



Sandia  
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# A hybrid mesh-based/element-free approach for analysis on geometrically complex domains without defeaturing

Joe Bishop

Engineering Sciences Center  
Sandia National Laboratories  
Albuquerque, NM



SAND2022-???? C



US Congress on Theoretical and Applied Mechanics  
June 19-24, 2022, Austin, TX



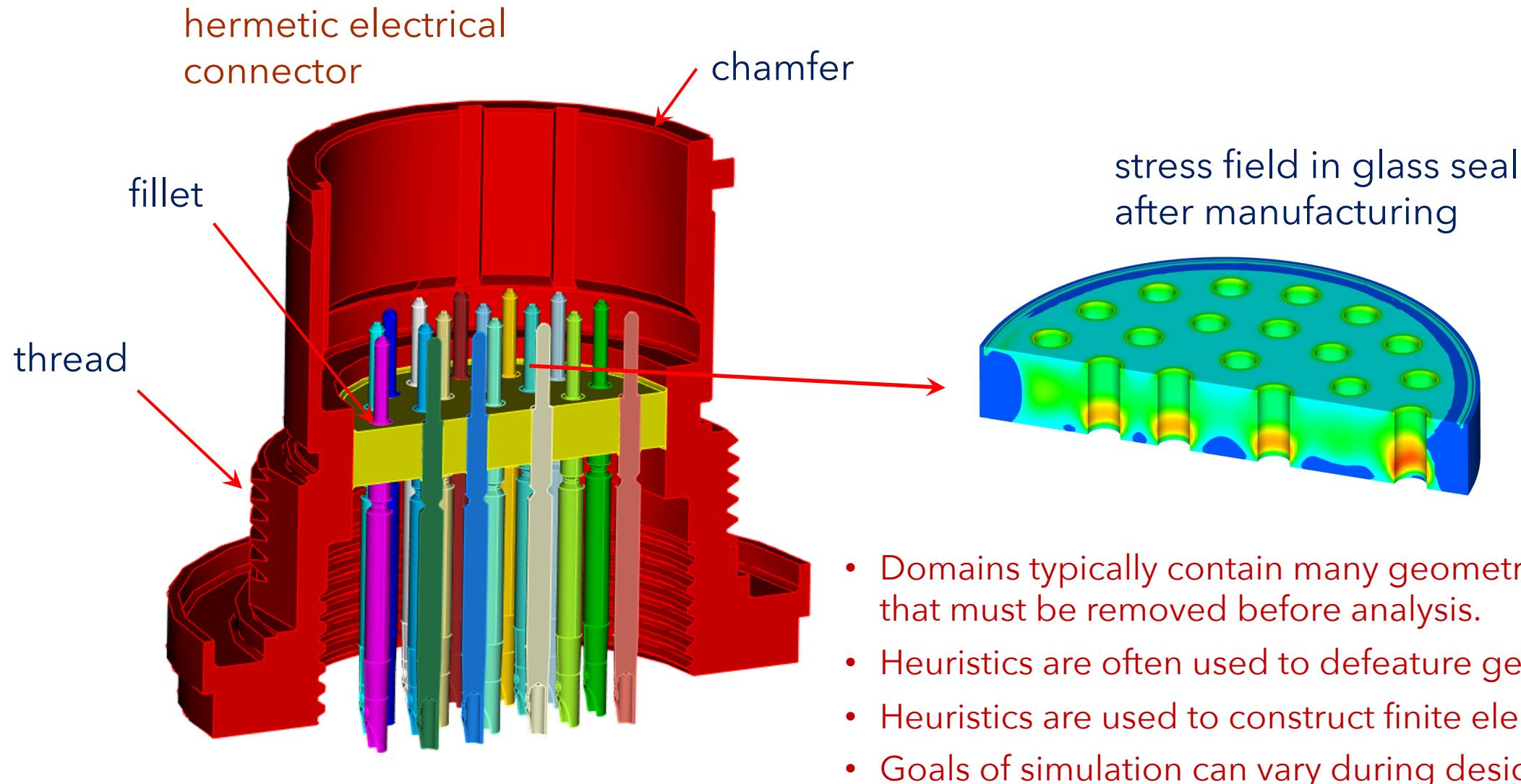
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# Outline

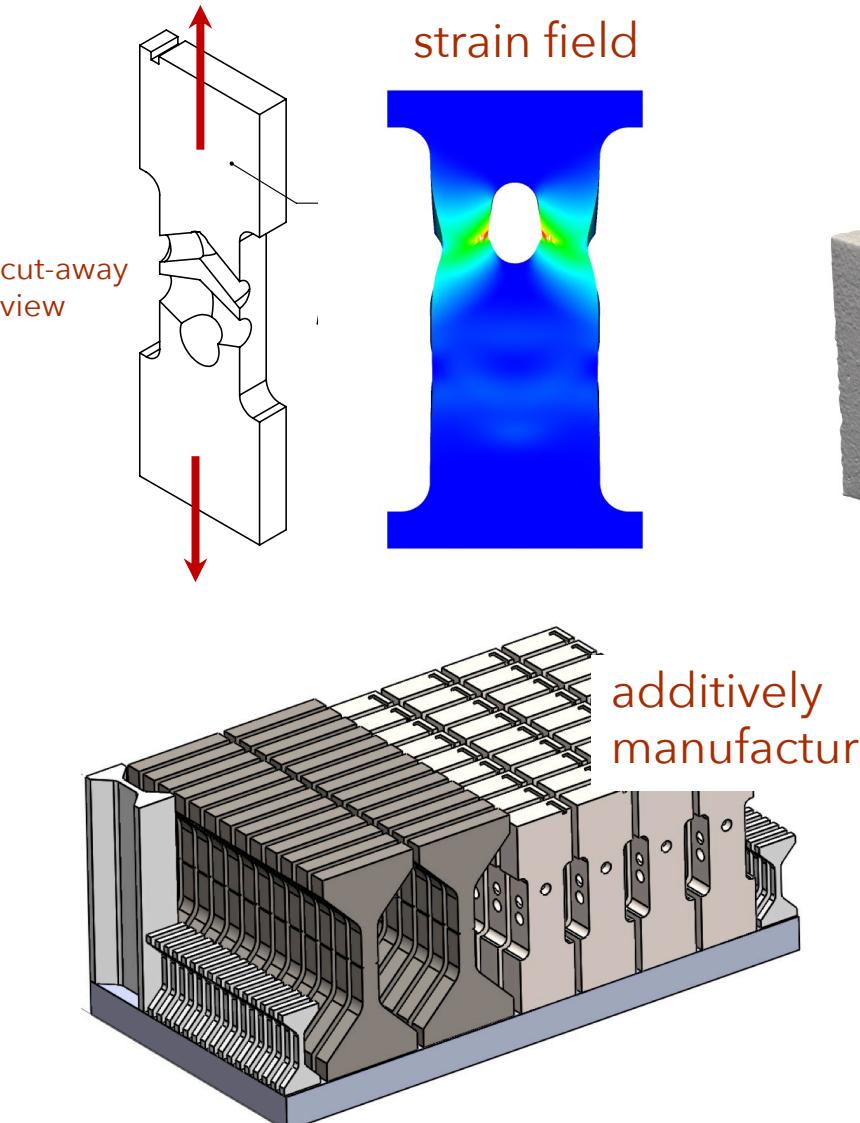


1. motivation
2. hybrid mesh/element-free discretizations
3. weight functions using manifold geodesics
4. quadrature via secondary basis functions
5. strain projections for polynomial consistency
6. verification example, linear elasticity
7. summary

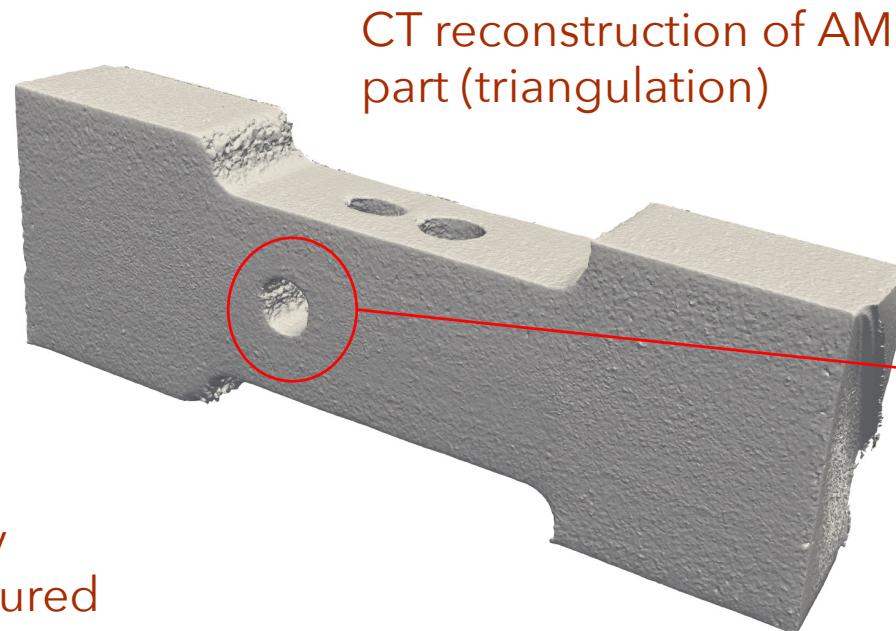
# Motivation: Agile simulation of complex assemblies



# Motivation: Image-based analysis

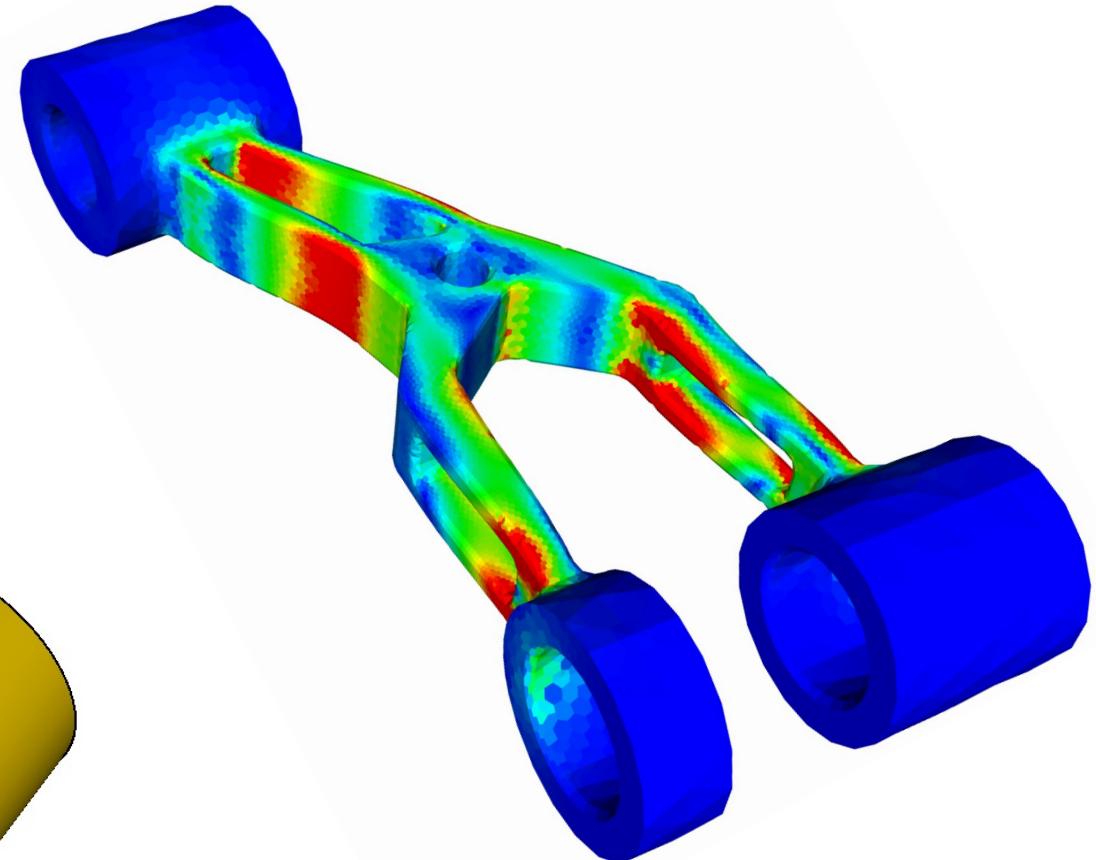
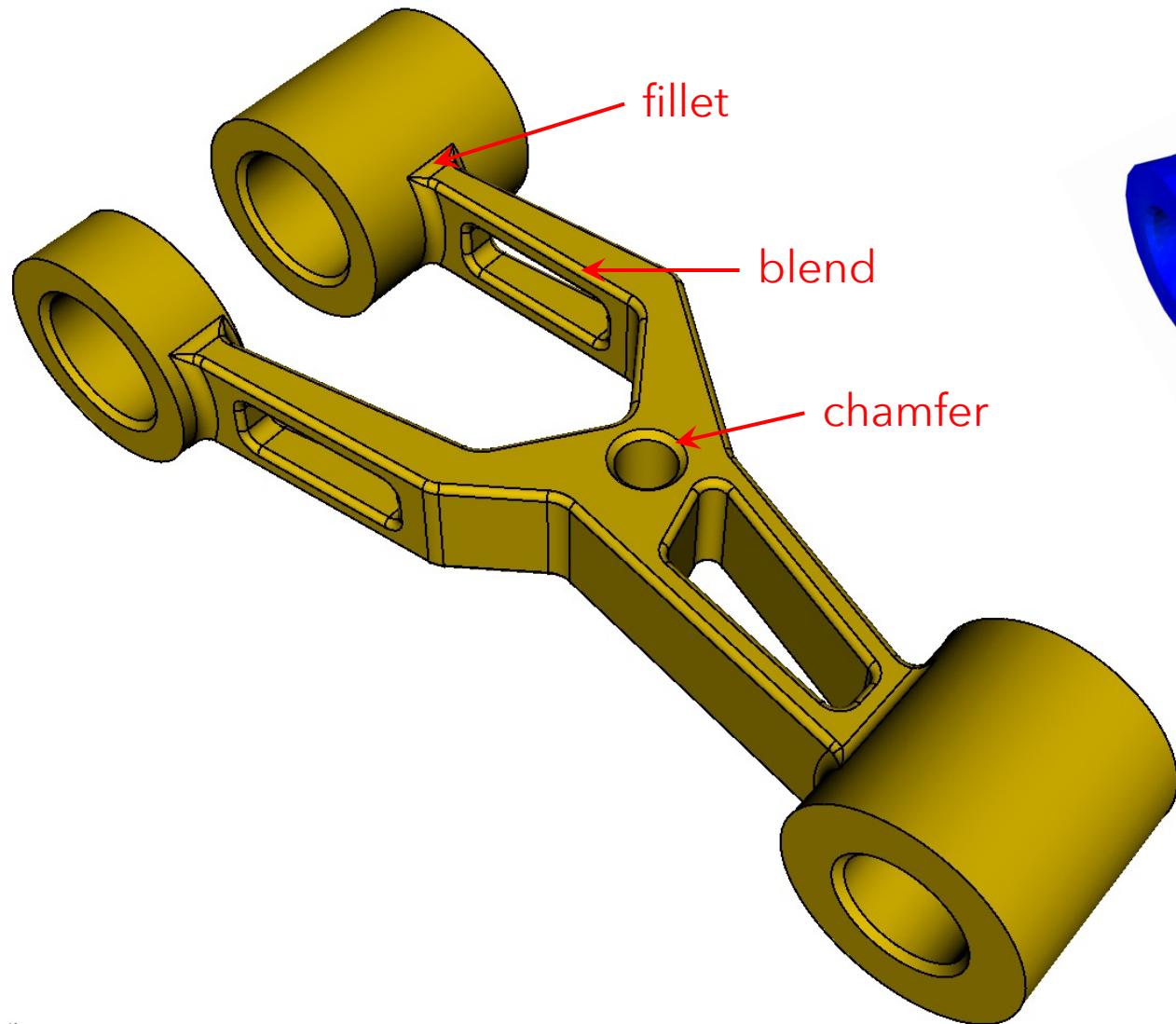


Johnson, et al., 2019, "Predicting the reliability of an additively-manufactured metal part for the third Sandia fracture challenge by accounting for random material defects," *International Journal of Fracture*, v. 218, pp. 231-243

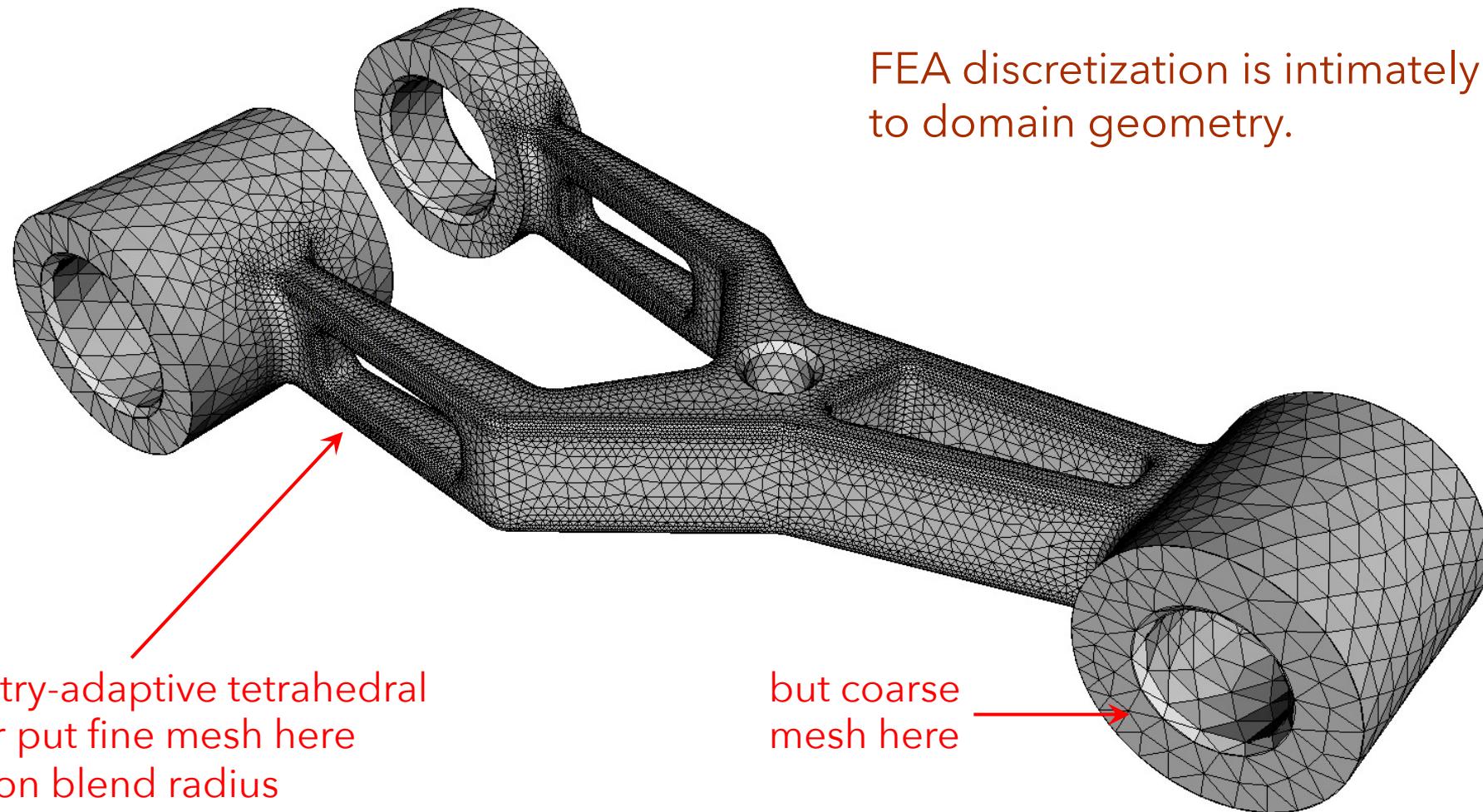


Typical geometric reconstructions require a smoothing or decimation process before modeling can commence.

