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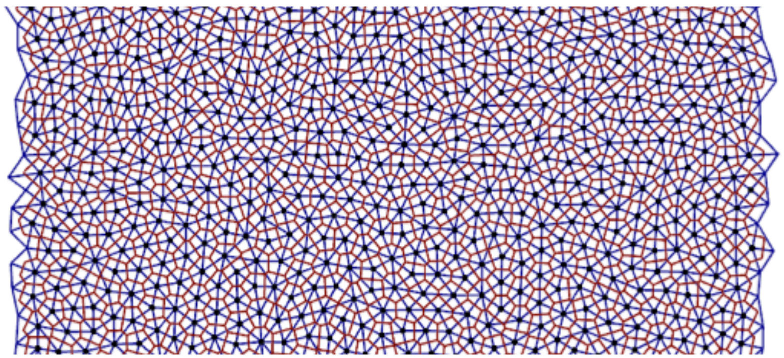

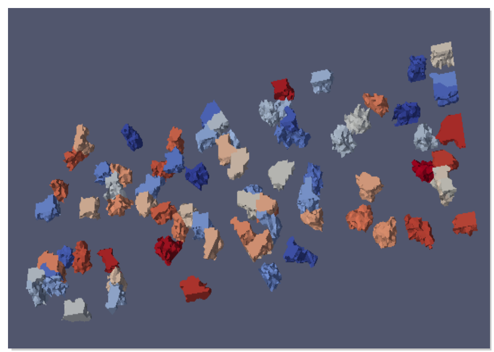

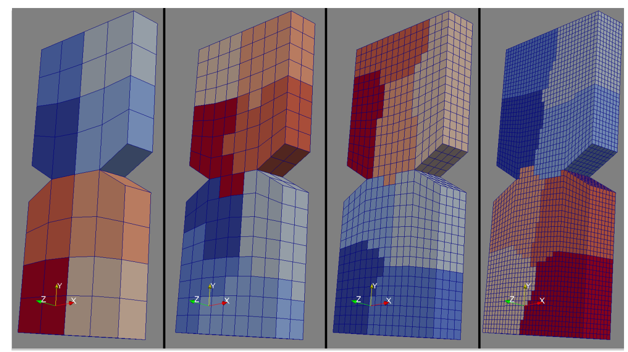

Nonlocal Regularization for Loss of Ellipticity in Inelastic Problems

Alejandro Mota, James W. Foulk III
Jakob T. Ostien, Tracy Vogler

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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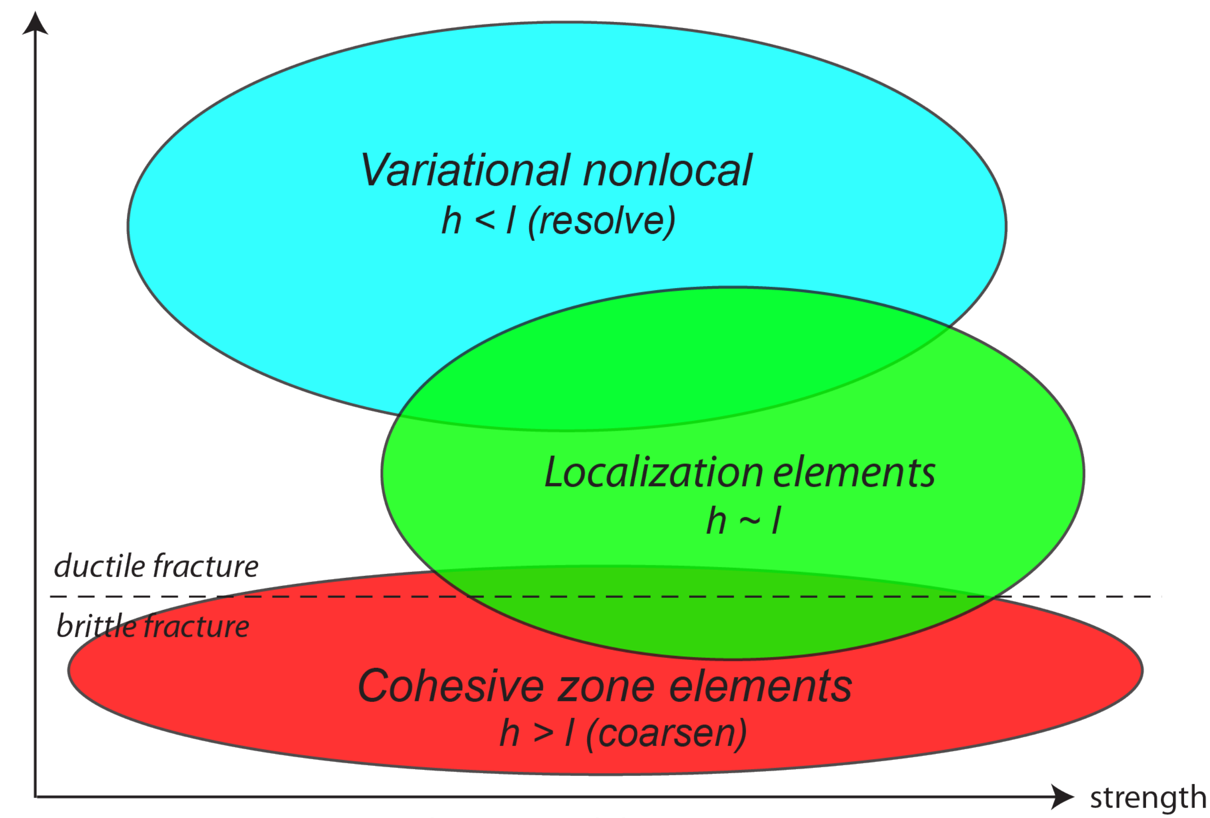
Methods broadly applicable

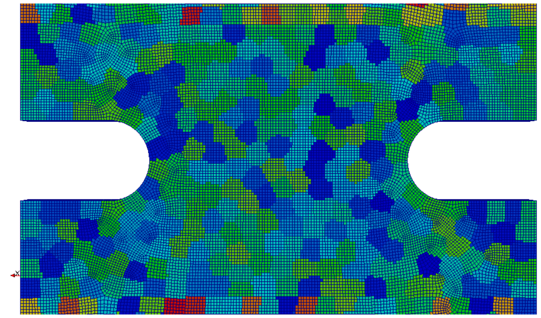
- Provide regularized techniques for modeling localization and fracture/failure
- For ductile failure, provide infrastructure for local damage models



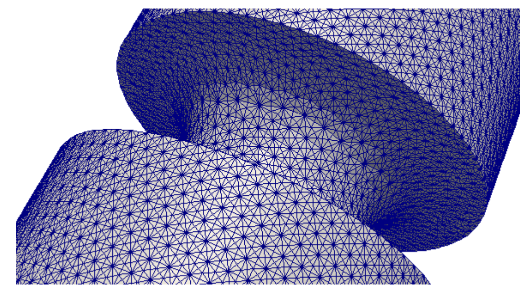
$$l = \text{length scale}_{\text{mode I}} = \frac{\text{toughness} * \text{modulus}}{\text{strength}^2}$$

h = element size

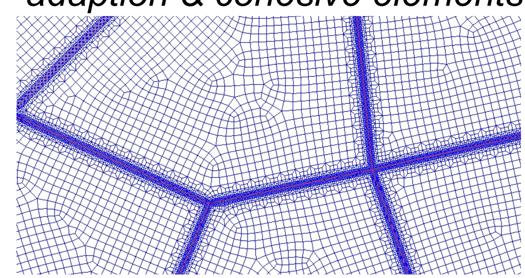
variational nonlocal



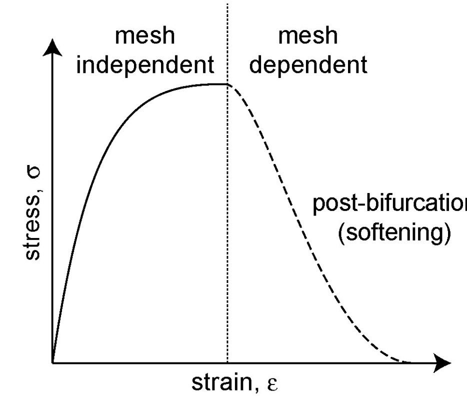
adaption & localization elements



adaption & cohesive elements



Loss of Ellipticity



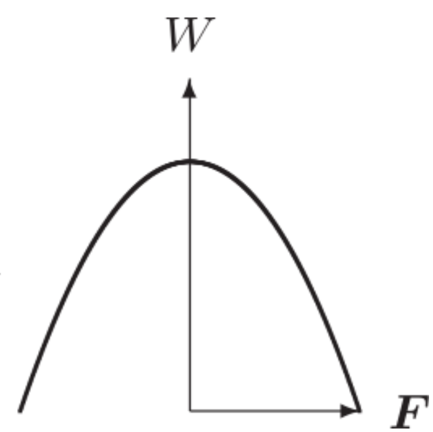
Softening behavior

Stress-strain curve has one or more peaks.

Loss of ellipticity

Governing partial differential equation changes character.

$$\operatorname{Div} \boldsymbol{P} + \boldsymbol{B} = \boldsymbol{0}$$



Loss of convexity

Stored energy function becomes non-convex.

$$\Phi[\boldsymbol{\varphi}] = \int_B W(\boldsymbol{F}, \boldsymbol{Z}, T)\, dV - \int_B \boldsymbol{B} \cdot \boldsymbol{\varphi}\, dV - \int_{\partial_T B} \bar{\boldsymbol{T}} \cdot \boldsymbol{\varphi}\, dS$$

Singular Acoustic Tensor

Tangent modulus becomes non-positive definite (singular acoustic tensor).

$$\mathbb{C} = 4 \frac{\partial^2 W}{\partial \boldsymbol{C}^2}$$

Variational Methods

- Begin from fundamental physical principles.
- Governing equations from optimization.
- Allow better analysis for uniqueness of solutions.
- Lead to robust numerical methods.
- Help identify correct conjugate fields.
- Et cetera.

