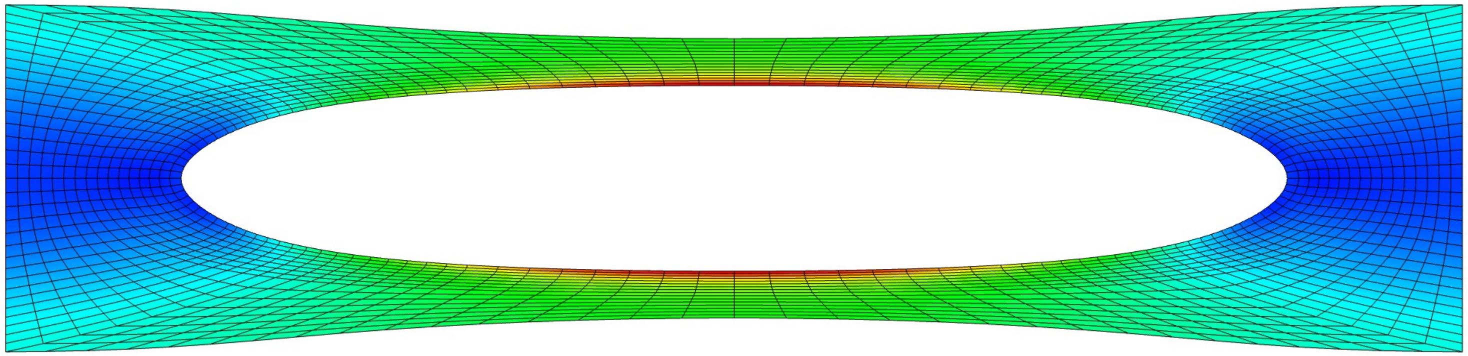
mapped hexagon mesh

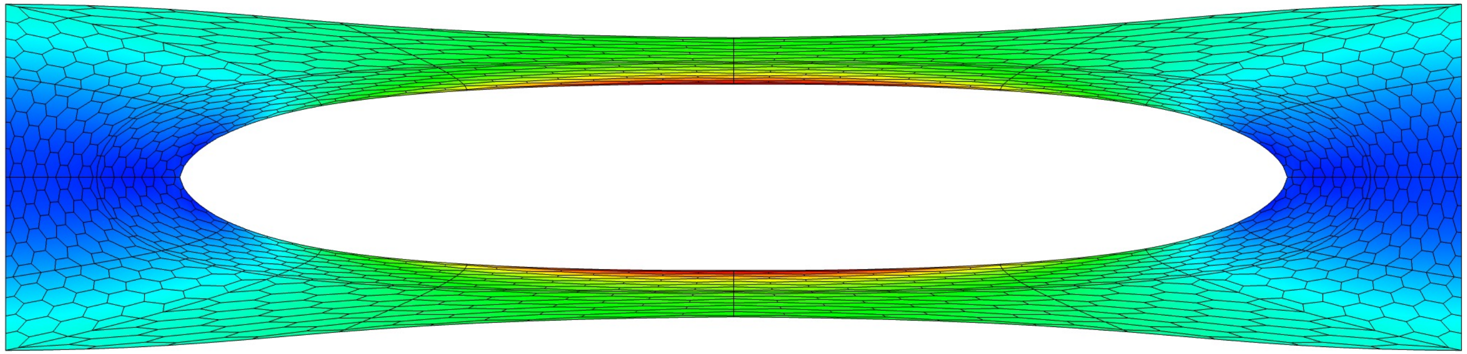


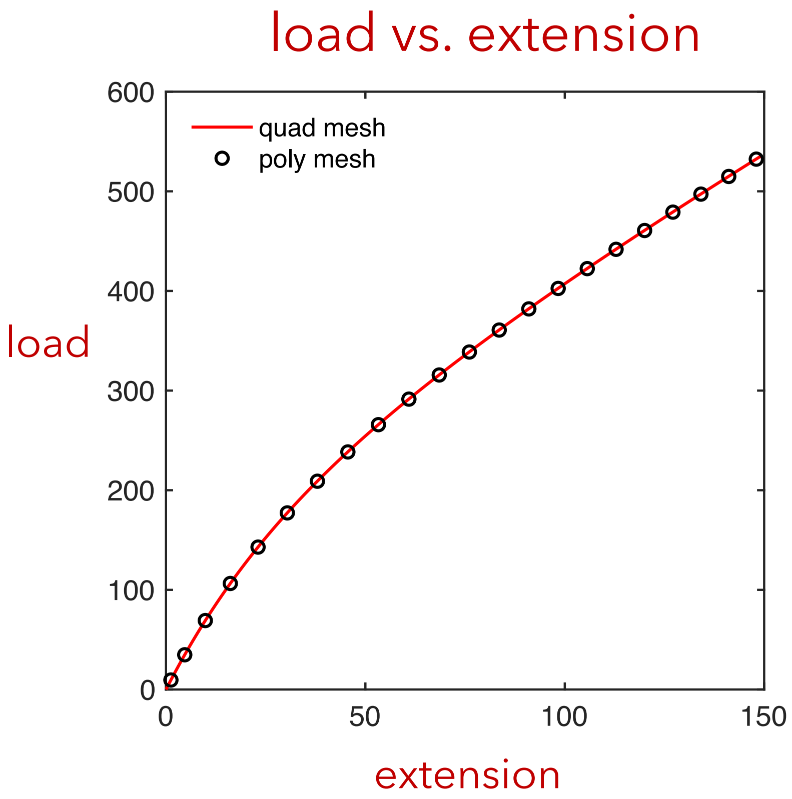
compressible neo-Hookean material

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

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





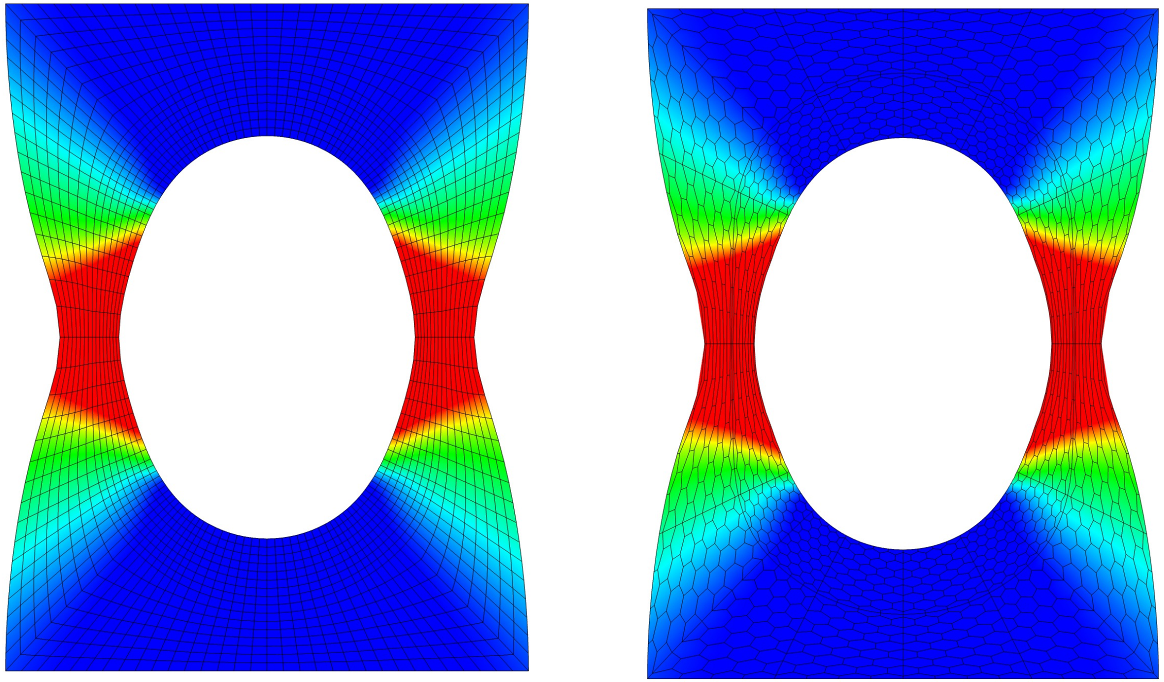

load vs. extension
quad mesh
poly mesh
load
extension
0
100
200
300
400
500
600
0
50
100
150

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

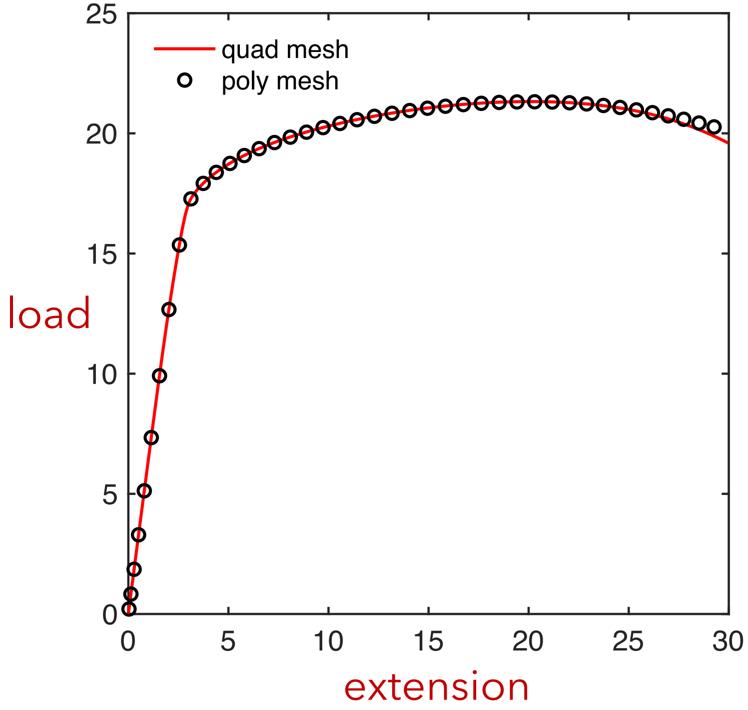
yield surface $f(\sigma, \bar{\varepsilon}^p) = \phi(\sigma) - \sigma_y(\bar{\varepsilon}^p) = 0$

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

plastic strain field



load vs. extension



(Use F-bar methods for inf-sup stability.)

Calculation of $(\nabla \phi_I, \phi_K)$

- Currently solving for derivative projection using a sub-triangulation and FEA.
- Can also use Green's identities to calculate these if shape functions are 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 Green's identities for calculating gradient projections of harmonic shape functions.