# Motivation: Typical domain (geometry) features



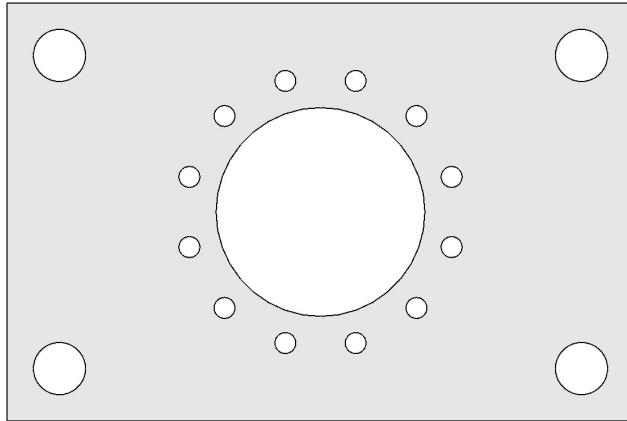
# Motivation: Domain discretization



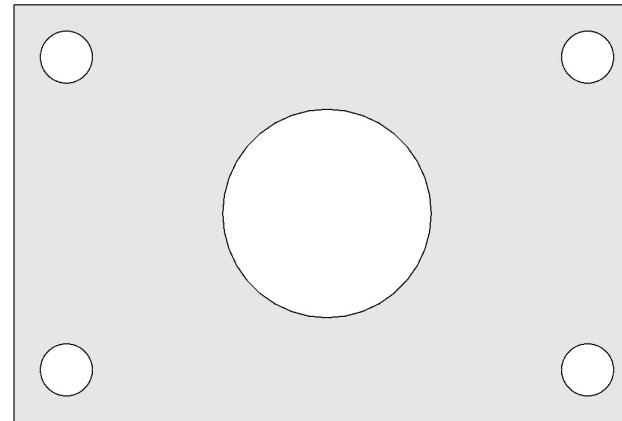
# Motivation: Separate domain discretization from solution discretization



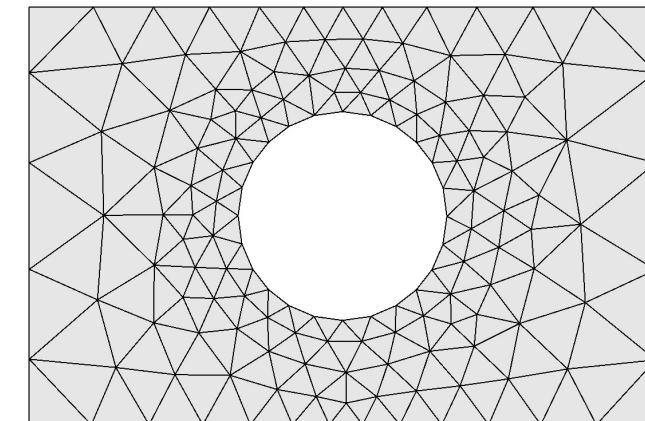
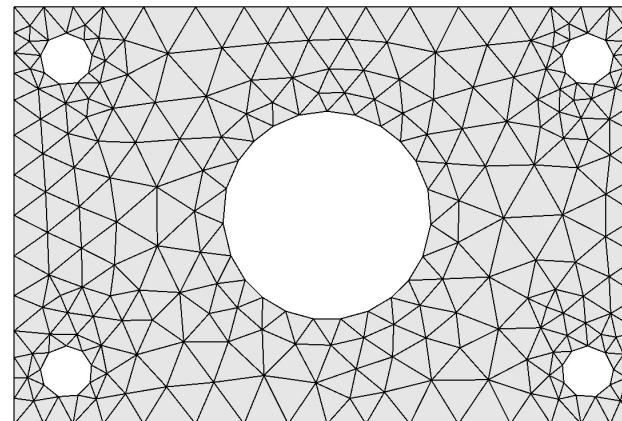
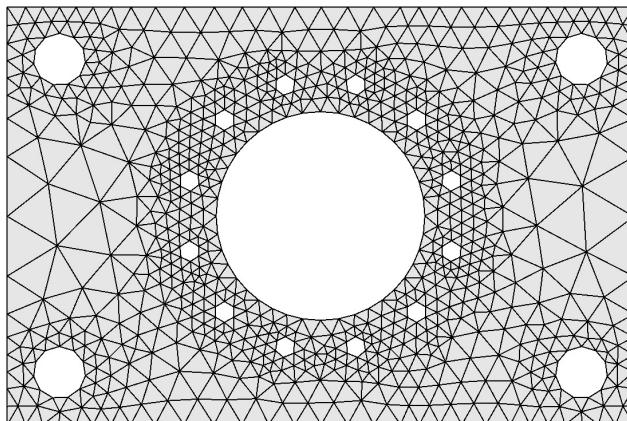
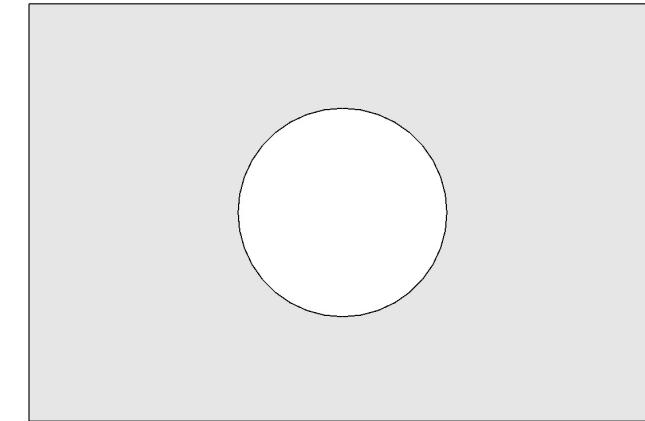
original domain



defeature



defeature



Impact of domain defeaturing? depends on goals of simulation

# Motivation: Separate domain discretization from solution discretization

- Domain defeaturing is needed to control FEA discretization quality, size, and critical time step (explicit dynamics)
- Domain defeaturing typically requires human intervention (heuristics).
- For FEA, domain discretization and solution discretization are synonymous (isoparametric).
- Geometric features can require a fine local discretization while solution does not.
- Heuristics are often used in mesh design.
- Meshes are typically designed with goal in mind, thus making it cumbersome to reuse.
- Adaptivity requires going back to geometric model of domain.

Alternative hybrid approach: separate domain discretization and solution approximation using an element-free formulation.

# A hybrid element-free approach



## finite-element approach

- defeature domain geometry based on goals
- create a mesh based on goals
- mesh discretizes domain and solution
- quadrature of weak form is easy
- visualization of results using mesh
- adaptivity of mesh is hard

## mesh-free approach

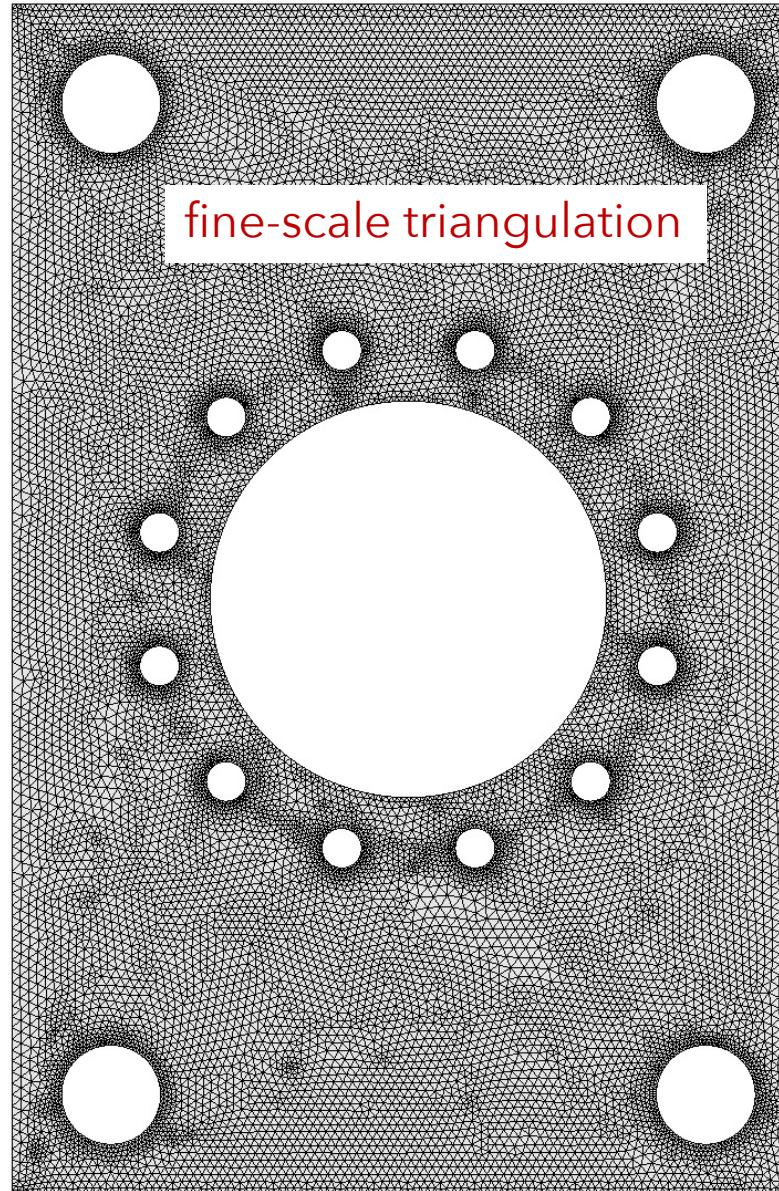
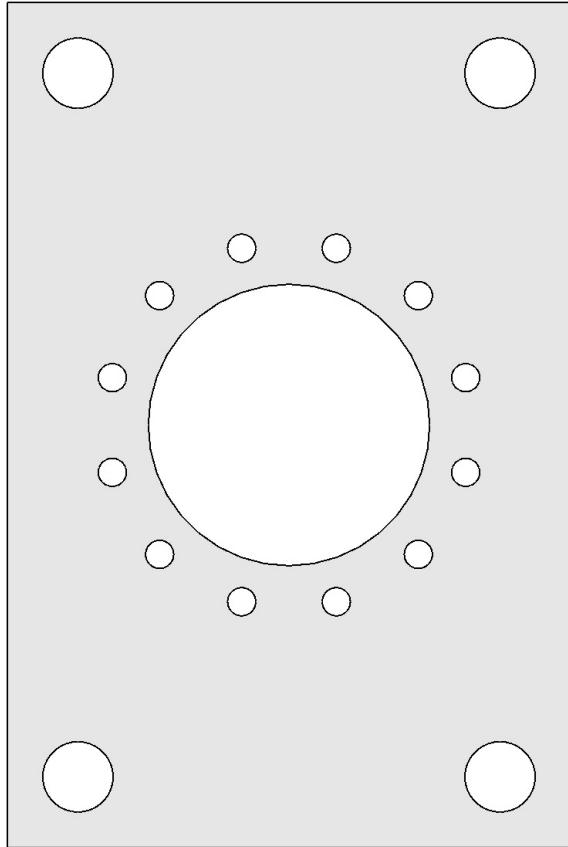
- no defeaturing of domain geometry
- no discretization of domain
- connectivity of domain is undefined (need computational geometry)
- quadrature of weak form is very hard
- visualization of results is cumbersome

Alternative hybrid approach: separate domain discretization and solution approximation using an element-free formulation.

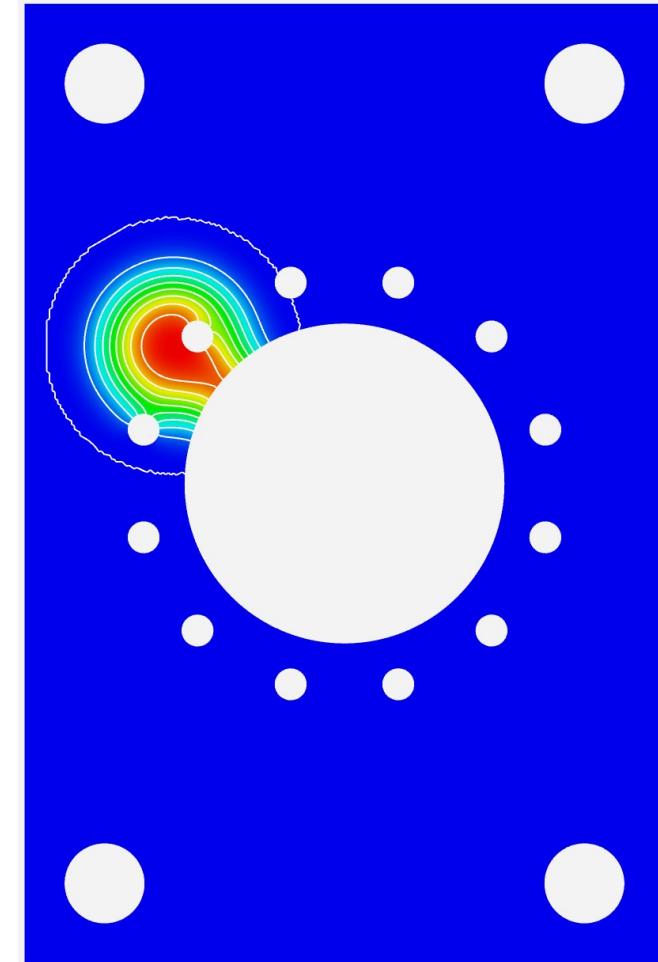
# Hybrid approach: fine-scale triangulation



original domain



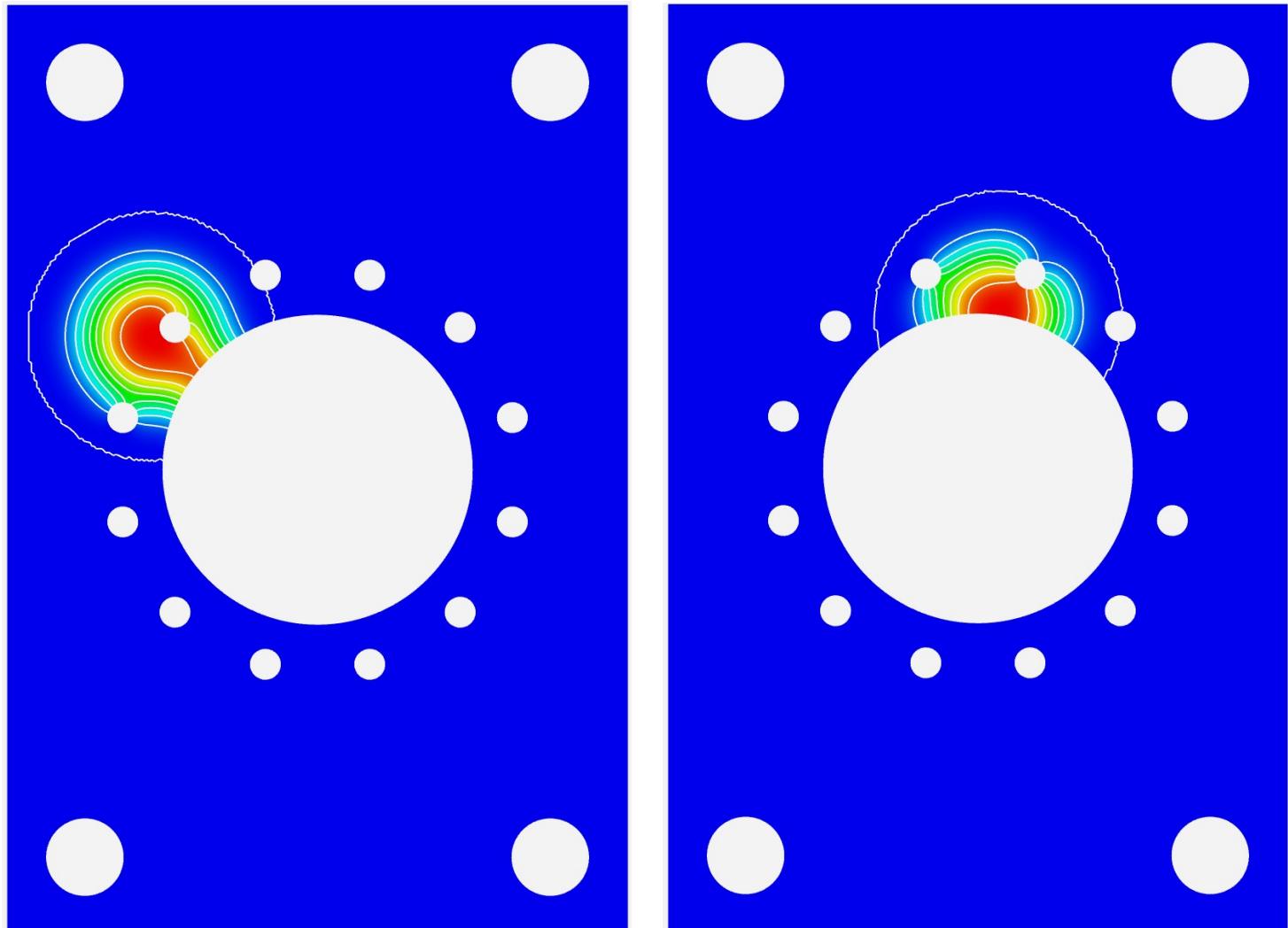
create an element-free basis using triangulation.



# Element-free basis functions



- Element-free basis functions automatically include geometric features at all scales.
- Solution discretization is separate from domain discretization.
- No need to defeature domain.