Variational Nonlocal Method

Three-Field Mixed Finite Element Formulation:

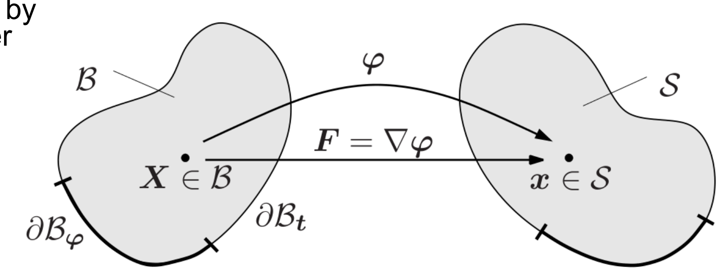
$$\Phi[\boldsymbol{\varphi}, \bar{\boldsymbol{Z}}, \bar{\boldsymbol{Y}}] := \int_B W(\boldsymbol{F}, \bar{\boldsymbol{Z}}, \boldsymbol{Q}, T)\, dV + \int_B \bar{\boldsymbol{Y}} \cdot (\bar{\boldsymbol{Z}} - \boldsymbol{Z})\, dV - \int_B \rho_0 \boldsymbol{B} \cdot \boldsymbol{\varphi}\, dV - \int_{\partial_T B} \boldsymbol{T} \cdot \boldsymbol{\varphi}\, dS$$

Deformation Mapping

Helmholtz Free Energy

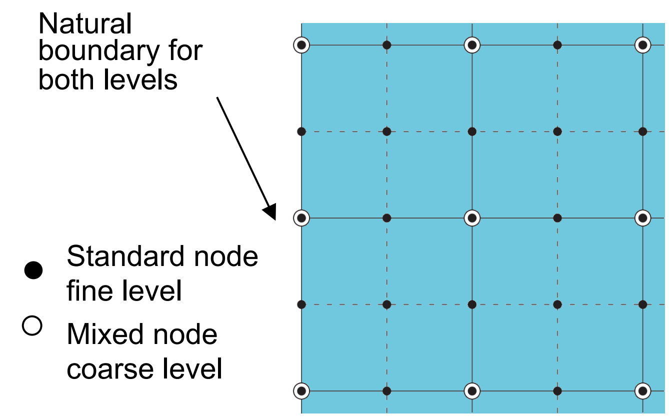
Nonlocal Internal Variable

Constraint Enforced by Lagrange Multiplier



Deformation Mapping

- Motivated through studies of non-locality
- Fully variational approach.
- Entirely by-passes ad hoc approaches.
- Does not require any modifications to constitutive models.
- Nonlocal domain is defined naturally by support of mixed interpolation functions.
- Natural parallelization by domain decomposition of coarse discretization.
- Does not require cut-off approaches at boundary.



Finite Element Formulation

Three-Field Mixed Finite Element Formulation:

$$\Phi[\boldsymbol{\varphi}, \bar{\boldsymbol{Z}}, \bar{\boldsymbol{Y}}] := \int_B W(\boldsymbol{F}, \bar{\boldsymbol{Z}}, \boldsymbol{Q}, T)\; dV + \int_B \bar{\boldsymbol{Y}} \cdot (\bar{\boldsymbol{Z}} - \boldsymbol{Z})\; dV - \int_B \rho_0 \boldsymbol{B} \cdot \boldsymbol{\varphi}\; dV - \int_{\partial_T B} \boldsymbol{T} \cdot \boldsymbol{\varphi}\; dS$$

Variations:

$$\boldsymbol{\varphi} \in V_\varphi := (W_2^1(B))^3,\; \bar{\boldsymbol{Z}} \in V_Z := (W_2^1(B))^q \text{ and } \bar{\boldsymbol{Y}} \in V_Y := (W_2^1(B))^q$$

$$\boldsymbol{\eta} \in V_\varphi,\; \boldsymbol{\zeta} \in V_Z \text{ and } \boldsymbol{\xi} \in V_Y$$

$$D\Phi[\boldsymbol{\varphi}, \bar{\boldsymbol{Z}}, \bar{\boldsymbol{Y}}](\boldsymbol{\eta}) = \int_B \boldsymbol{P} : \operatorname{Grad} \boldsymbol{\eta}\; dV - \int_B \rho_0 \boldsymbol{B} \cdot \boldsymbol{\eta}\; dV - \int_{\partial_T B} \boldsymbol{T} \cdot \boldsymbol{\eta}\; dS = 0,$$

$$D\Phi[\boldsymbol{\varphi}, \bar{\boldsymbol{Z}}, \bar{\boldsymbol{Y}}](\boldsymbol{\zeta}) = \int_B (\bar{\boldsymbol{Y}} - \boldsymbol{Y}) \cdot \boldsymbol{\zeta}\; dV = 0,$$

$$D\Phi[\boldsymbol{\varphi}, \bar{\boldsymbol{Z}}, \bar{\boldsymbol{Y}}](\boldsymbol{\xi}) = \int_B (\bar{\boldsymbol{Z}} - \boldsymbol{Z}) \cdot \boldsymbol{\xi}\; dV = 0,$$

$$\boldsymbol{P} := \partial W / \partial \boldsymbol{F} \qquad \boldsymbol{Y} := -\partial W / \partial \bar{\boldsymbol{Z}}$$

Regularization

Discrete Statement of Equilibrium, Internal Variables and Conjugate Forces:

$$\int_B \boldsymbol{P} \cdot \mathrm{Grad}\, N_a \; dV - \int_B \rho_0 \boldsymbol{B} N_a \; dV - \int_{\partial_T B} \boldsymbol{T} N_a \; dS = \boldsymbol{0},$$

$$\bar{\boldsymbol{Y}} = \lambda_\alpha \left(\int_B \lambda_\alpha \lambda_\beta \; dV \right)^{-1} \int_B \lambda_\beta \boldsymbol{Y} \; dV,$$

$$\bar{\boldsymbol{Z}} = \lambda_\alpha \left(\int_B \lambda_\alpha \lambda_\beta \; dV \right)^{-1} \int_B \lambda_\beta \boldsymbol{Z} \; dV,$$

Unit Interpolation, Regularized Variables:

$$\lambda_\alpha = 1, \; \lambda_\beta = 1 \quad \Rightarrow \quad \bar{\boldsymbol{Y}} = \frac{1}{\mathrm{vol}(D)} \int_D \boldsymbol{Y} \; dV, \quad \bar{\boldsymbol{Z}} = \frac{1}{\mathrm{vol}(D)} \int_D \boldsymbol{Z} \; dV,$$

$$\mathrm{vol}(\bullet) := \int_{(\bullet)} dV,$$

Volume averaging provides nonlocal regularization

Connection to Gradients

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Expansion in Taylor Series:

$$\boldsymbol{Z} = \boldsymbol{Z}_0 + \frac{\partial \boldsymbol{Z}}{\partial \boldsymbol{X}}(\boldsymbol{X}_0) \cdot (\boldsymbol{X} - \boldsymbol{X}_0) + \frac{1}{2}(\boldsymbol{X} - \boldsymbol{X}_0) \cdot \frac{\partial^2 \boldsymbol{Z}}{\partial \boldsymbol{X}^2}(\boldsymbol{X}_0) \cdot (\boldsymbol{X} - \boldsymbol{X}_0) + \cdots$$

Apply to Regularized Variables:

$$\bar{\boldsymbol{Z}} = \boldsymbol{Z}_0 + \frac{1}{2\,\mathrm{vol}(D)} \frac{\partial^2 \boldsymbol{Z}}{\partial \boldsymbol{X}^2}(\boldsymbol{X}_0) : \int_D (\boldsymbol{X} - \boldsymbol{X}_0) \otimes (\boldsymbol{X} - \boldsymbol{X}_0)\; dV + \cdots$$

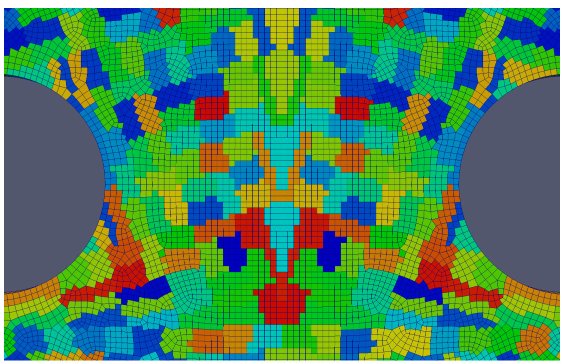
Obtain Gradient Regularization:

$$\bar{\boldsymbol{Z}} = \boldsymbol{Z}_0 + \nabla^2 \boldsymbol{Z}(\boldsymbol{X}_0) : \boldsymbol{H}(D) + \cdots$$