# Hybrid approach: fine-scale triangulation



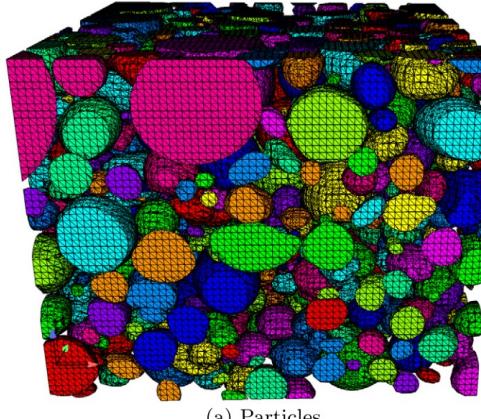
## Tet-meshing methods

- Delaunay
- advancing front
- background grid
- envelope

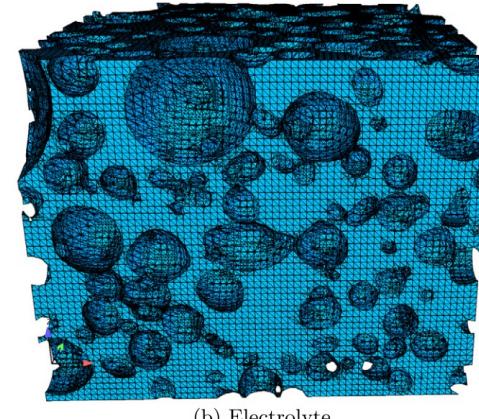
## CDFEM

A verified conformal decomposition finite element method for implicit, many-material geometries

Scott A. Roberts \*, Hector Mendoza, Victor E. Brunini, David R. Noble



(a) Particles



(b) Electrolyte

## Fast Tetrahedral Meshing in the Wild

YIXIN HU, New York University, USA

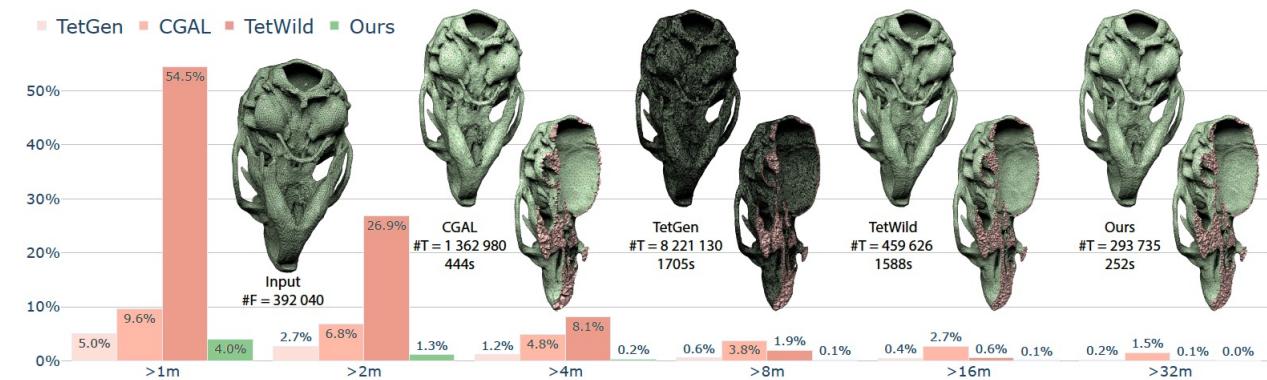
TESEO SCHNEIDER, New York University, USA

BOLUN WANG, Beihang University, China and New York University, USA

DENIS ZORIN, New York University, USA

DANIELE PANIZZO, New York University, USA

ACM Trans. Graph. 2020  
vol. 39 Issue 4 Article 117



TetWild

# Hybrid element-free approach



- no defeaturing of domain
- discretize domain using fine-scale triangulation (a mesh, but poor quality is okay)
- use hp-cloud to define solution discretization (GBC, RK)
- use second hp-cloud to define quadrature and ensure coercivity
- projection of solution gradient to obtain polynomial consistency
- visualization of results using fine-scale mesh

## pros

- symmetric, Galerkin
- linear or nonlinear
- implicit or explicit dynamics
- can do higher order
- can do direct or mixed formulation
- adaptivity is seamless
- can use poor quality tet mesh
- adaptivity is facilitated
- should work for  $H(\text{div})$  and  $H(\text{curl})$  spaces
- reduced order modeling through coarse discretizations

## cons

- constant material properties within a domain
- material interfaces: have to use weak enforcement such as mortar method
- less sparse

# Hybrid element-free approach



INTERNATIONAL JOURNAL FOR NUMERICAL METHODS IN ENGINEERING, VOL. 37, 229–256 (1994)

## ELEMENT-FREE GALERKIN METHODS

T. BELYTSCHKO, Y. Y. LU AND L. GU

*Department of Civil Engineering, Robert R. McCormick School of Engineering and Applied Science,  
The Technological Institute, Northwestern University, Evanston IL 60208-3109, U.S.A.*

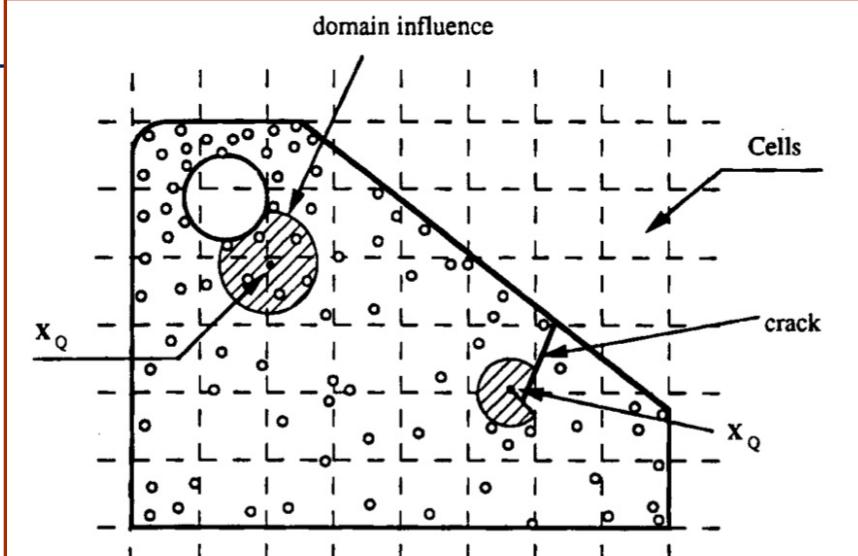


Figure 1. Cell structure for quadrature in EFGM and domains of quadrature point

# Moving Least Squares (Reproducing Kernel)



The MLS shape functions  $\phi_I(\mathbf{X})$  are defined as a spatial modulation of the nodal weight functions.

$$\phi_I(\mathbf{X}) = c_I(\mathbf{X})w_I(\mathbf{X})$$

where the modulation function  $c_I(\mathbf{X})$  is found through a least square minimization process resulting in

$$c_I(\mathbf{X}) = \mathbf{g}^T(\mathbf{X})\mathbf{A}^{-1}(\mathbf{X})\mathbf{g}(\mathbf{X}_I)$$

where

$$\mathbf{A}(\mathbf{X}) = \sum_{I \in \mathcal{N}} w_I(\mathbf{X})\mathbf{g}(\mathbf{X}_I)\mathbf{g}^T(\mathbf{X}_I) \quad (\text{sum over neighbors})$$

$$\mathbf{g}^T(\mathbf{X}) = \{ 1 \ X_1 \ X_2 \} \quad (\text{linear reproducibility})$$

Note: shape function construction is algebraic.

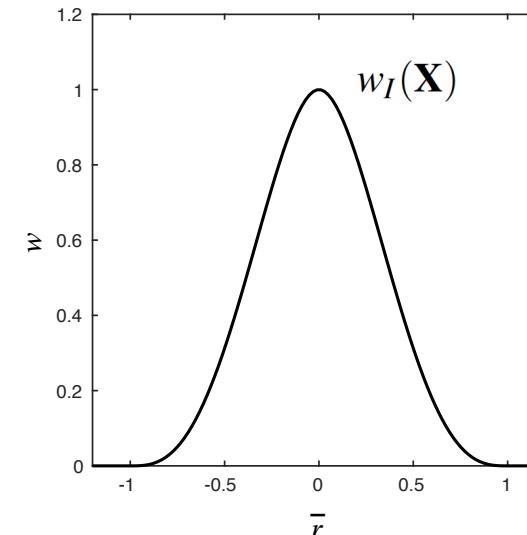
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nodal weight function

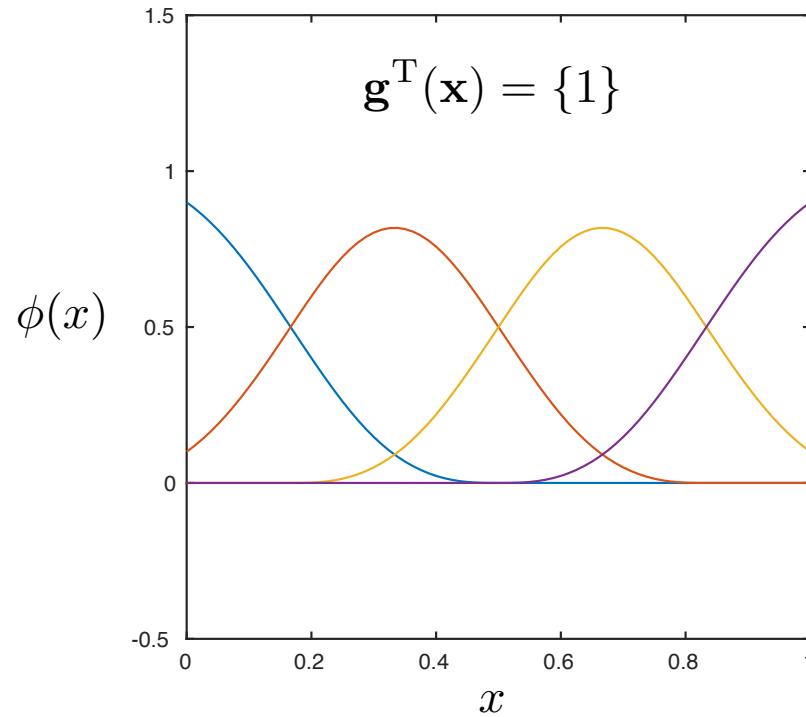


circular or rectangular support

# Moving Least Squares

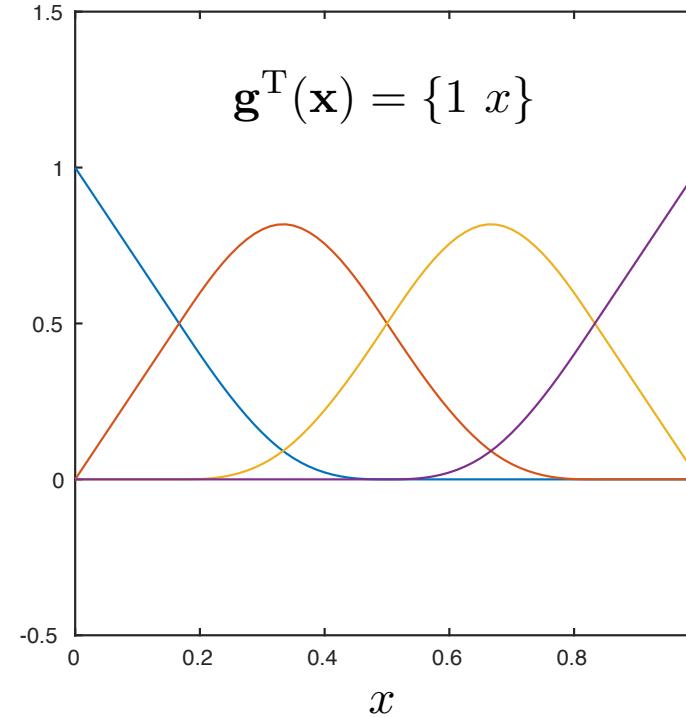


$$\sum_K \phi_K(x) = 1$$



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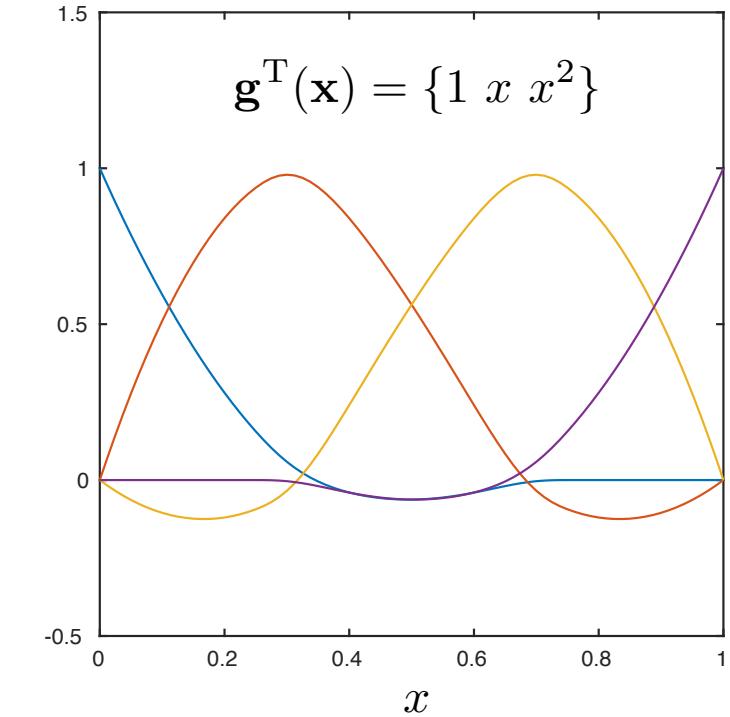
$$\sum_K x_K \phi_K(x) = x$$



$$\sum_K \phi_K(x) = 1$$

$$\sum_K x_K \phi_K(x) = x$$

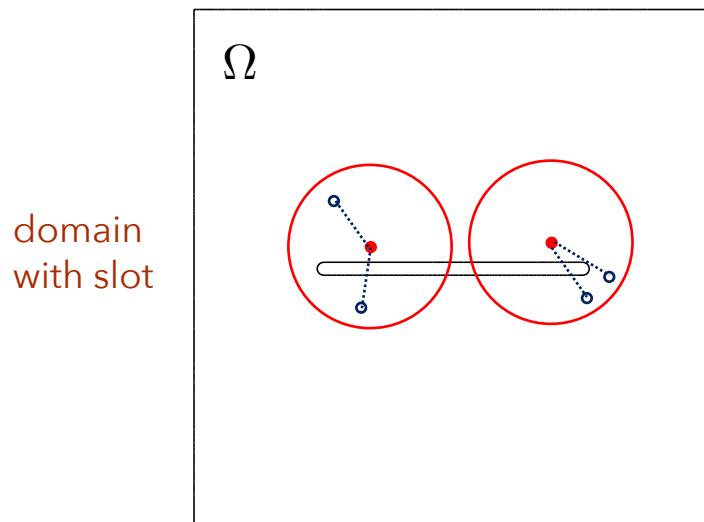
$$\sum_K x_K^2 \phi_K(x) = x^2$$



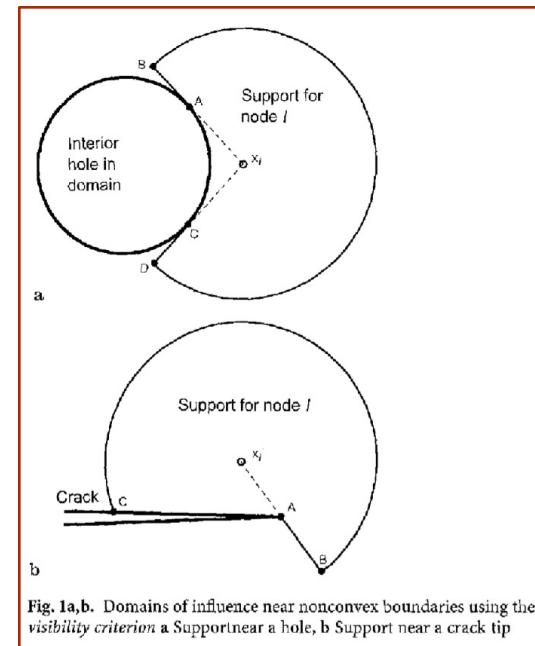


# Continuous meshless approximations for nonconvex bodies by diffraction and transparency

D. Organ, M. Fleming, T. Terry, T. Belytschko



visibility criterion



visibility criterion

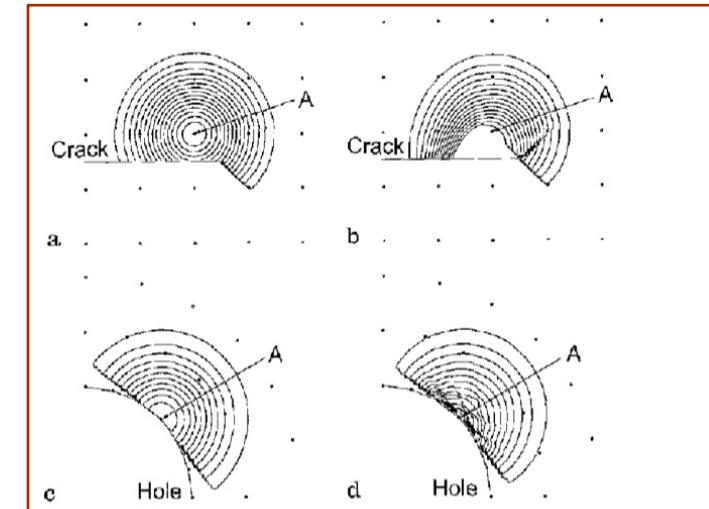


Fig. 2a-d. Contours for weight and shape functions associated with node A constructed using the *visibility criterion*. a Weight function near a crack tip, b Shape function near a crack tip, c Weight function near a hole, d Shape function near a hole

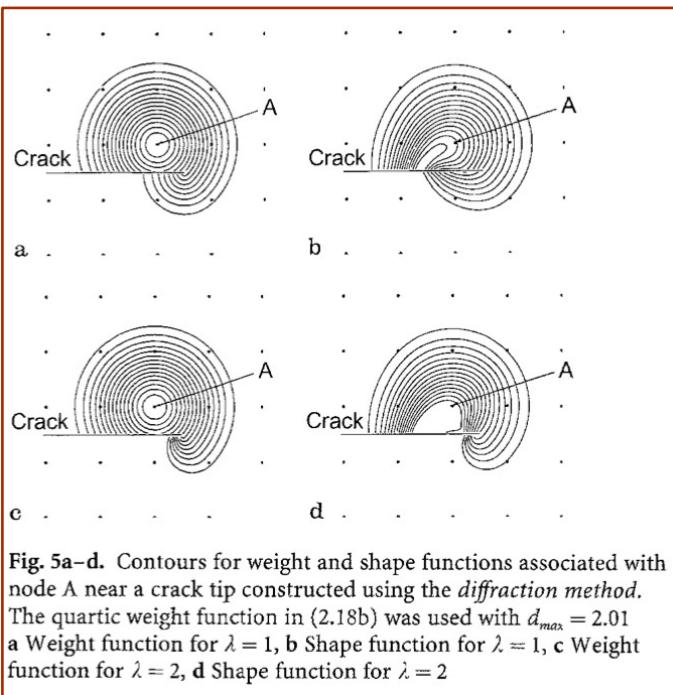
All these methods (visibility, transparency, diffraction) require use of computational geometry.



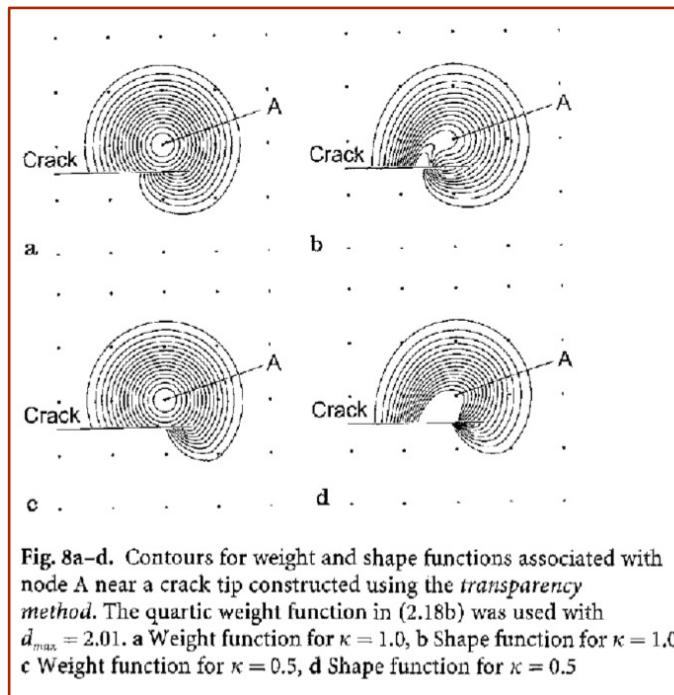
# Continuous meshless approximations for nonconvex bodies by diffraction and transparency

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diffraction method



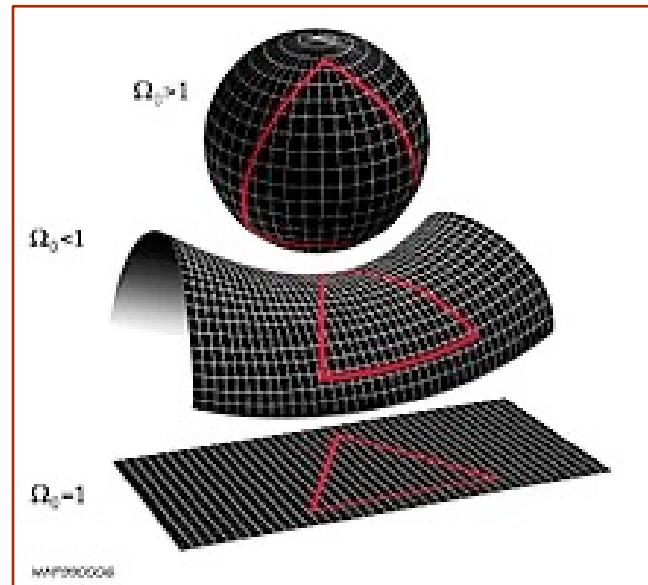
transparency method



All these methods (visibility, transparency, diffraction) require use of computational geometry.

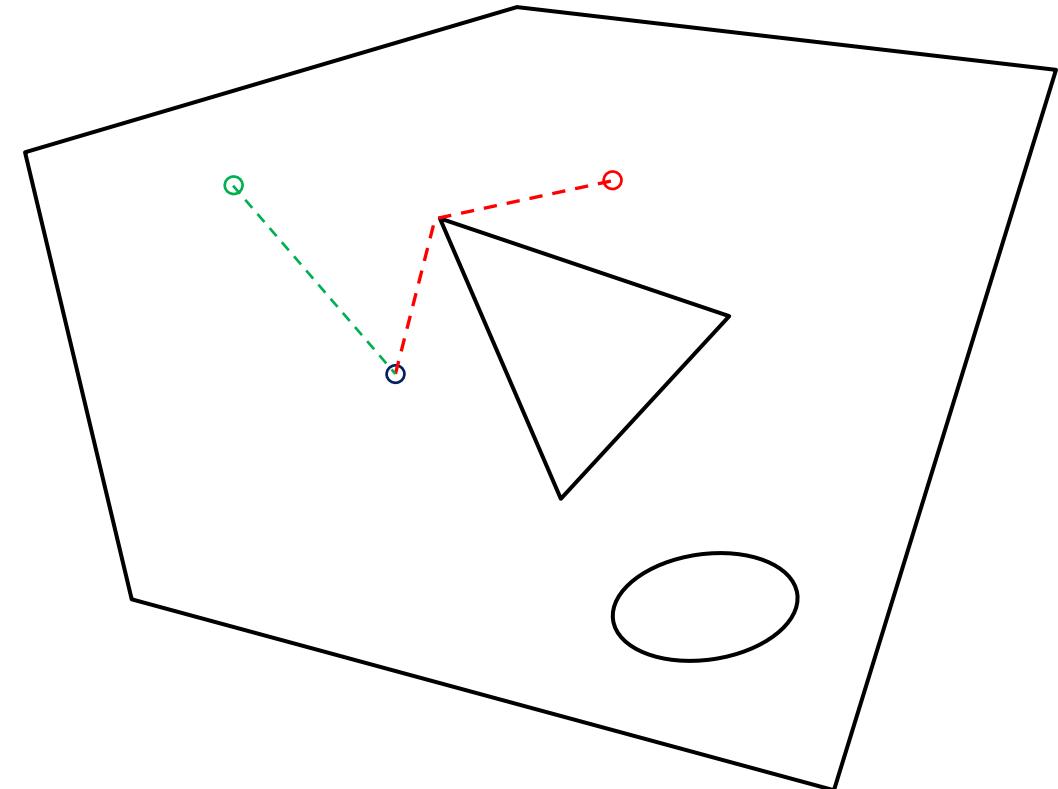
# Manifold geodesic

Geodesic: path that provides the shortest distance along a manifold



<https://en.wikipedia.org/wiki/Geodesic>

Euclidean manifold with boundary



# Geodesics in Heat: A New Approach to Computing Distance Based on Heat Flow

KEENAN CRANE

Caltech

and

CLARISSE WEISCHEDEL and MAX WARDETZKY,  
University of Göttingen

ACM Trans. Graph. 2013 Vol. 32 Issue 5 Pages Article 152

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## ALGORITHM 1: The Heat Method

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- I. Integrate the heat flow  $\dot{u} = \Delta u$  for some fixed time  $t$ .
- II. Evaluate the vector field  $X = -\nabla u / |\nabla u|$ .
- III. Solve the Poisson equation  $\Delta \phi = \nabla \cdot X$ .

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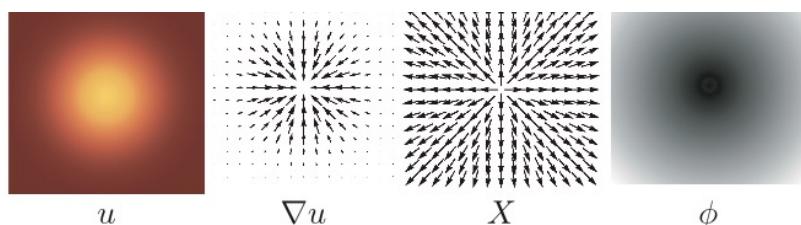


Fig. 5. Outline of the heat method. (I) Heat  $u$  is allowed to diffuse for a brief period of time (left). (II) The temperature gradient  $\nabla u$  (center left) is normalized and negated to get a unit vector field  $X$  (center right) pointing along geodesics. (III) A function  $\phi$  whose gradient follows  $X$  recovers the final distance (right).

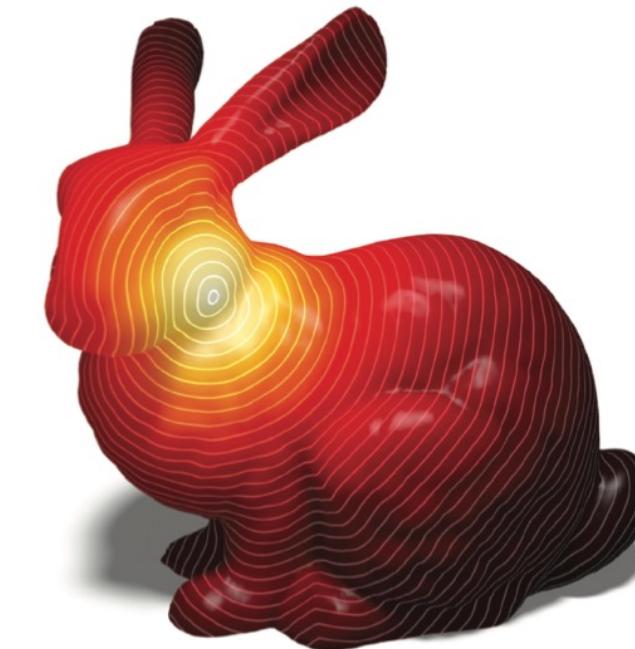
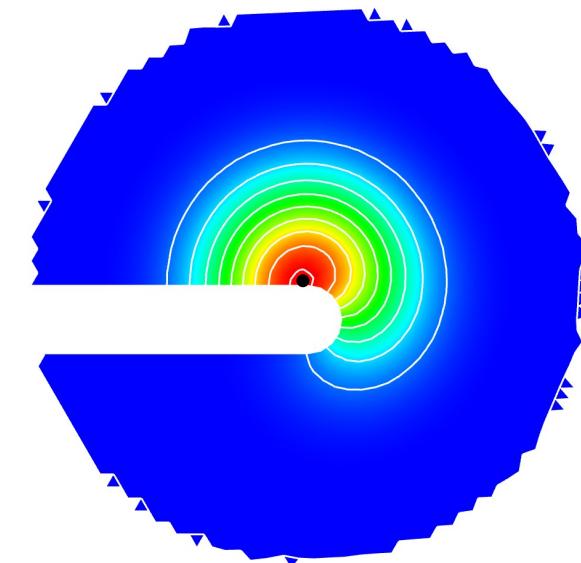
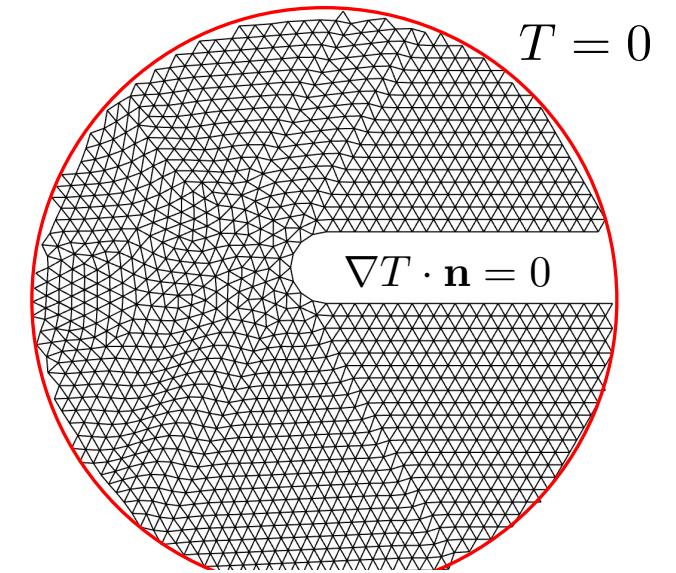
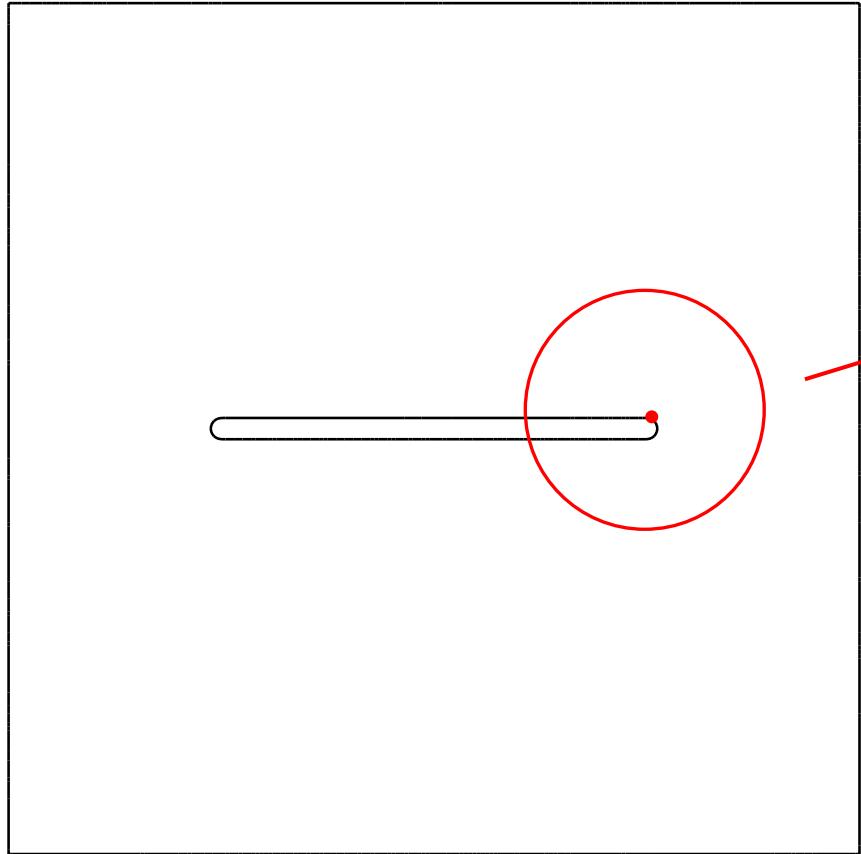
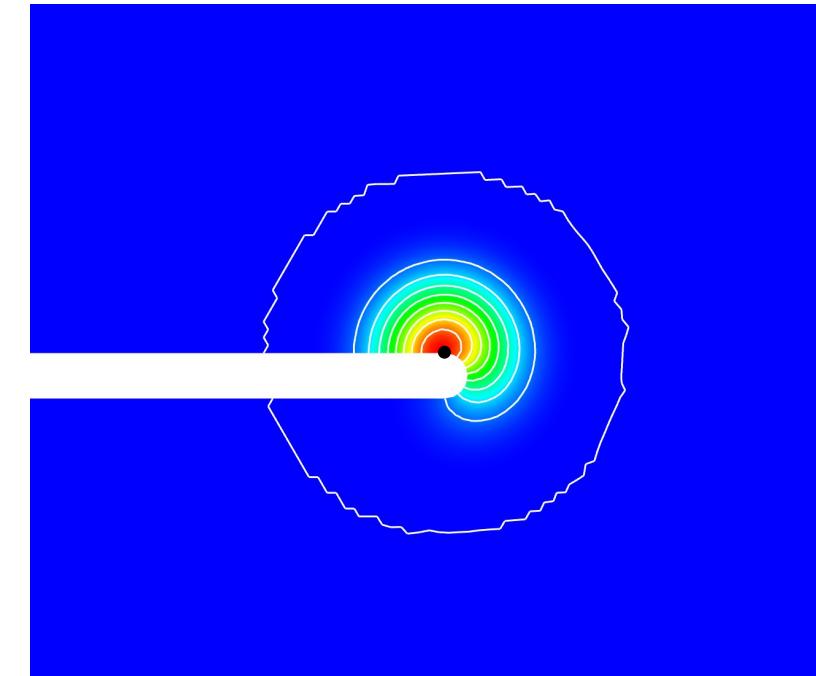
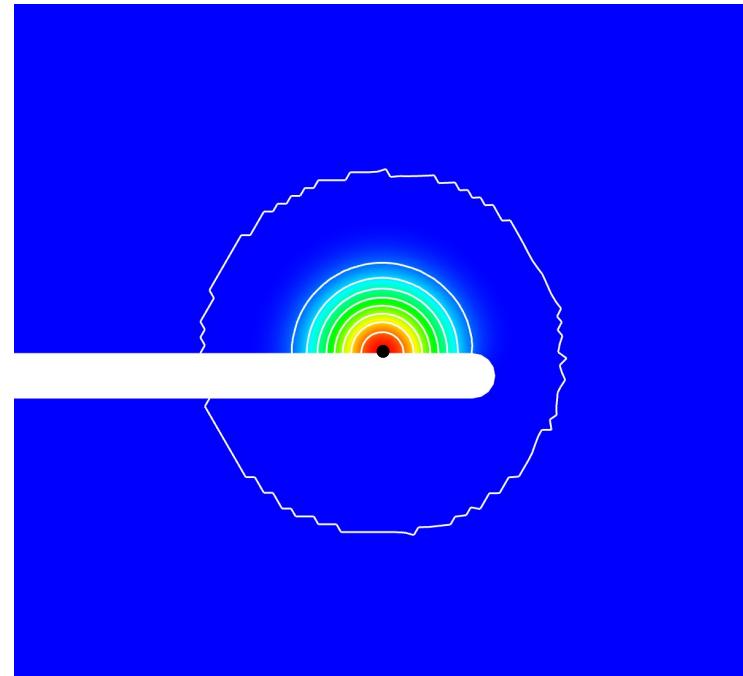
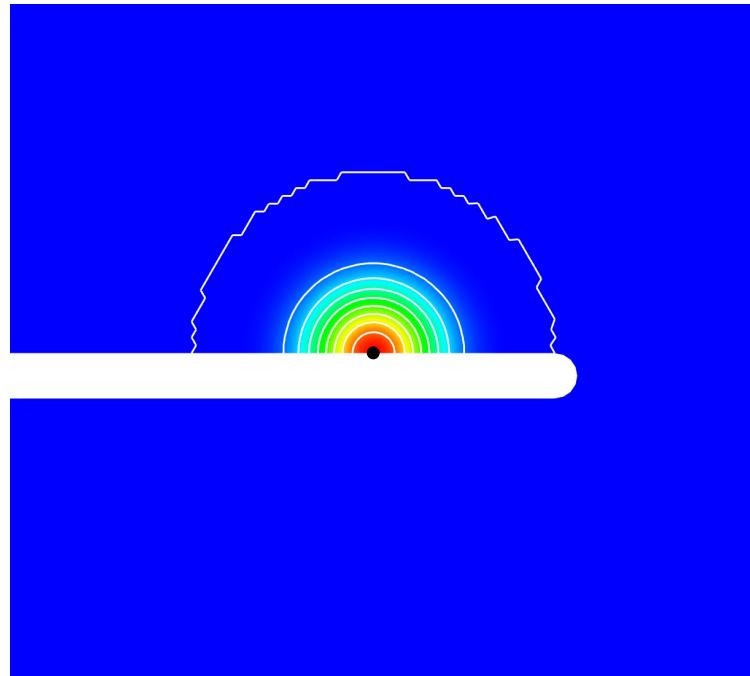


Fig. 1. Geodesic distance from a single point on a surface. The heat method allows distance to be rapidly updated for new source points or curves.