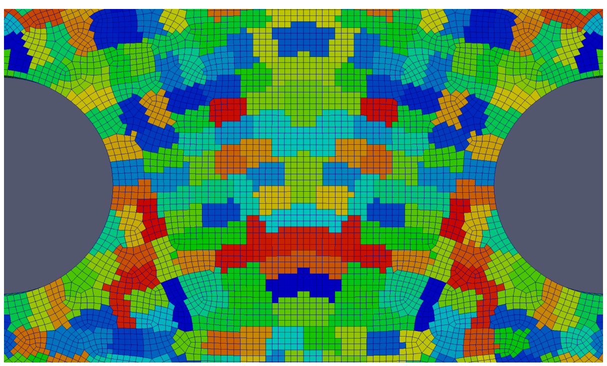
Leverage domain decomposition

IDEA: Simple volume averaging enables non-conformal meshes. We can leverage an entire community devoted to domain decomposition

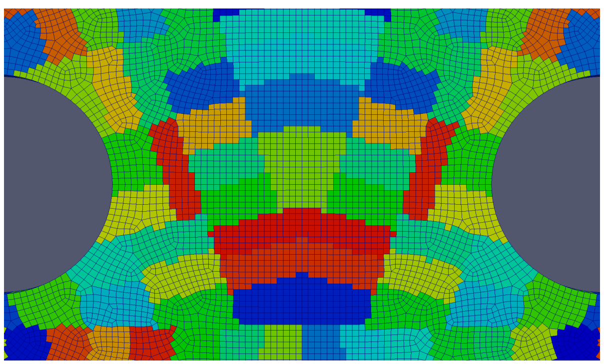
- *Domain decomposition algorithms minimize communication*
  - *Geometric partitions (Zoltan RCB, Zoltan RIB)*
  - *Graph-based partitions (Zoltan Hypergraph, Metis)*
- *We can constrain domains to be of common volume, l^3*



Zoltan RCB



Zoltan RCB w/bounding box

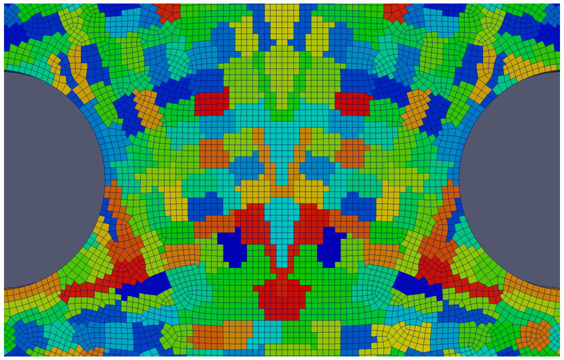


Zoltan RCB w/bounding box, larger l

Initial analysis illustrates that domain shape can affect the solution. We are introducing anisotropy into nonlocal ISV evolution!

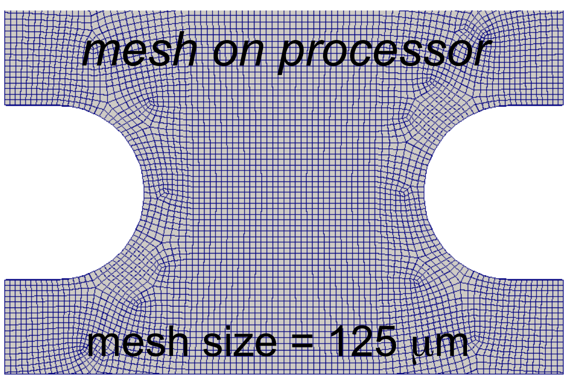
NOTE: Meyerhenke and co-authors have considered domain shape. "A New Diffusion-based Multilevel Algorithm for Computing Graph Partitions", H. Meyerhenke, B. Monien, T. Sauerwald, JPDC 69, 2009.

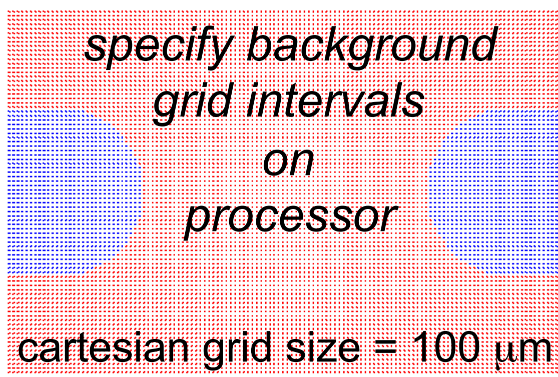
Rethinking domain shape

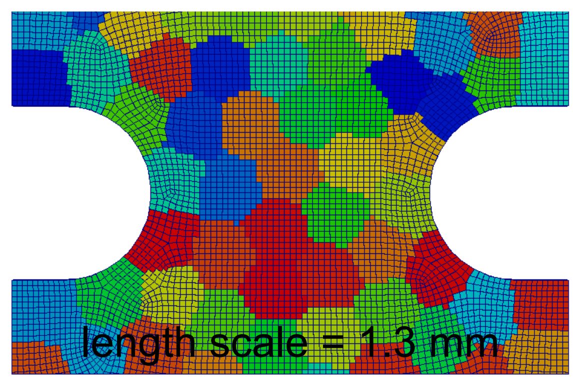


- *Geometric and graph-based partitioners are not adequate*
- *Using these methods outside space of applicability*
- *Domains must have common volume and be isotropic*
- *Boundary volumes can be critical to crack initiation*
- *Consider Centroidal Voronoi Tesselation (Burkardtetal, 2002)*

- *Create a background grid to establish boundaries of general domain*
- *Employ graph based decomposition algorithms to find an initial guess*
- *Use Lloyd's algorithm to iteratively find CVT – use background grid for clustering*
- *When finished with CVT – find element centroids closest to partition centroids*







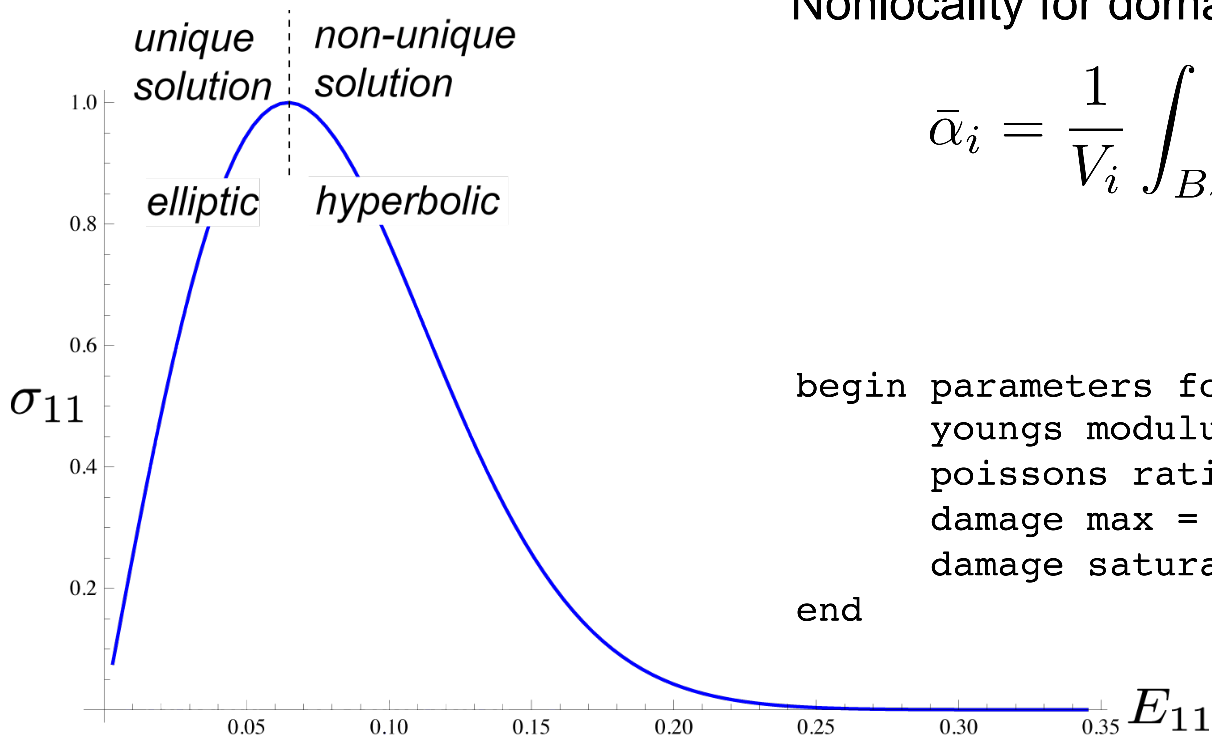
Learn with hyperelastic damage

$$\Psi = \Psi(\boldsymbol{C}, \phi) = (1 - \phi)\Psi_0(\boldsymbol{C})$$

(Holzapfel, Miehe, Simo)

$$\phi = \phi_{max}(1 - \exp(-\alpha/\iota))$$

$$\alpha(t) = \max(\Psi_0)$$



ISV for nonlocality: α

Nonlocality for domain i:

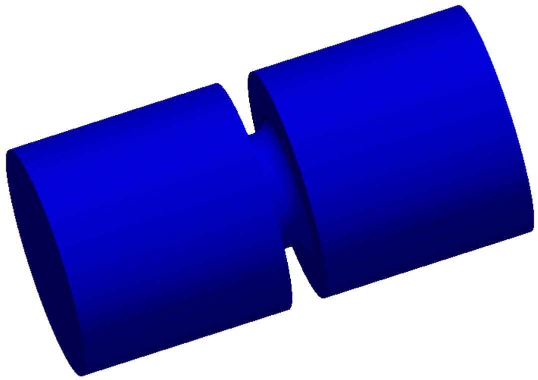
$$\bar{\alpha}_i = \frac{1}{V_i}\int_{B_i} \alpha dV$$

```
begin parameters for model hyperelastic_damage
      youngs modulus = 200e9
      poissons ratio = 0.25
      damage max = 1.0
      damage saturation = 1.0e9
end
```