# Weight functions using heat flow

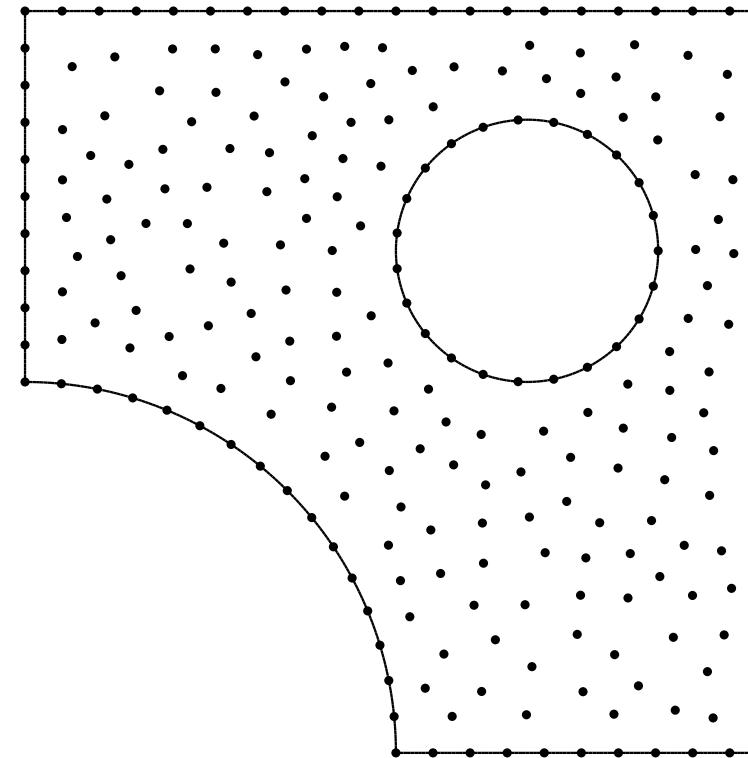
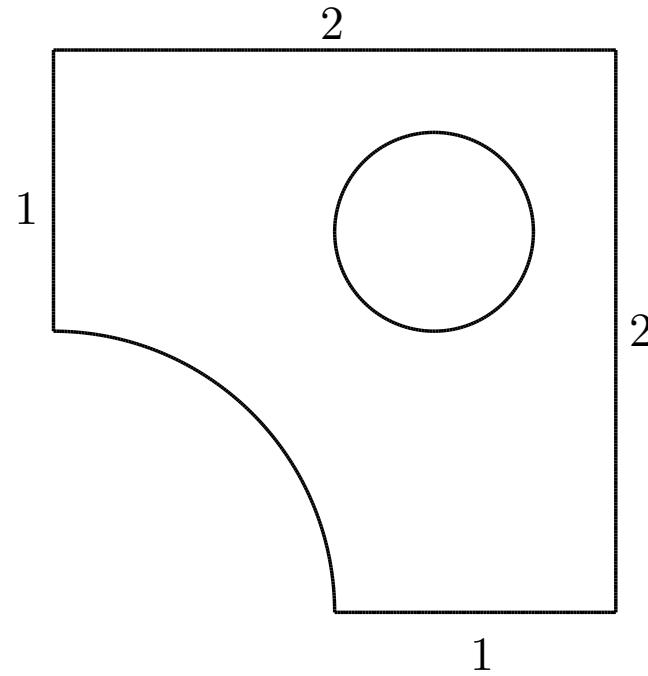


# Weight functions using heat flow



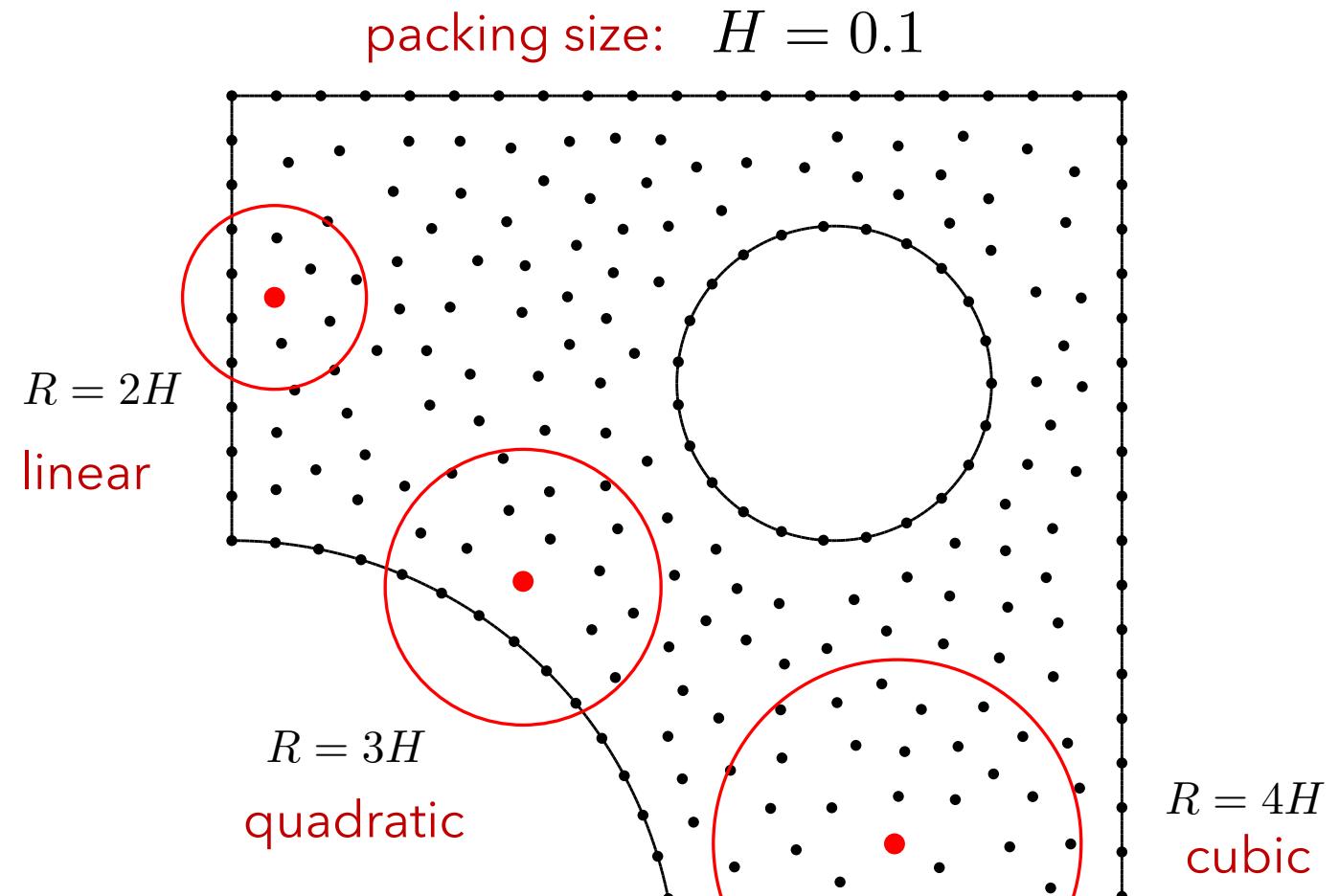
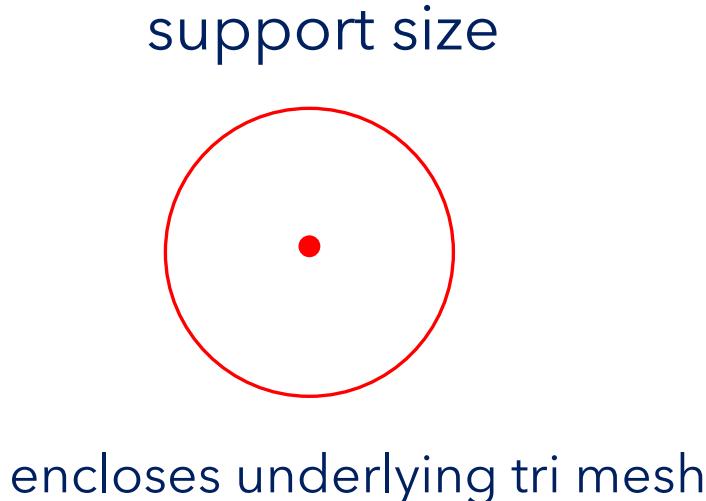
# Node placement

- uniform on boundary
- random close packing on interior (maximal Poisson sampling)

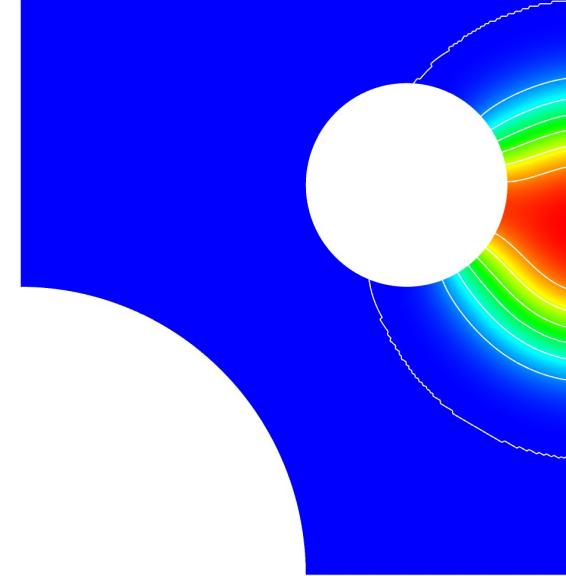
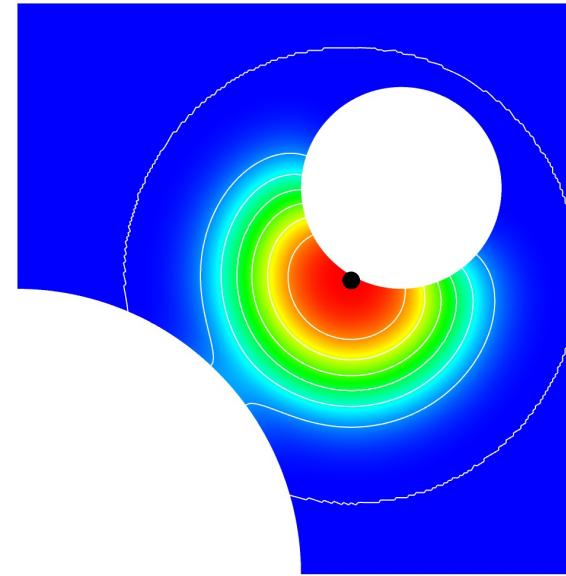
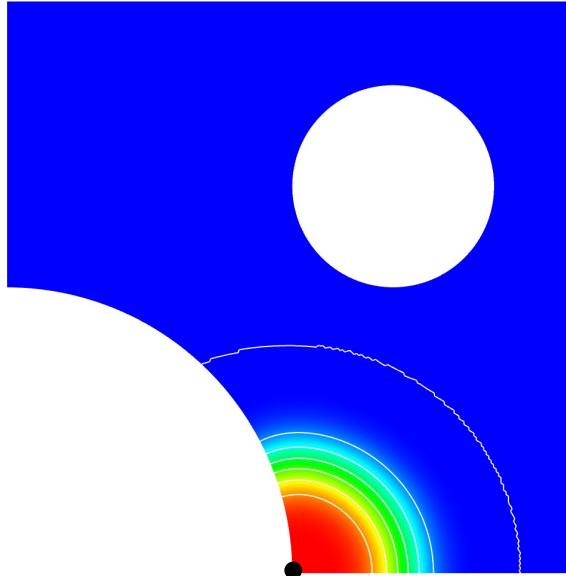


packing size:  
 $H = 0.1$

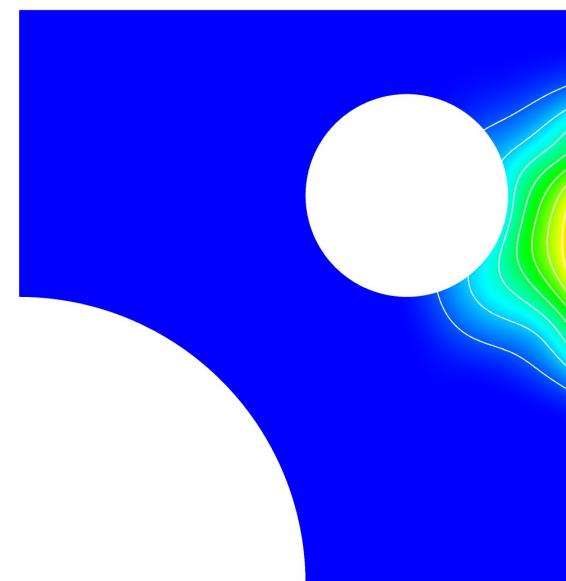
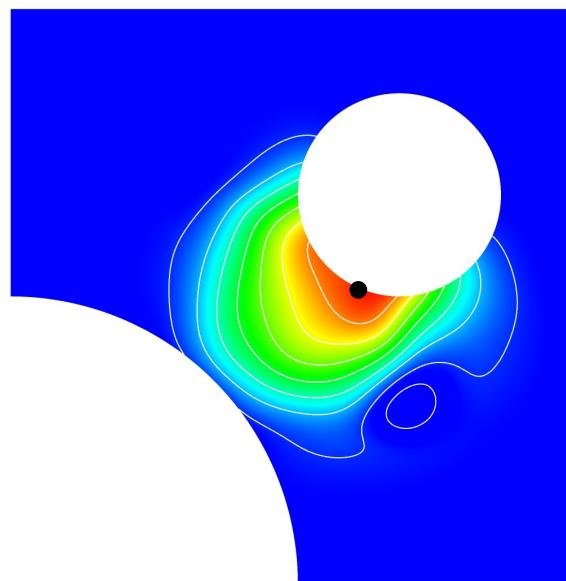
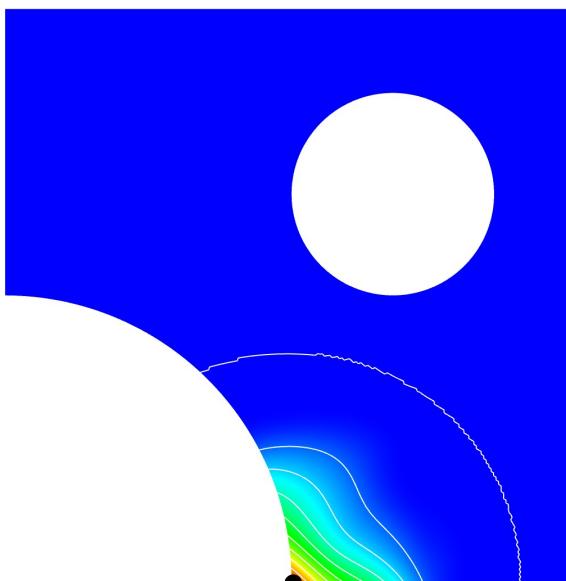
# Weight function support size



weight  
functions



shape  
functions  
(basis)



# How to do quadrature?



Observe that partition-of-unity property allows us to approximate any continuous function arbitrarily closely using only point evaluations as long as basis functions have local support.

Given  $\sum_K \phi_K(\mathbf{x}) = 1$  then it follows that  $f(\mathbf{x}) \approx \sum_K f(\mathbf{x}_K) \phi_K(\mathbf{x}) := f_h(\mathbf{x})$  *non-interpolatory approximation*

**Theorem:** For every  $\varepsilon > 0$  and  $\mathbf{x} \in \bar{\Omega}$ , there exists  $h(\varepsilon) > 0$  such that  $|f_h(\mathbf{x}) - f(\mathbf{x})| < \varepsilon$ .

It follows that  $\int f(\mathbf{x}) d\Omega \approx \int f_h(\mathbf{x}) d\Omega$

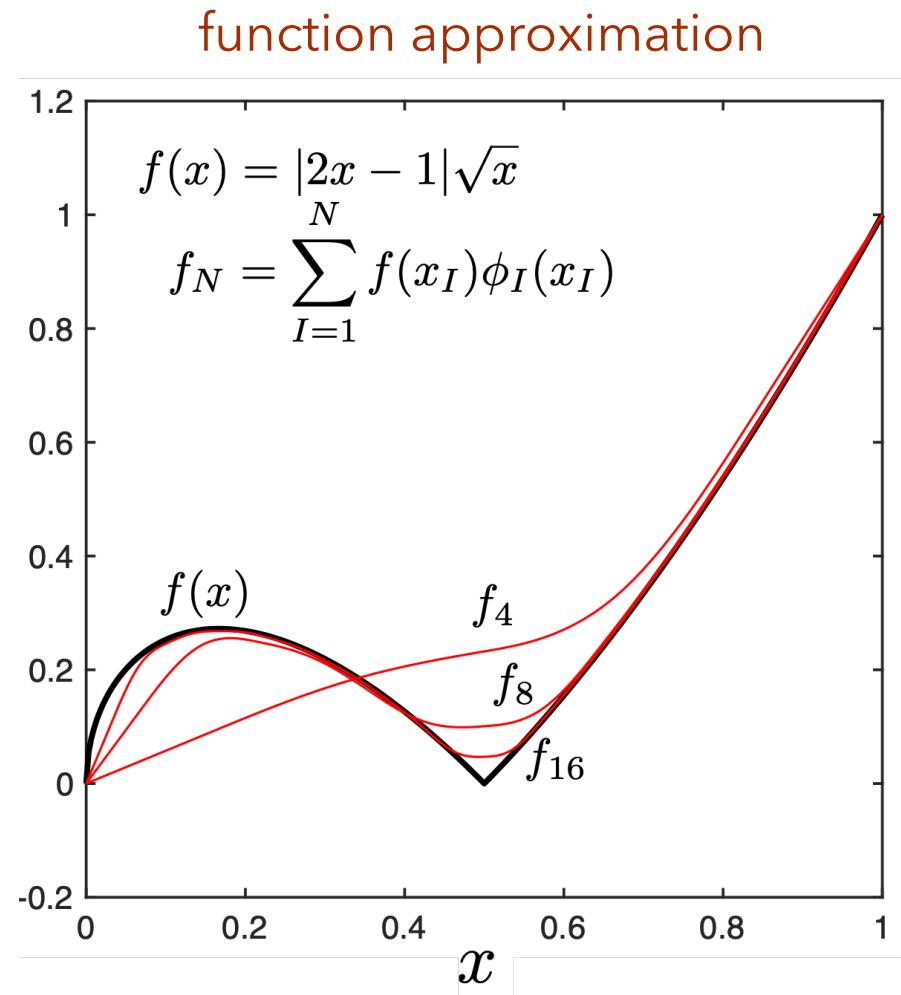
with  $\left| \int f_h(\mathbf{x}) d\Omega - \int f(\mathbf{x}) d\Omega \right| \leq \int |f_h(\mathbf{x}) - f(\mathbf{x})| d\Omega \leq \int \varepsilon d\Omega = V \cdot \varepsilon$

Can obtain rates of convergence using Taylor's theorem.

# Approximation property

let  $f(x) = |2x - 1|\sqrt{x}$

$$f_N = \sum_{K=1}^N f(x_K) \phi_K(x)$$



# Quadrature



$$\int f(\mathbf{x}) d\Omega \approx \int f_h(\mathbf{x}) d\Omega = \int \sum_K f(\mathbf{x}_K) \phi_K(\mathbf{x}) d\Omega = \sum_K f(\mathbf{x}_K) \int \phi_K(\mathbf{x}) d\Omega$$

Define quadrature weight as

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

$$\int f(\mathbf{x}) d\Omega \approx \sum_K w_K f(\mathbf{x}_K)$$

Can show that

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

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

# Quadrature

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

Also, since  $\sum_K \mathbf{x}_K \phi_K(\mathbf{x}) = \mathbf{x}$

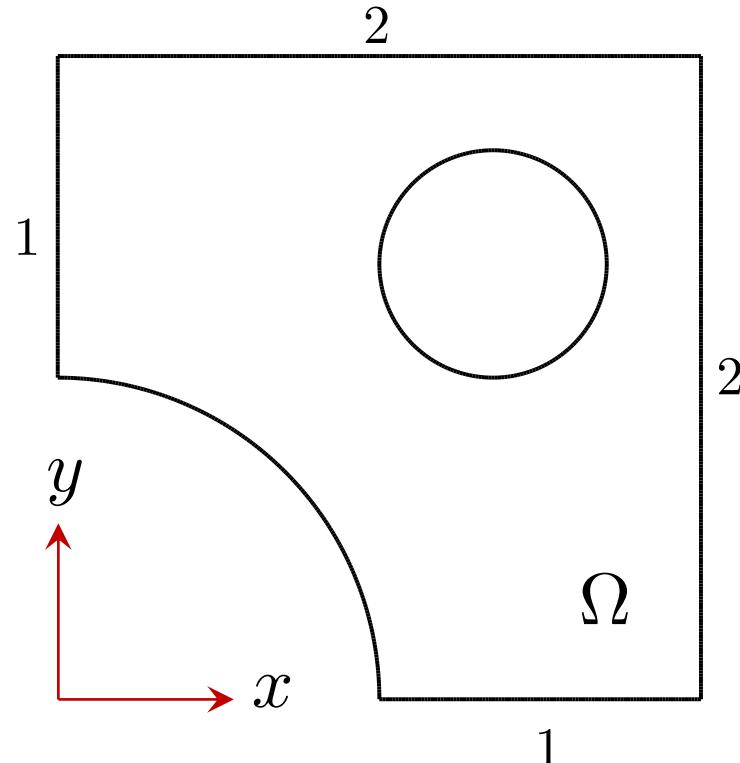
then  $\sum_K w_K \mathbf{x}_K = \sum_K \int_{\Omega} \phi_K(\mathbf{x}) \mathbf{x}_K d\Omega = \int_{\Omega} \sum_K \mathbf{x}_K \phi_K(\mathbf{x}) d\Omega = \int_{\Omega} \mathbf{x} d\Omega$

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

$$\sum_K w_K = V \quad \sum_K w_K \mathbf{x}_K = \int_{\Omega} \mathbf{x} d\Omega$$

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

# Quadrature example

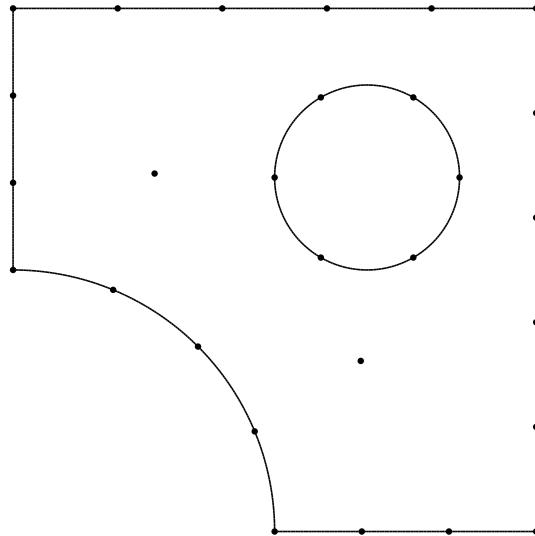


$$f(x, y) = \sin(\pi x/2) \sin(\pi y)$$

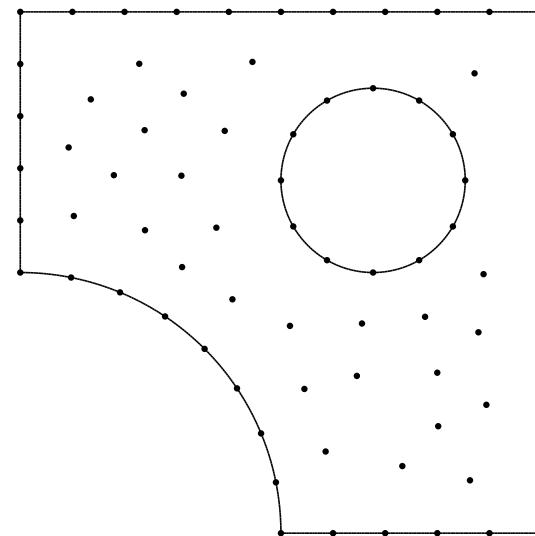
$$\text{error} := \left| \sum_K w_K f(\mathbf{x}_K) - \int_{\Omega} f \, d\Omega \right|$$

# Quadrature example

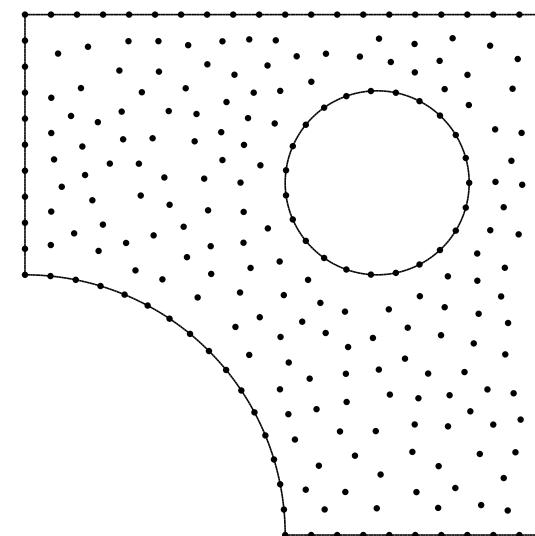
$H = 0.4$



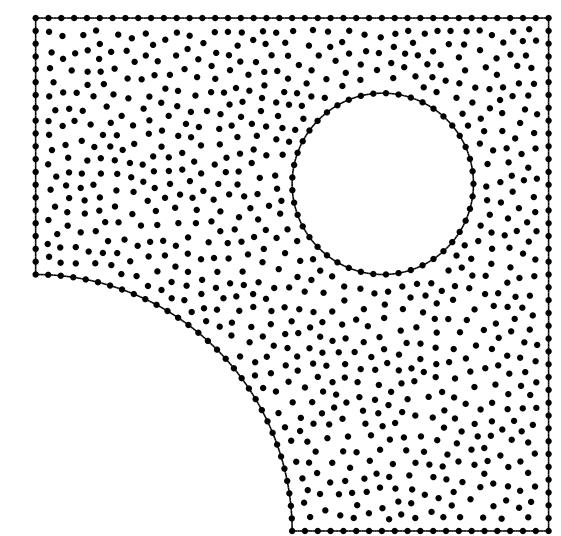
$H = 0.2$



$H = 0.1$



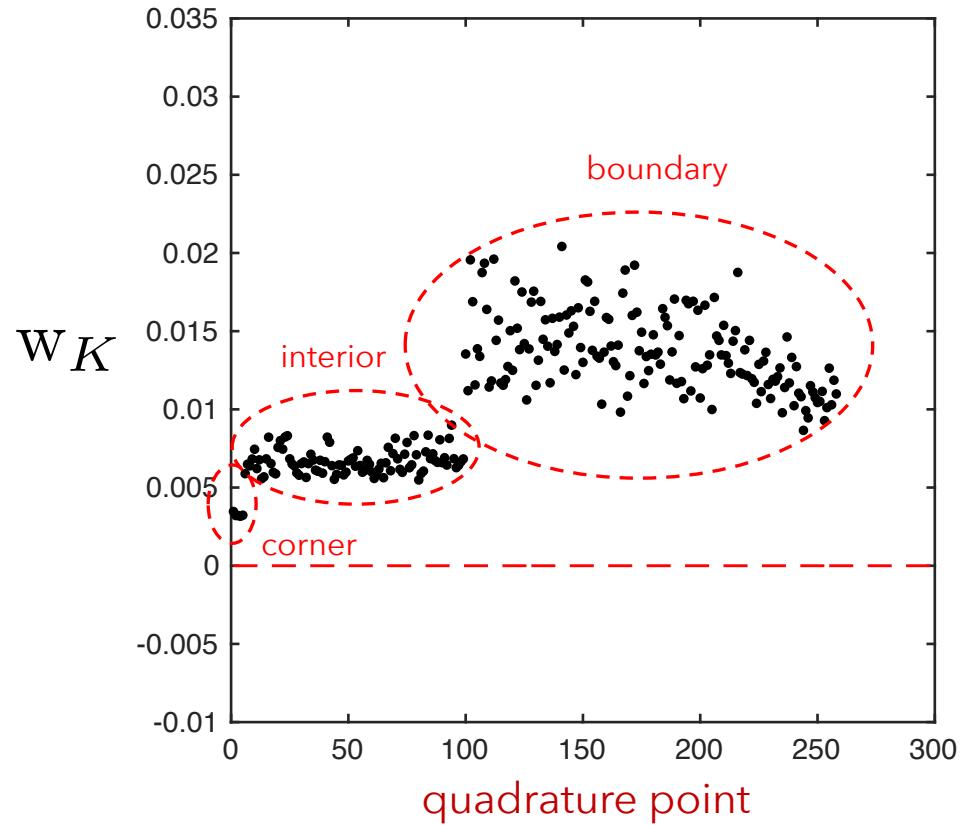
$H = 0.05$



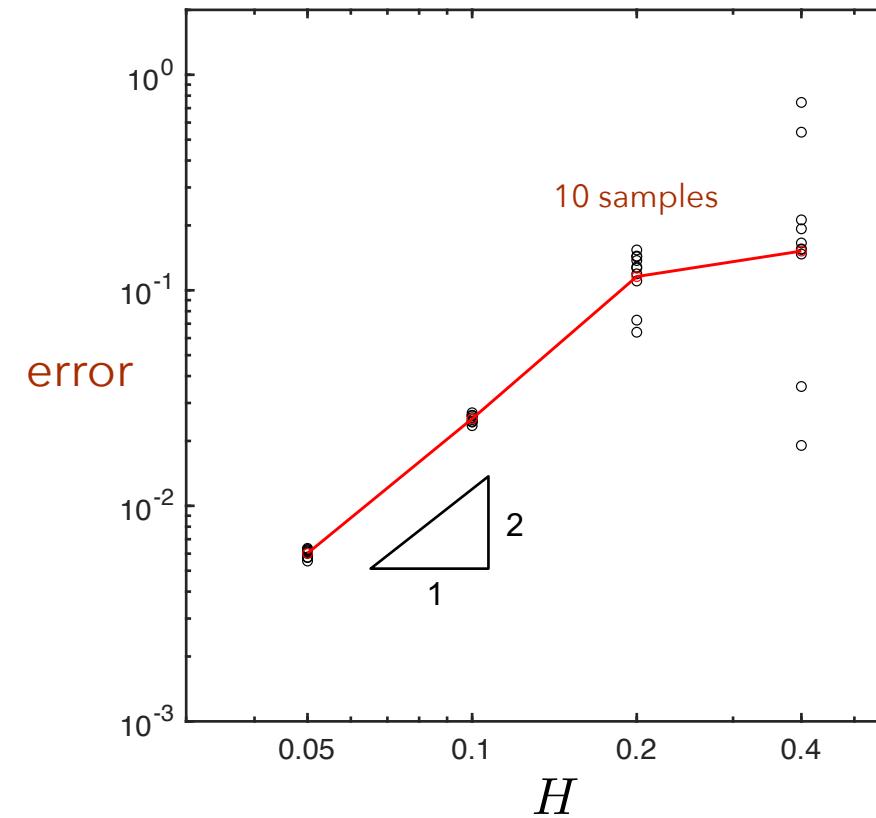
Evaluate error for 10 realizations.

# Quadrature weights

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



$$\text{error} := \left| \sum_K w_K f(\mathbf{x}_K) - \int_{\Omega} f d\Omega \right|$$



# Governing equations for solid mechanics (Lagrangian)

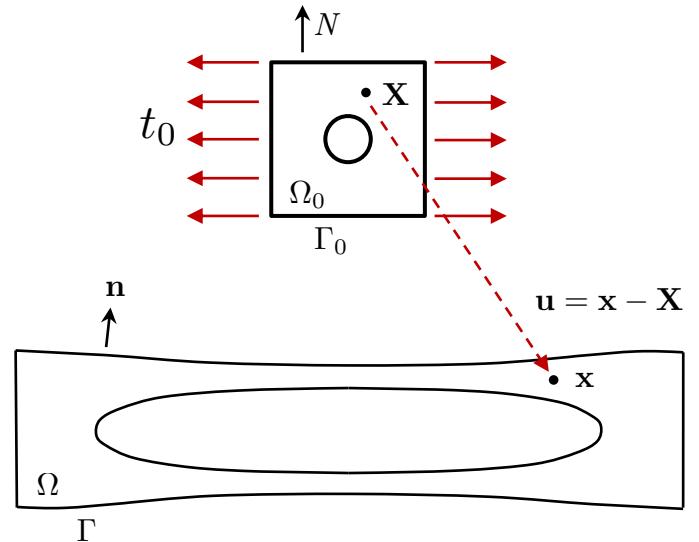


strong form

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

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

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



weak form

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

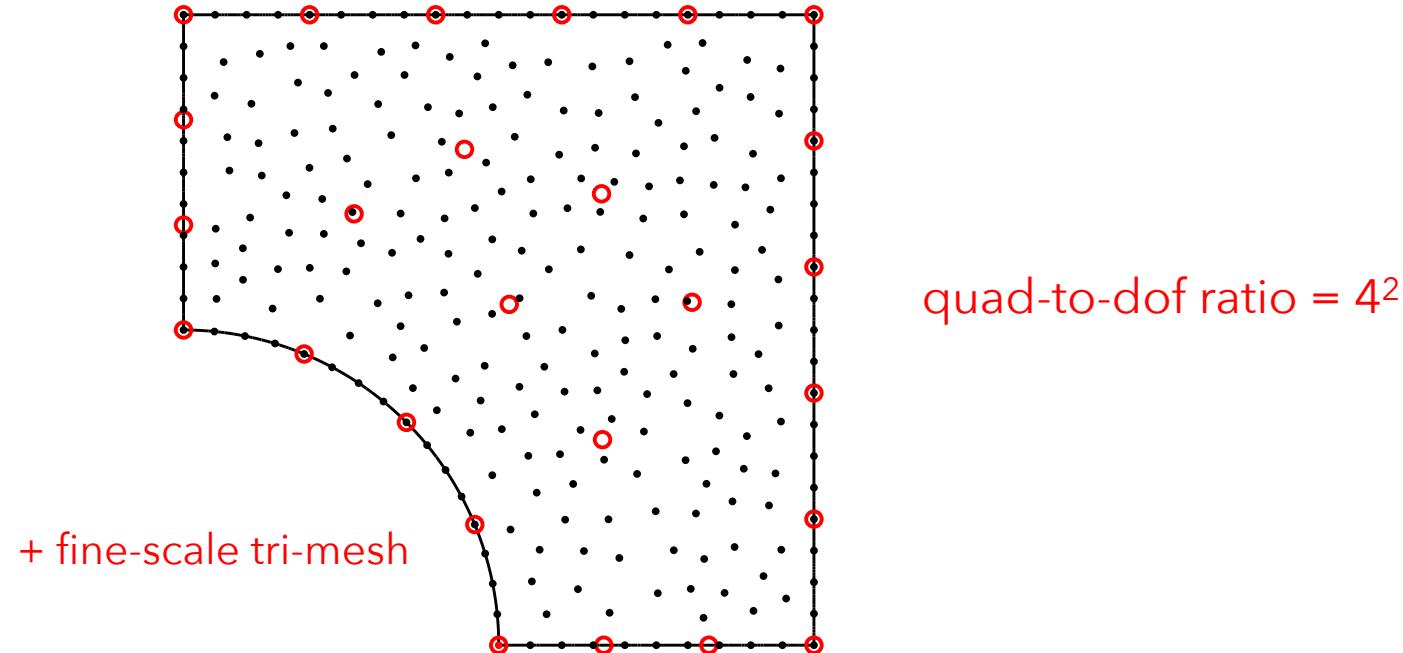
$$\int_{\Gamma_0^t} \mathbf{t}_0 \cdot \mathbf{v} \, dS - \int_{\Omega_0} \mathbf{P} : (\partial \mathbf{v} / \partial \mathbf{X}) \, d\mathbf{X} = \int_{\Omega_0} \rho_0 \ddot{\mathbf{u}} \cdot \mathbf{v} \, d\mathbf{X}$$

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

# Element-free approach to solve BVPs

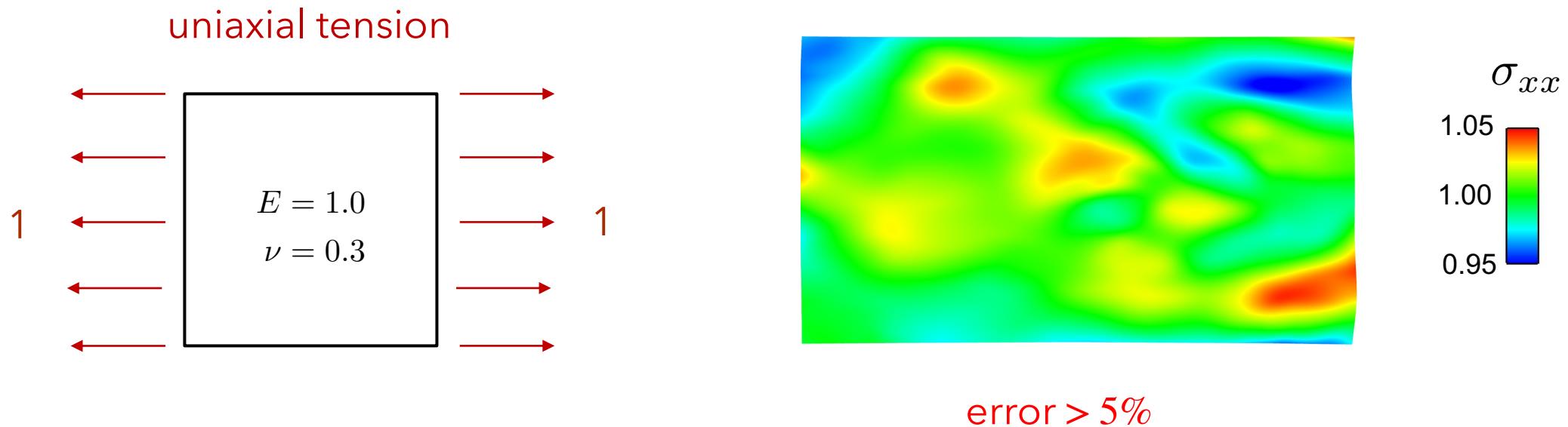
Use two meshfree clouds: one for solution discretization (DoF) and one for quadrature.

- DoF point
- quadrature point



What ratio of quad points to dof points is needed for stability (coercivity of bilinear form)?

# Patch test (linear consistency)



# Consistency of discrete form (integration)

- For convergence of discrete approximation, need to ensure consistency of discrete and continuous bilinear forms.
- Requires polynomial consistency of shape-function gradients (including quadrature).
- To obtain quadrature consistency, project the DoF shape function gradients to the subspace of quadrature shape functions.
- Only performed once in a pre-processing step.