- Softening causes a transition in the partial differential equation and yields non-uniqueness
- Local material models will yield this behavior for any numerical method

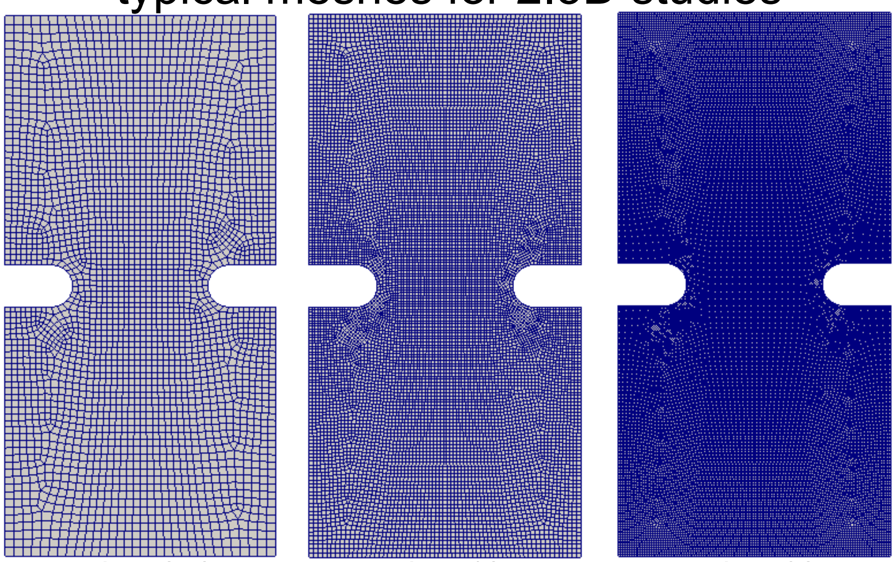
Notched geometries

Motivated to employ the notched bars for characterizing ductile fracture



geometry: notched tension
length: 25.4 mm
diameter: 12.7 mm
notch radius: 0.99 mm

typical meshes for 2.5D studies

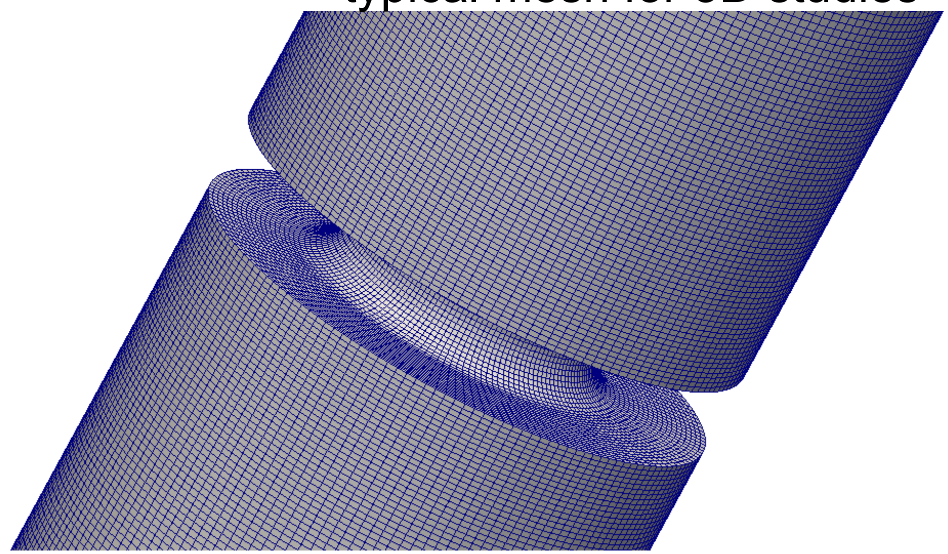


elem. size: 250 μm
nodes: 6,574
elements: 3,150

elem. size: 125 μm
nodes: 25,410
elements: 12,436

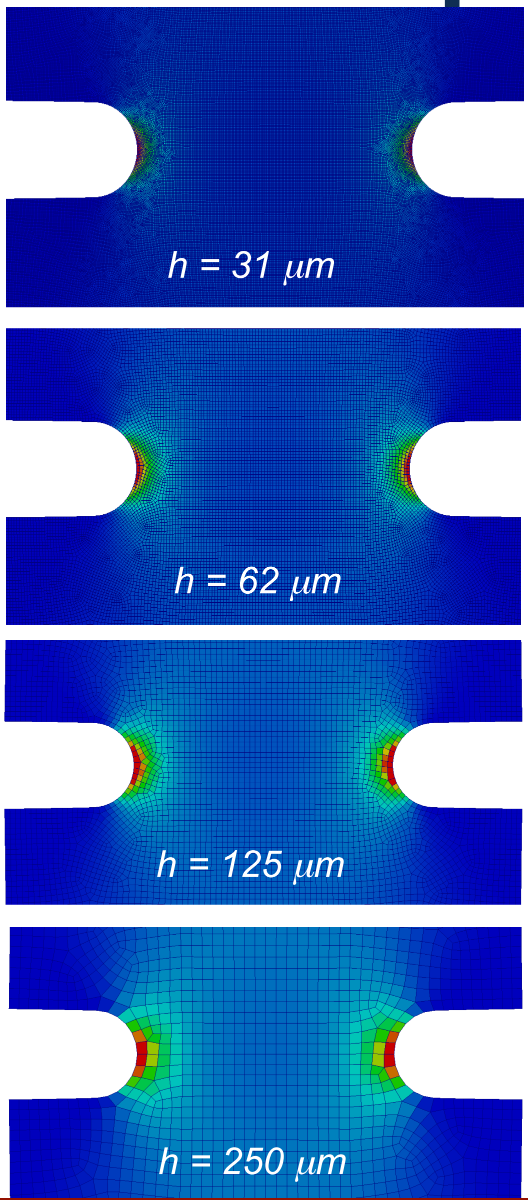
elem. size: 62.5 m
nodes: 100,562
elements: 49,744