$\{\phi_I, I = 1, \dots, N\}$  *DoF basis (shape functions)*

$\{\Phi_K, K = 1, \dots, M\}$  *Quadrature basis (shape functions)*

$$\nabla \phi_I := \arg \min \int_{\Omega} \left( \nabla \phi_I - \sum_{K=1}^M a^K \Phi_K \right)^2 d\Omega \quad (L_2 \text{ projection})$$

The projection can be written in terms of the dual or conjugate basis  $\{\Phi^J\}$

$$(\Phi_K, \Phi^J) = \delta_K^J \quad \text{bi-orthogonal}$$

$$\bar{\nabla} \phi_I = \sum_K (\nabla \phi_I, \Phi_K) \Phi^K = \sum_K (\nabla \phi_I, \Phi^K) \Phi_K$$


  
*covariant components*      *contravariant components*

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

Theorem:  $\int_{\Omega} \mathbf{p} \bar{\nabla} \phi_I d\Omega = \int_{\Omega} \mathbf{p} \nabla \phi_I d\Omega \quad \text{for all } \mathbf{p} \in \mathbb{P}_k(\Omega)$

*This ensures satisfaction of the patch test.*

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

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

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

$$\bar{a}(u, v) = \int_{\Omega} \left[ \sum_I (\nabla u, \Phi_I) \Phi^I \right] \mathbb{C} \left[ \sum_J (\nabla v, \Phi_J) \Phi^J \right] \, d\Omega$$

$$\bar{a}(u, v) = \sum_{I, J} (\nabla u, \Phi_I) \mathbb{C} (\nabla v, \Phi_J) \int_{\Omega_e} \Phi^I \Phi^J \, d\Omega$$


 $G^{IJ}$

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

where  $G_{IJ} = \int_{\Omega_e} \Phi_I \Phi_J d\Omega$  is the Gram matrix for the basis  $\{\Phi_K\}$

Can show that  $\Phi^I = G^{IJ} \Phi_J$  and  $\Phi_I = G_{IJ} \Phi^J$  *"raising" and "lowering" of indices*

$$\bar{a}(u, v) = \sum_{I,J} G^{IJ} (\nabla u, \Phi_I) \mathbb{C} (\nabla v, \Phi_J) = \sum_K (\nabla u, \Phi^K) \mathbb{C} (\nabla v, \Phi_K)$$



*Looks like a sum over quadrature points.*

Since  $G^{IJ} = (G_{IJ})^{-1}$  is dense:



Replace  $G_{IJ}$  with row-sum lumped version:  $G_{IJ}^L := \sum_J G_{IJ} = \text{diag}\{w_K\}$

where recall  $w_K = \int_{\Omega} \phi_K(\mathbf{x}) d\Omega$

Then  $\bar{a}(u, v) \rightarrow \bar{a}^L(u, v) = \sum_K \frac{1}{w_K} (\nabla u, \Phi_K) \mathbb{C} (\nabla v, \Phi_K)$  where  $(G_{IJ}^L)^{-1} = \text{diag} \left\{ \frac{1}{w_K} \right\}$

Can write  $\bar{a}^L(u, v)$  as

$$\bar{a}^L(u, v) = \sum_K w_K (\bar{\nabla} u)_K : \mathbb{C} (\bar{\nabla} v)_K$$

where

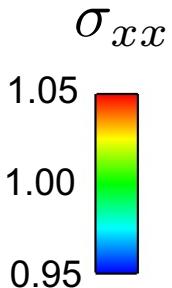
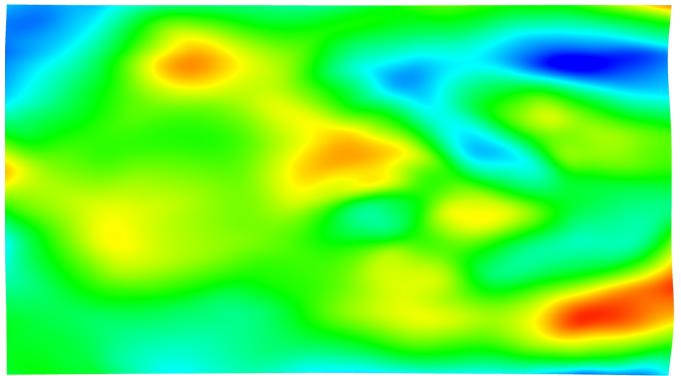
$$(\bar{\nabla} u)_K := \frac{1}{w_K} \int_{\Omega} (\nabla u) \Phi_K d\Omega$$

which has the form of a discrete derivative at a quadrature point  $K$ .

Our discrete bilinear form is now "sparse."

# Patch test (linear consistency)

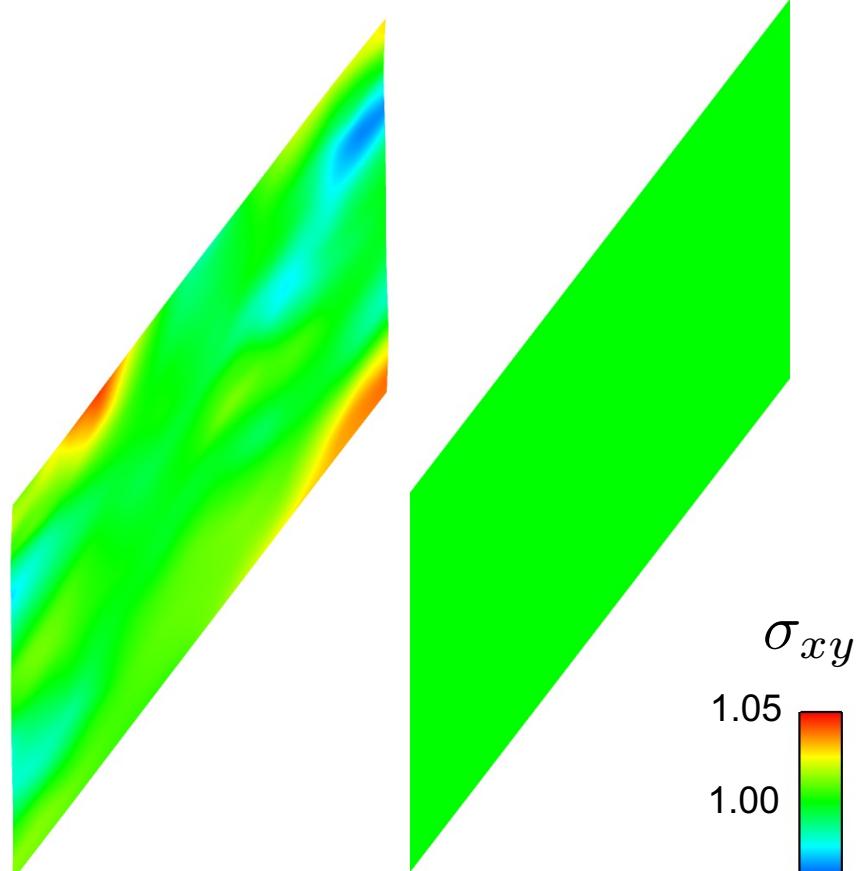
no projection



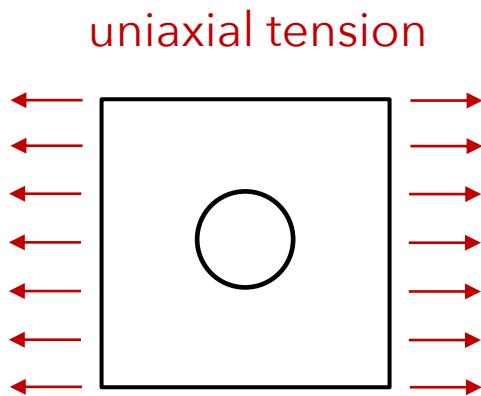
with projection



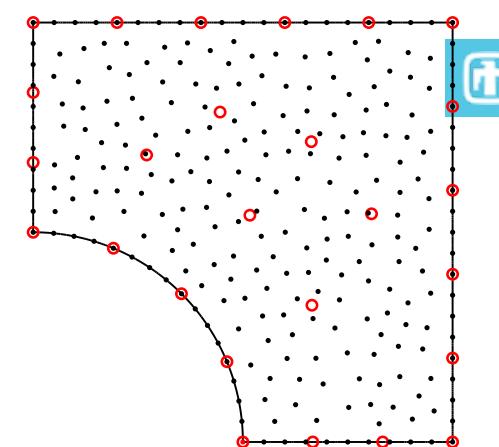
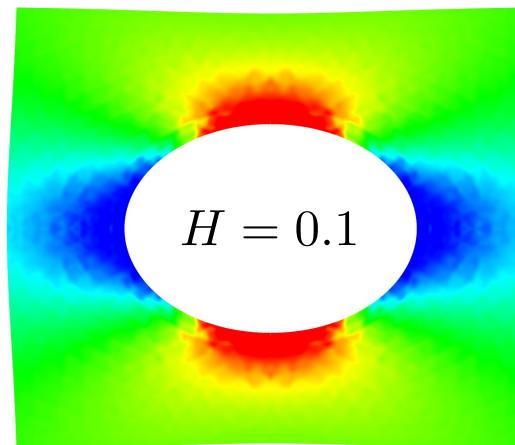
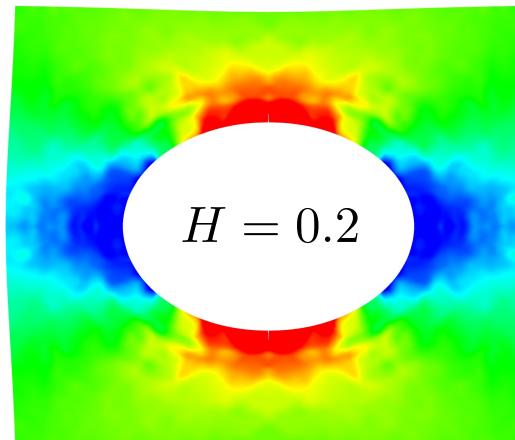
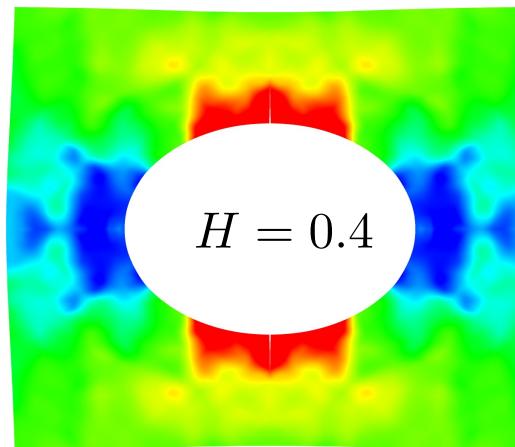
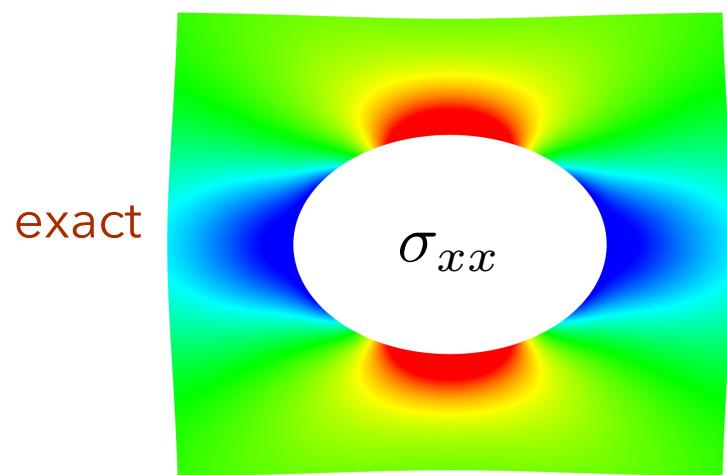
pure shear



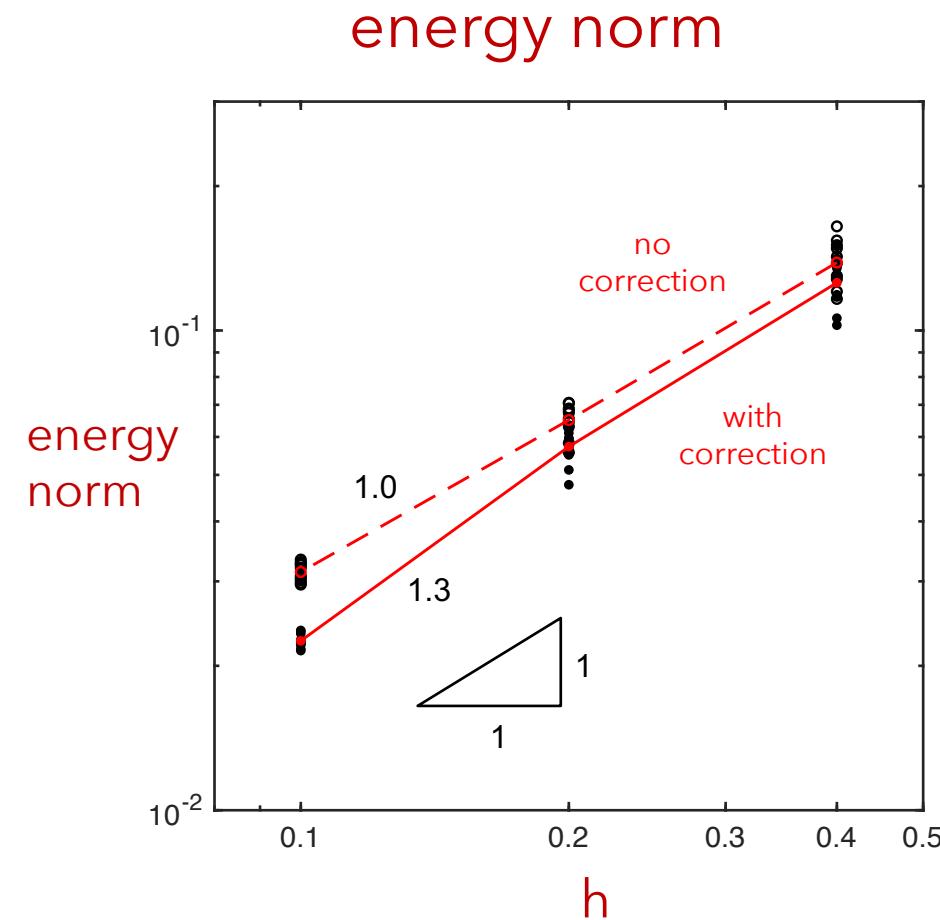
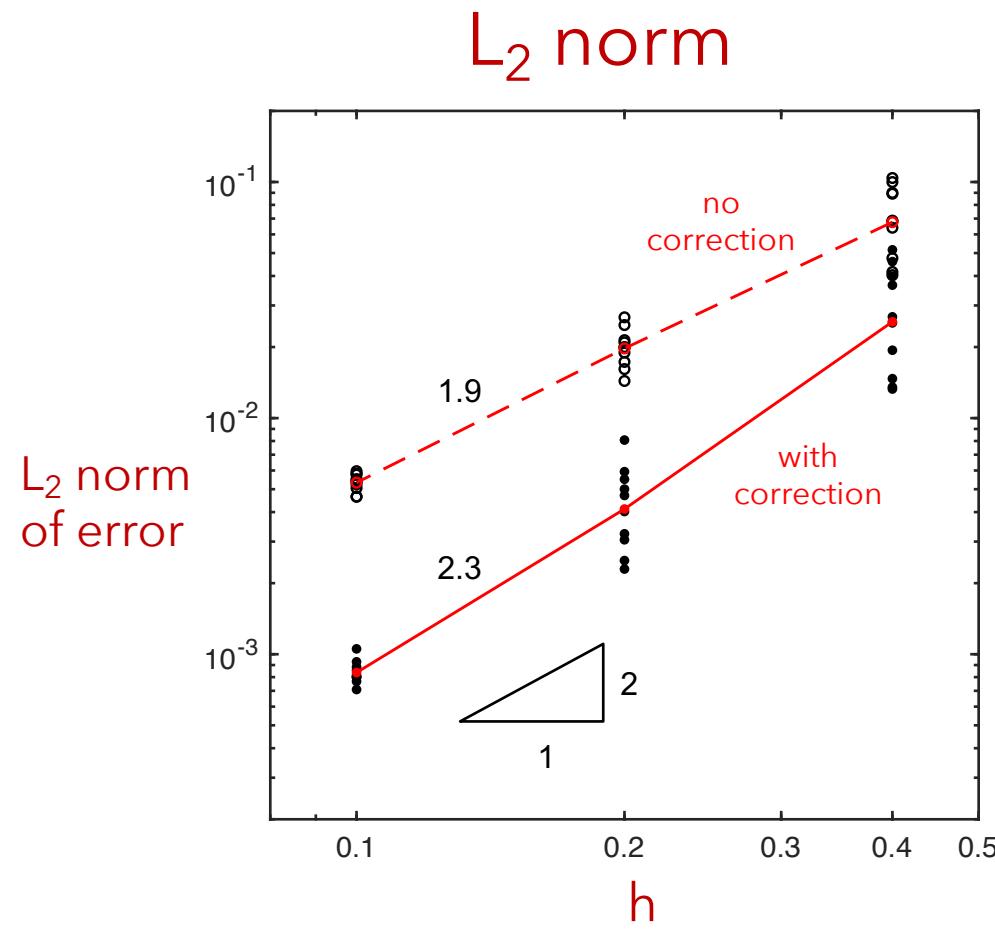
# Example: plate with hole



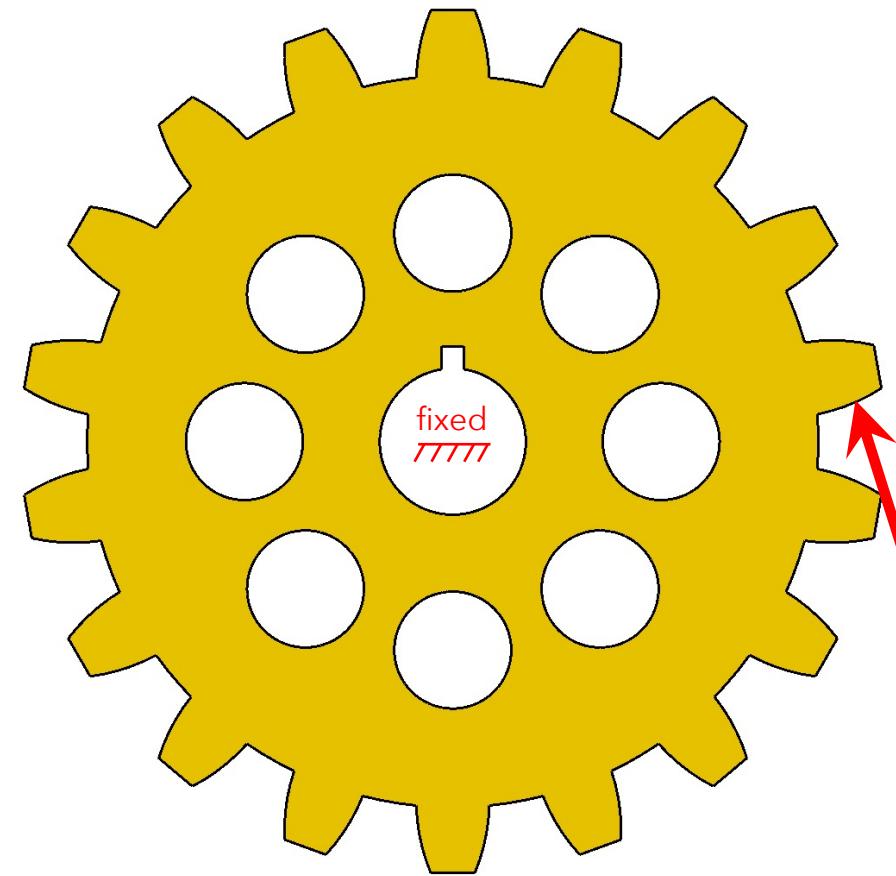
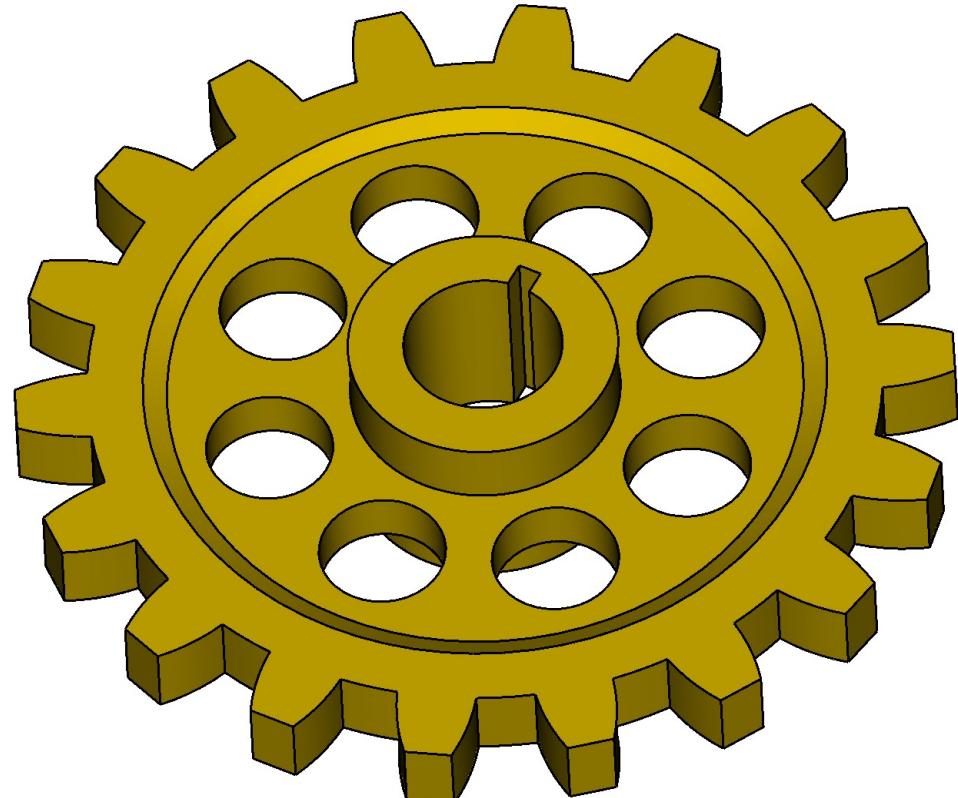
$$E = 1.0$$
$$\nu = 0.3$$