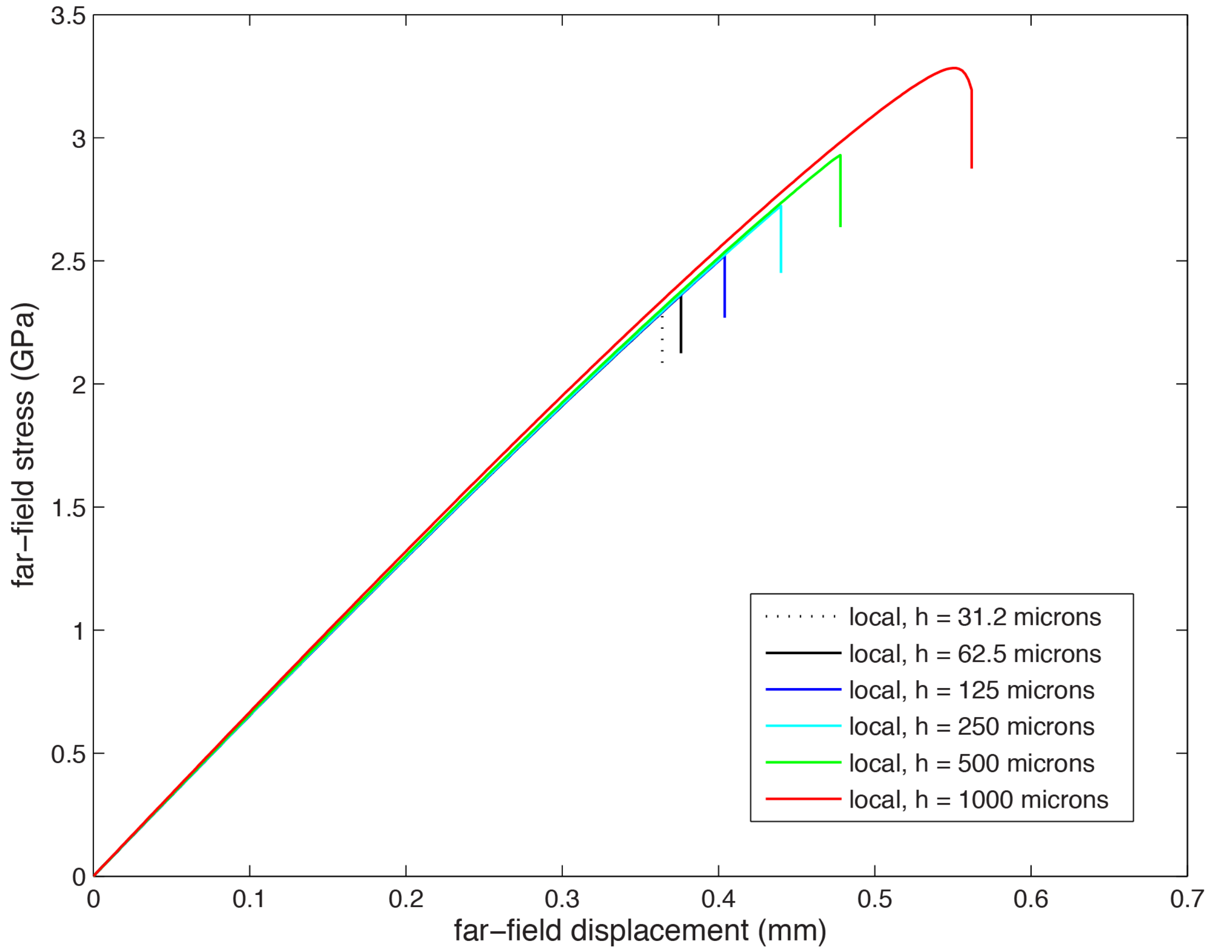
typical mesh for 3D studies



element size: 125 μm
nodes: 807,177
elements: 786,560

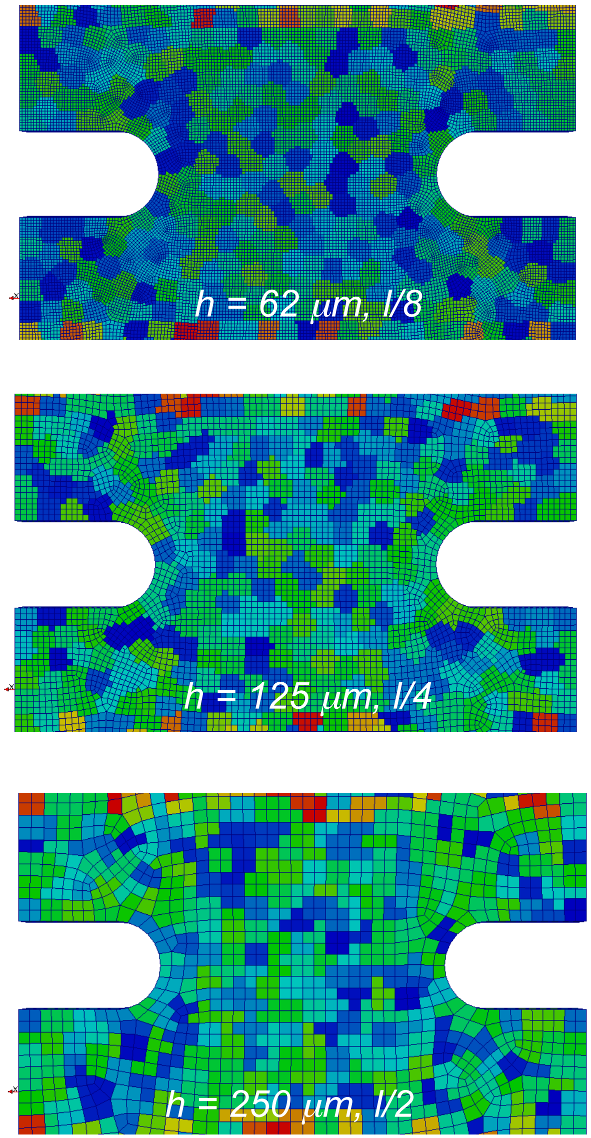
Mesh-dependent local damage

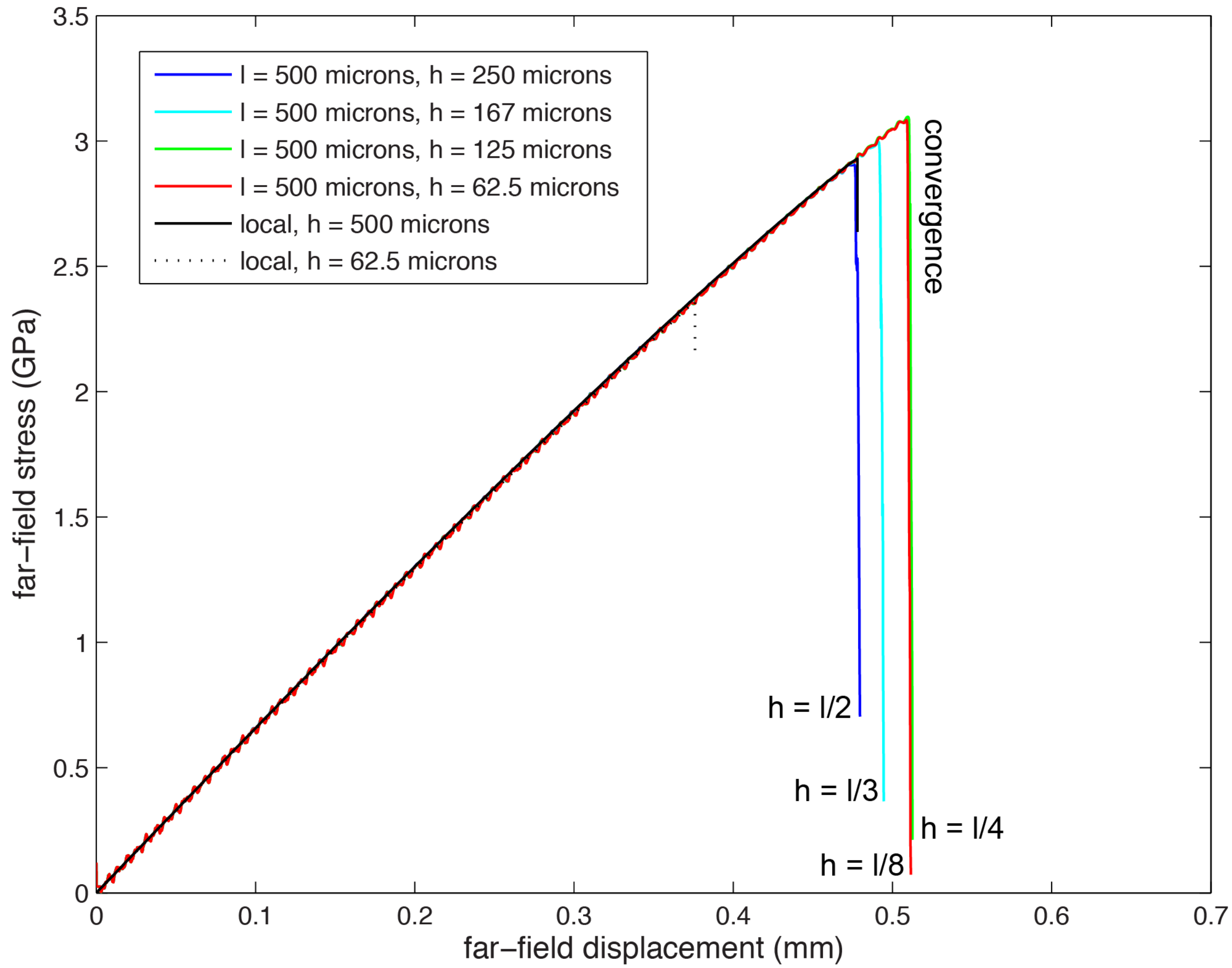




Quasi-statics. The crack nucleation process is unstable. Drop added for visualization. Dynamics employed for solution.

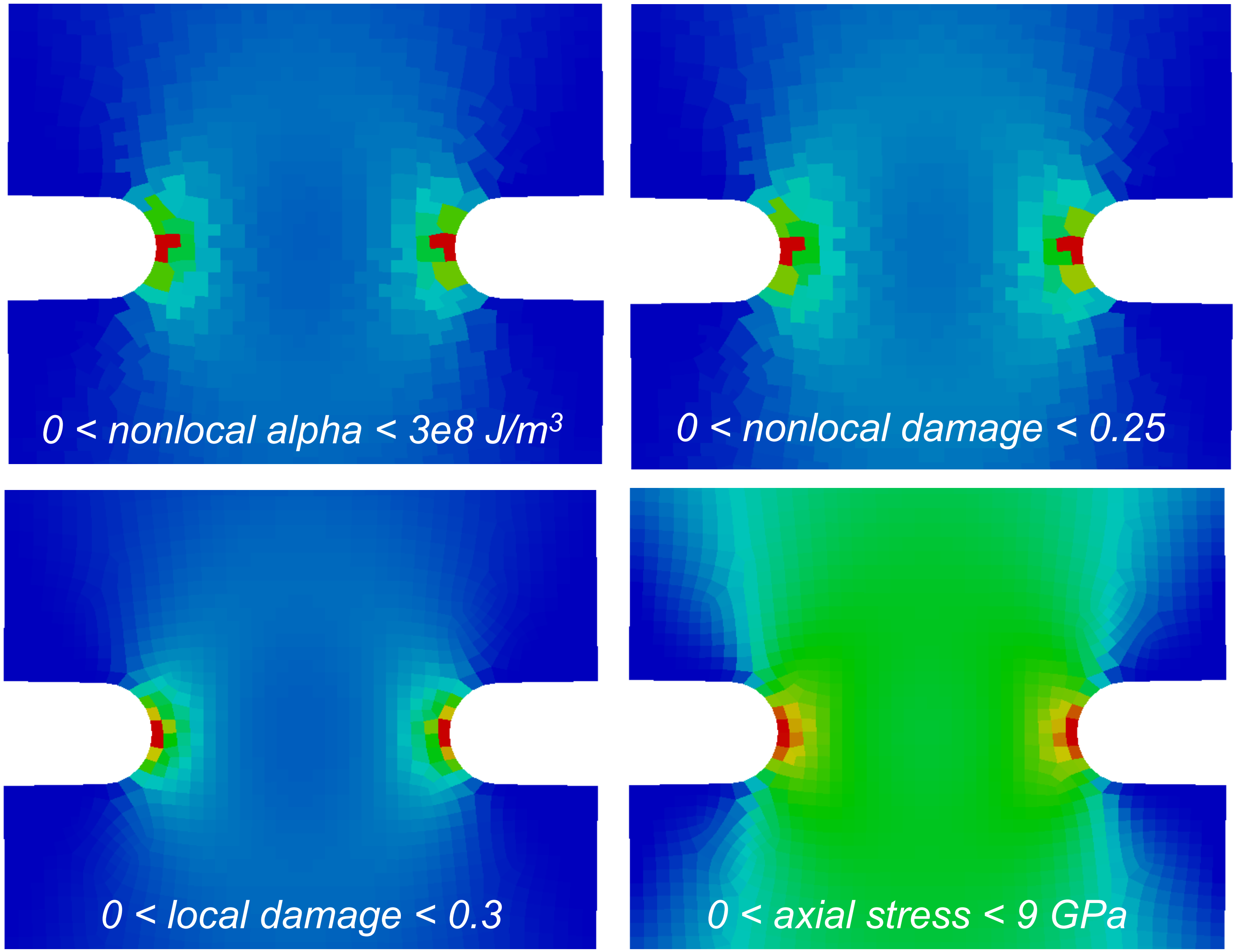
Nonlocality regularizes solution





Nonlocal length scale is 500 μm. Consider element discretizations of 250 μm, 167μm, 125 μm, and 62 μm.

Nonlocality in IVs

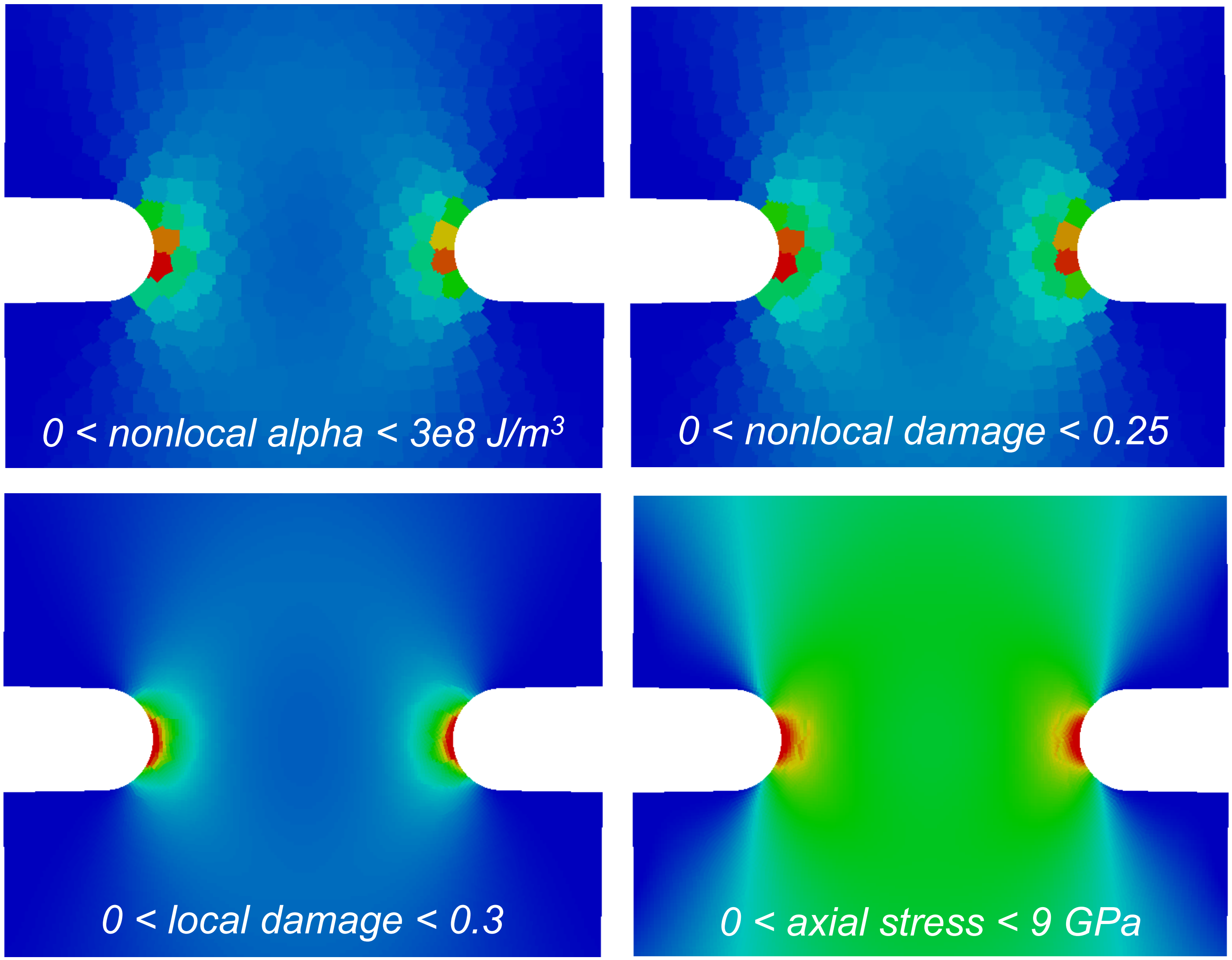


$$\bar{\alpha}_i = \frac{1}{V_i} \int_{B_i} \alpha dV$$

l = 500 μm
h = 250 μm
h = l/2

Converged nonlocality in ISV

$$\bar{\alpha}_i = \frac{1}{V_i} \int_{B_i} \alpha dV$$



l = 500 μm
h = 62 μm
h = l/8

Length scale governs nucleation

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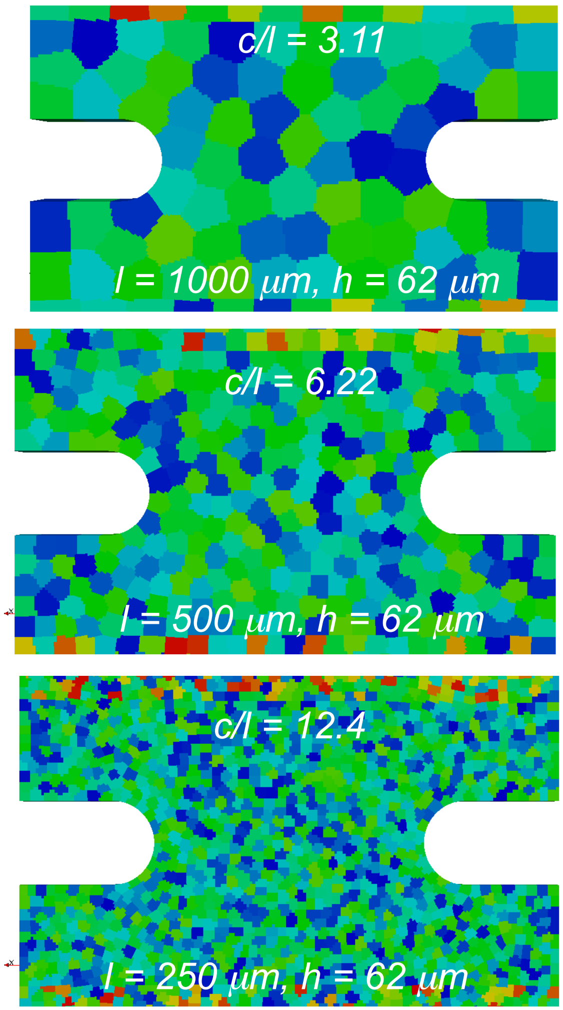

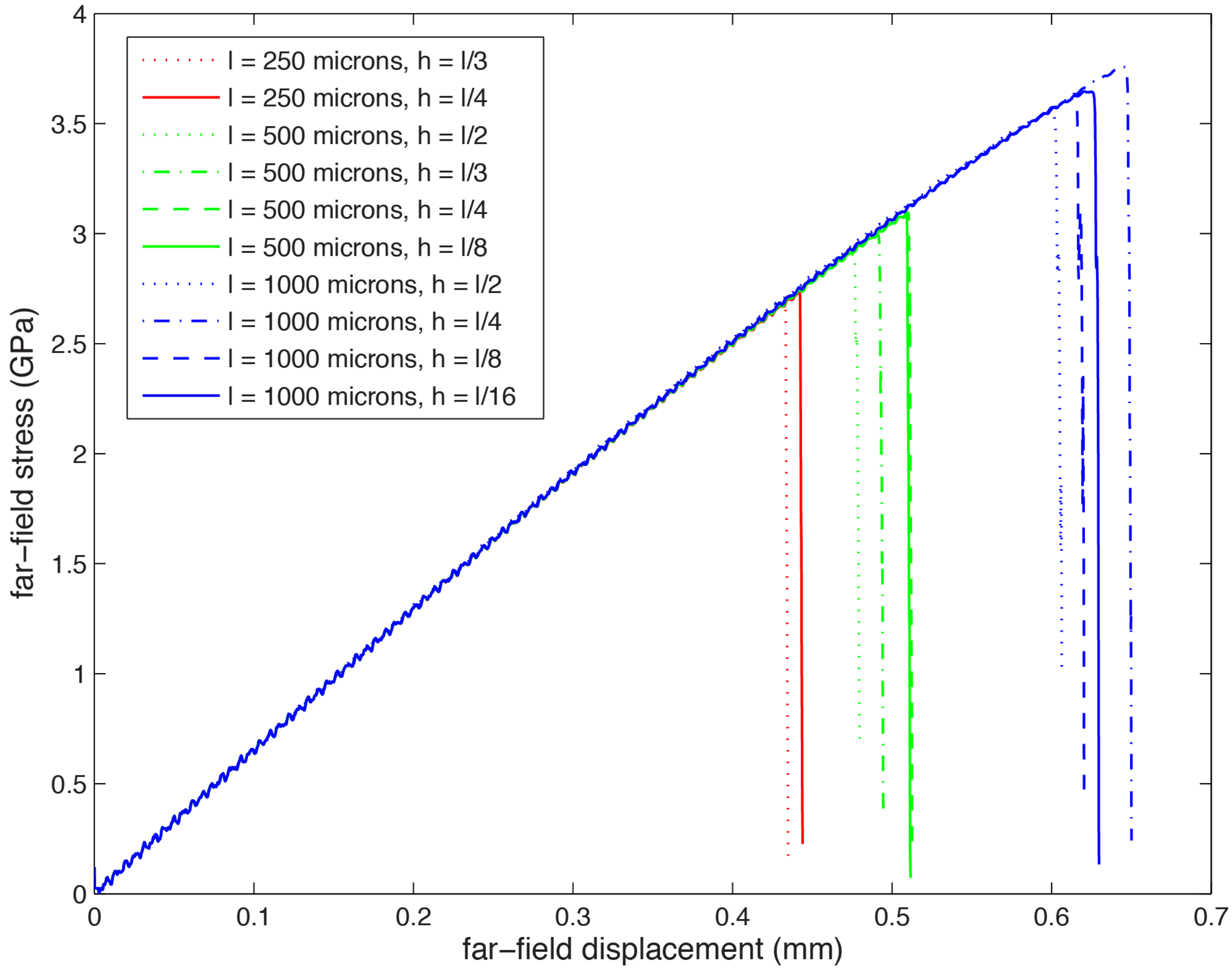

radius of notch, r: 991 μm
arc length of notch, c : 3112 μm

Nonlocal length scale l governs crack nucleation. Variability increases as l approaches geometric dimensions of body. *More work needed.*