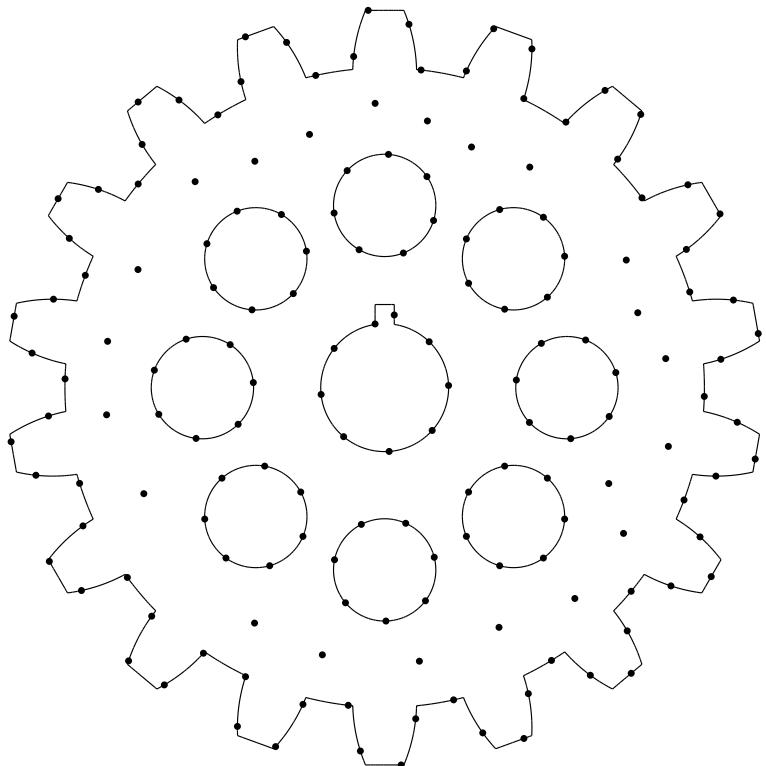
# Example: plate with hole



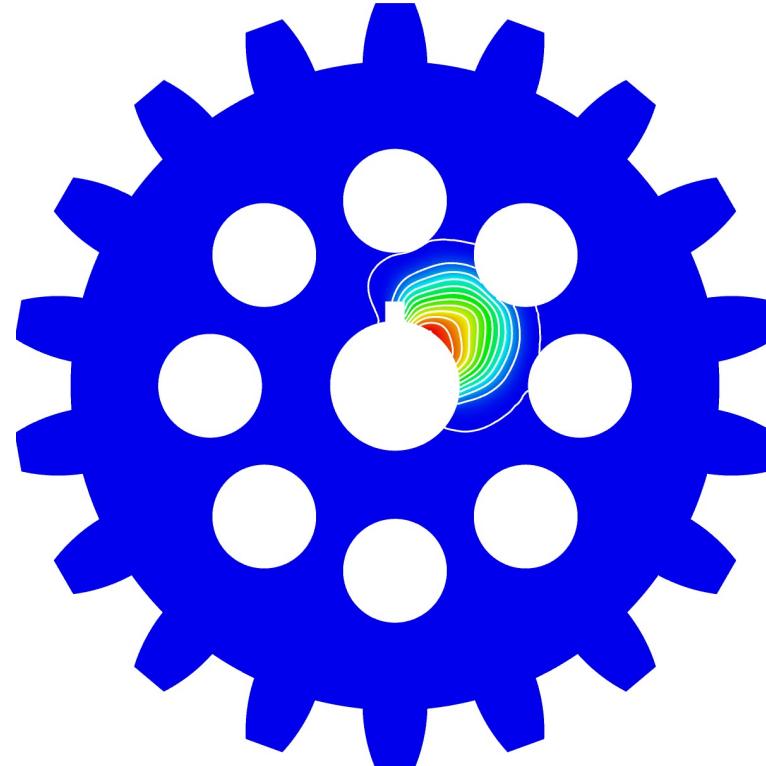
# Example



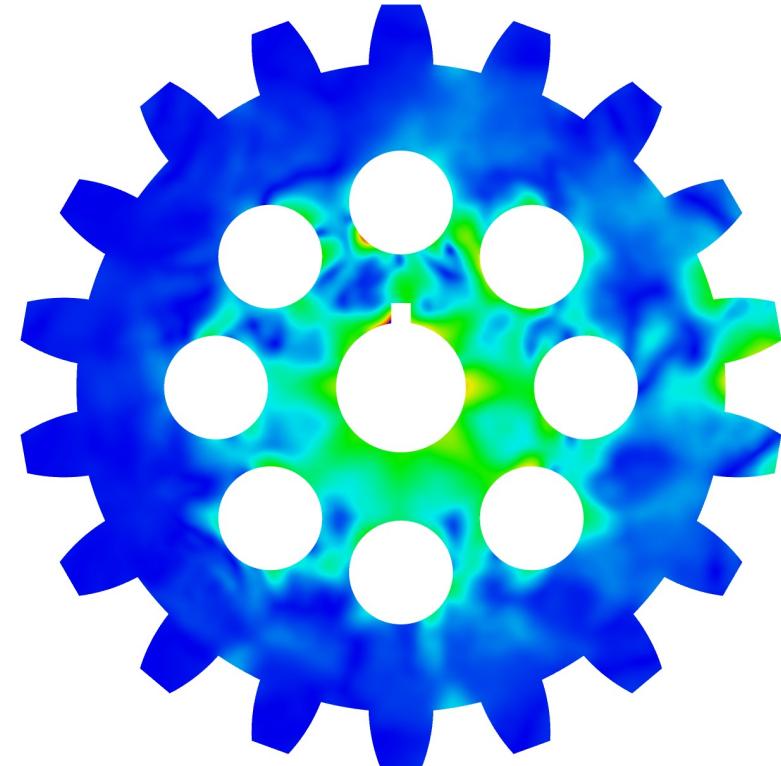
dof nodes

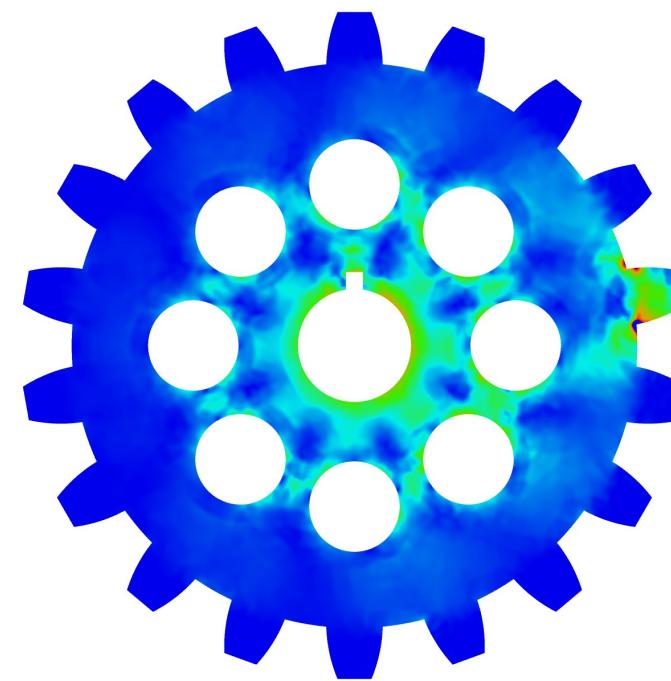
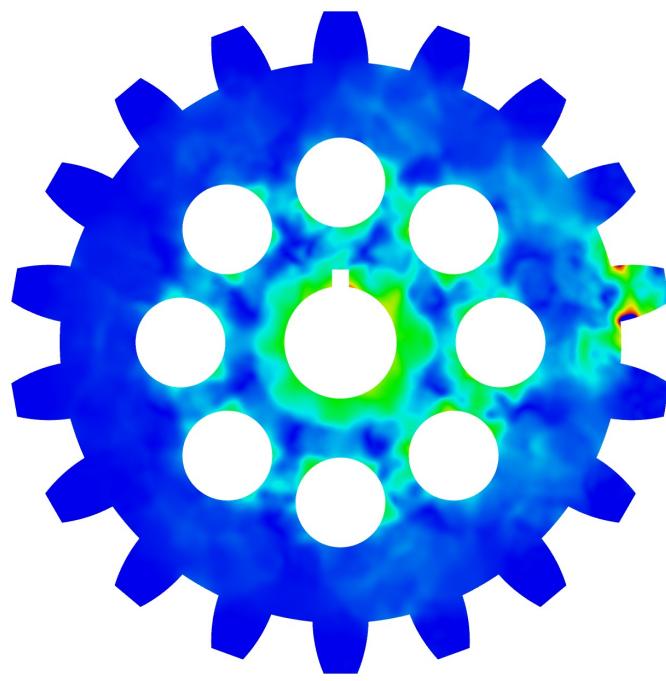
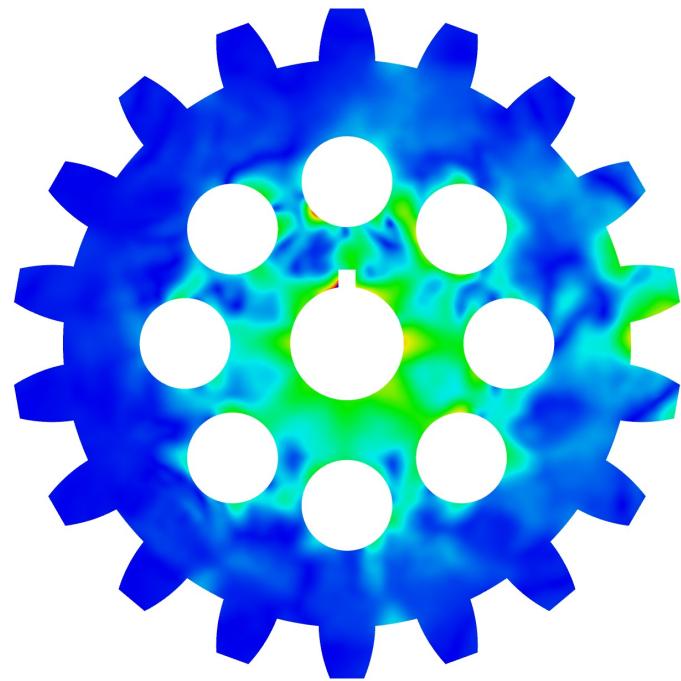
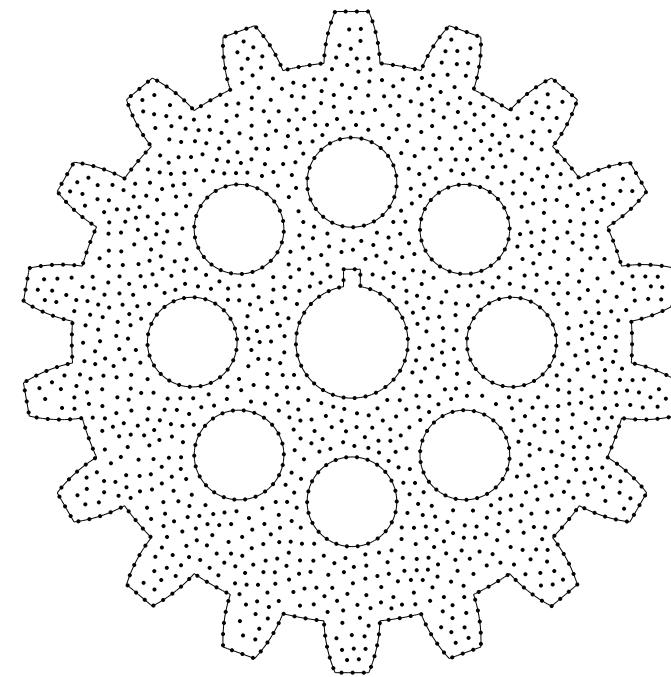
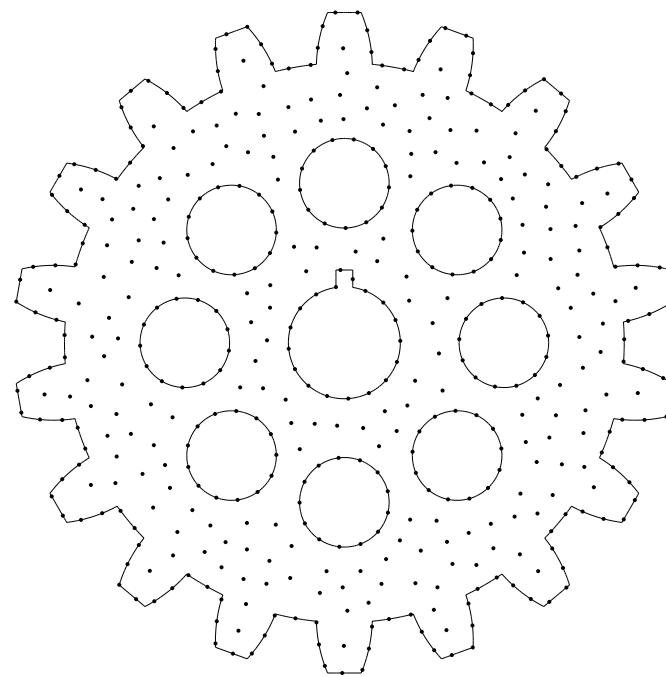
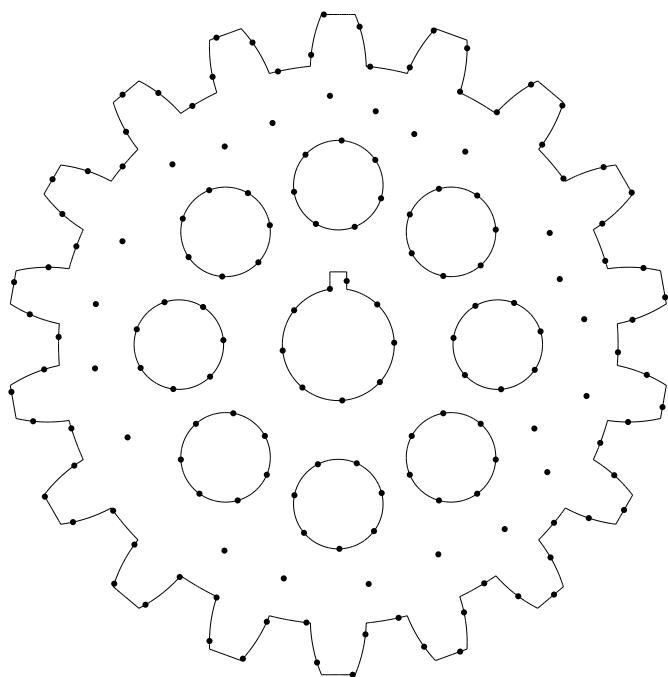


basis functions



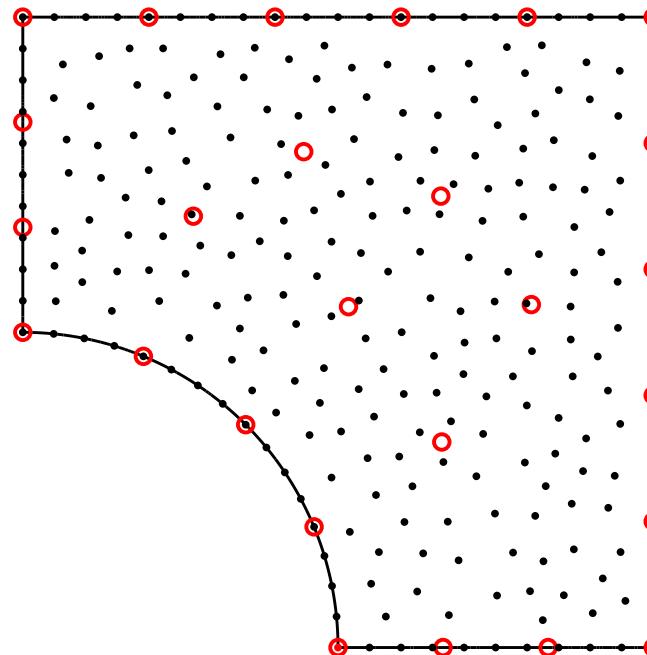
stress field (vm)





# Nearly incompressible limit

- Can extend approach to handle nearly incompressible materials
- Use a “generalized” B-Bar/F-bar approach.
- Project dilatational portion of deformation gradient to smaller subspace, e.g. use original DOF points as quadrature basis.



- DoF node and dilatational quadrature node
- deviatoric quadrature node

# Summary

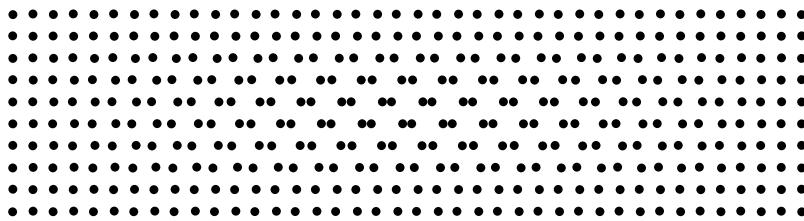
1. Separate domain discretization from solution discretization (fine-scale domain triangulation with coarse-scale solution discretization).
2. Example of discretization-based reduced order model.
3. Generation of meshfree weight functions using manifold geodesics.
4. New approach to quadrature for meshfree methods based on secondary basis.
5. Projected shape-function gradients using dual basis for polynomial consistency.
6. Observed optimal convergence rates for 2D elasticity.
7. Applicable to nonlinear solid mechanics too (plasticity).
8. Examples here were in  $H^1$ , also can be extended to  $H(\text{div})$  and  $H(\text{curl})$

# Coercivity

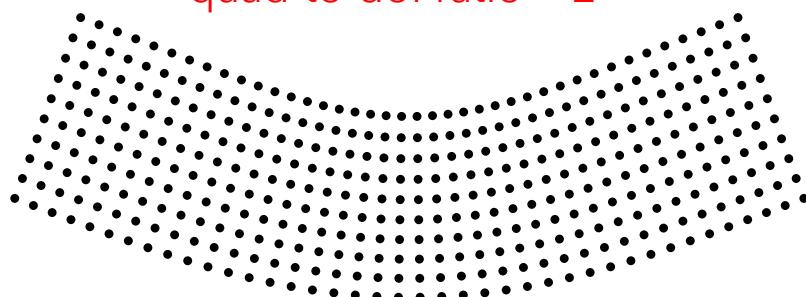
For Lax-Milgram theorem (existence and uniqueness)  
need coercivity of the bilinear form

There exists  $C$  such that  $a(u, u) \geq C\|u\|^2$  for all  $u \in H_0^1$

quad-to-dof ratio = 1



quad-to-dof ratio = 2<sup>2</sup>



minimum eigenvalue (nonzero)