Nucleation in 3D

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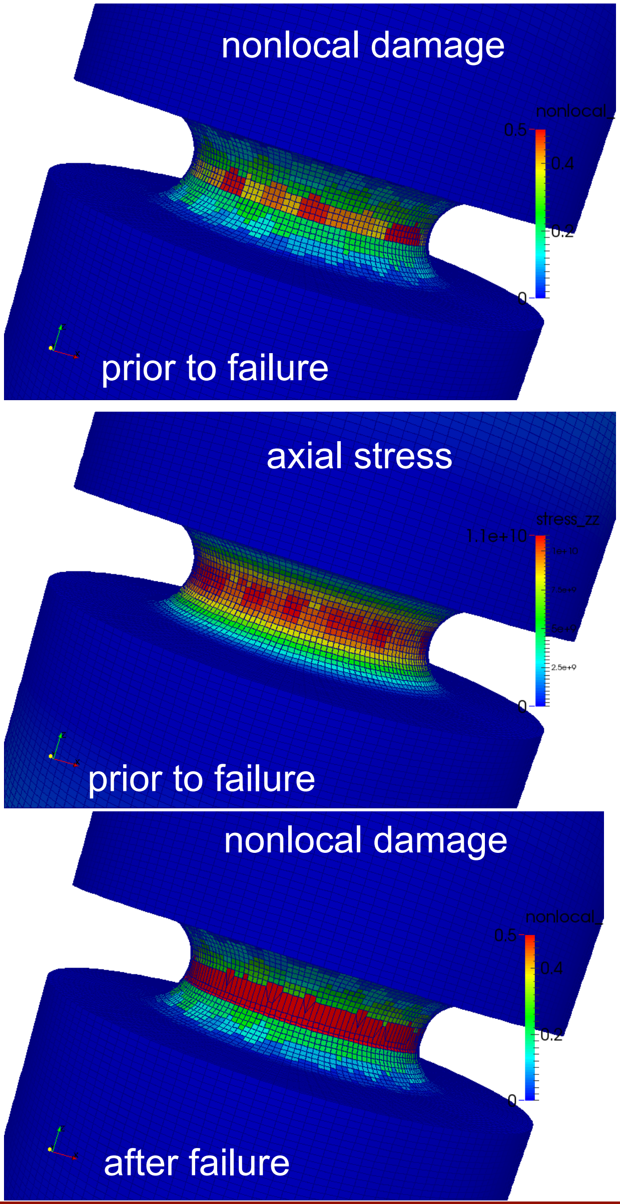
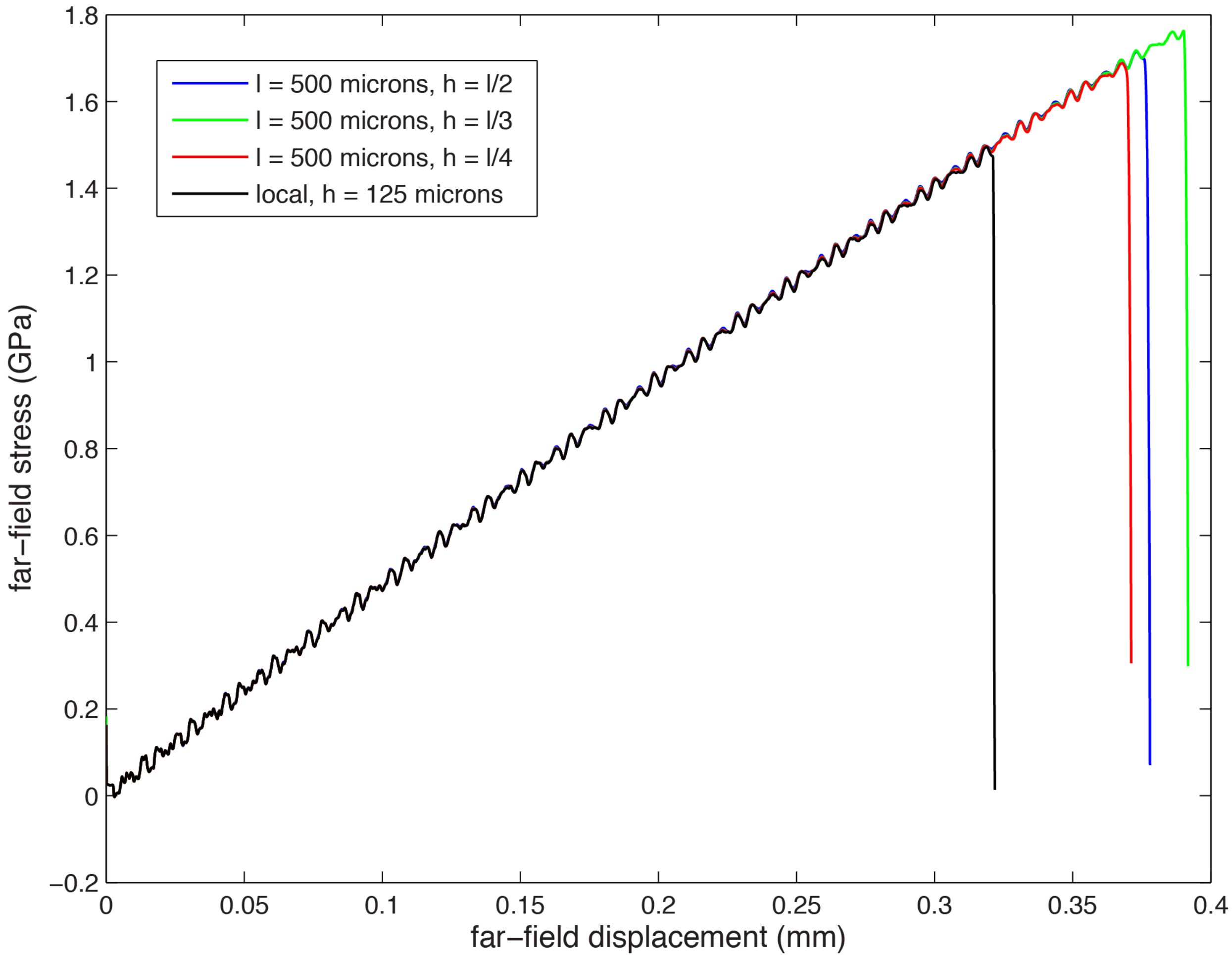




Larger simulations are forthcoming to examine convergence.
Debugging many processor simulations.

Conclusions

- *Employ the micromechanics dictated by the dominant mechanism*
- *Variational nonlocal method convergent – effective for regularization*
- *Future work will consider void growth in ductile metals*
- *Derived naturally from variational principle.*
- *Strong connection to gradient methods.*
- *No special boundary considerations.*
- *Simple form with unit interpolation functions.*

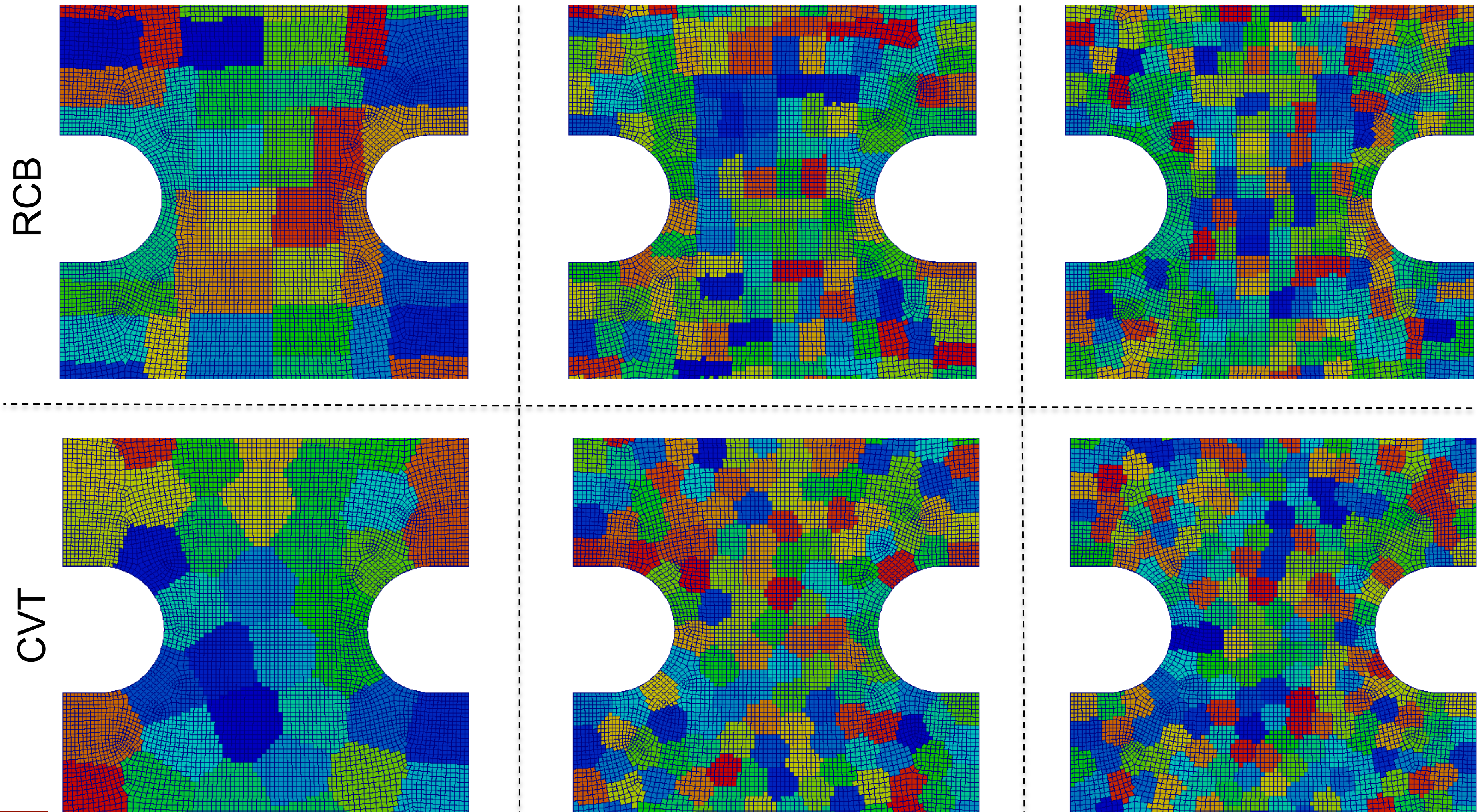
```
begin parameters for block block_1
      material simo
      solid mechanics use model hyperelastic_damage
      section = solid_1
      nonlocal regularization on alpha with length scale = 0.0005
      nonlocal regularization partitioning scheme = kmeans
      nonlocal regularization kmeans cell size = 0.00005
      nonlocal regularization kmeans maximum iterations = 128
      nonlocal regularization kmeans tolerance = 0.1 # percentage of cell size
end parameters for block block_1
```

Acknowledgments: *This works was partially funded by the DOD Joint Munitions Program.* Many thanks to the Sierra Code Team & Devin O'Connor (Northwestern). Devin investigated the weaknesses of currently available domain decomposition algorithms.

EXTRA SLIDES

Focus on a length scale

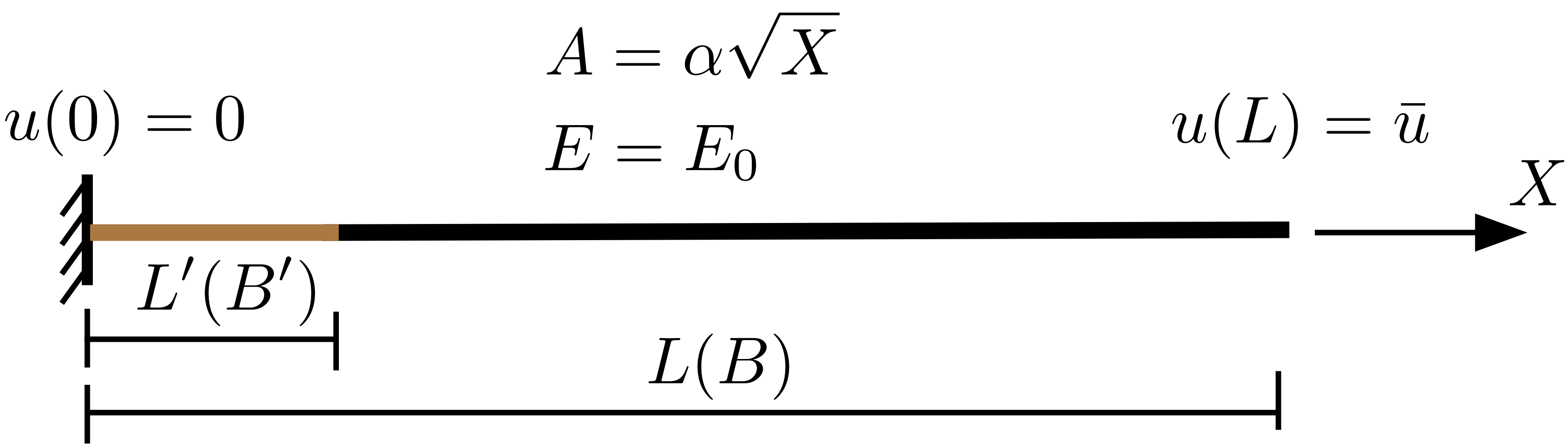
Centroidal voronoi tesselation (CVT) is independent of discretization – looks good.



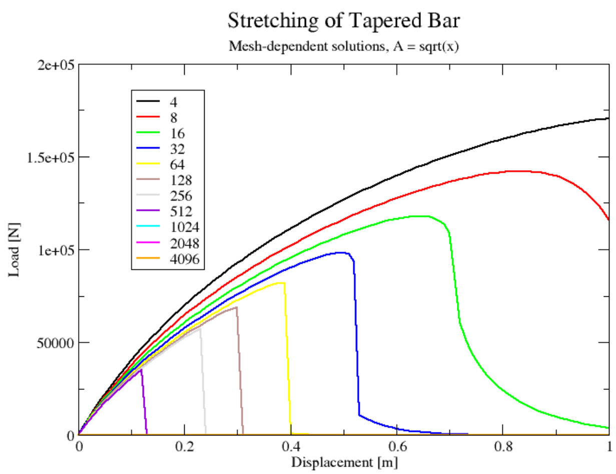
l_c= 2.0 mm, h = 125 μm | l_c= 1.0 mm, h = 125 μm | l_c= 660 μm, h = 125 μm

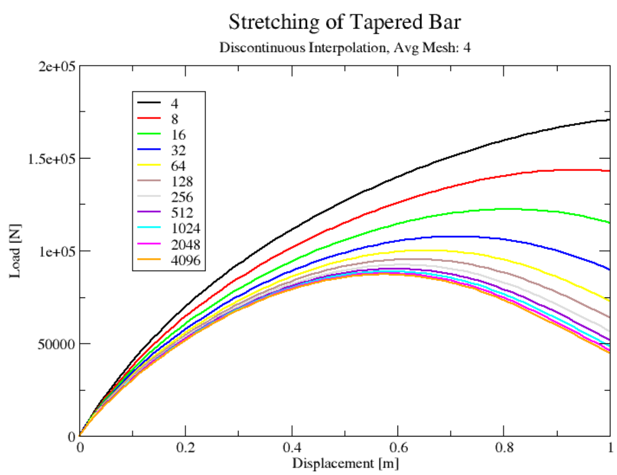
Example: Foulk's Singular Bar

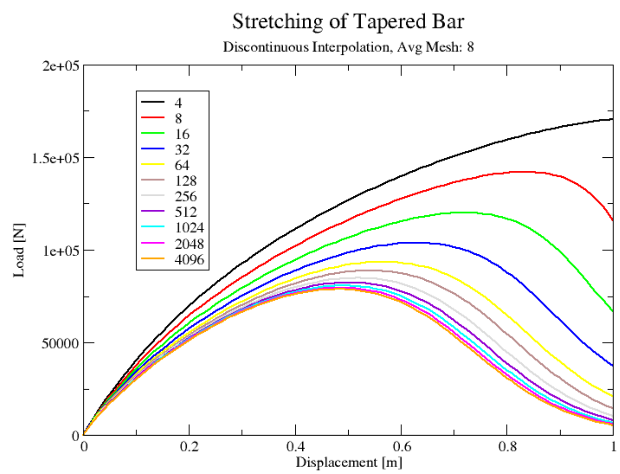
- 1D Proof of concept problem.
- Area proportional to square root of length.
- Strong singularity on left end of bar.
- Simple hyperelestic model with damage.
- Code written in Matlab.

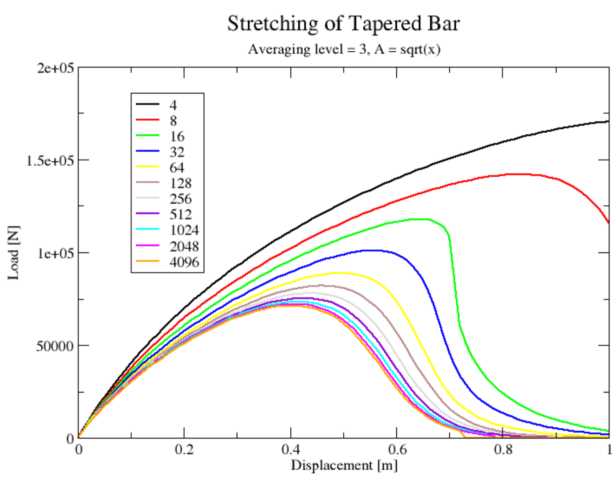


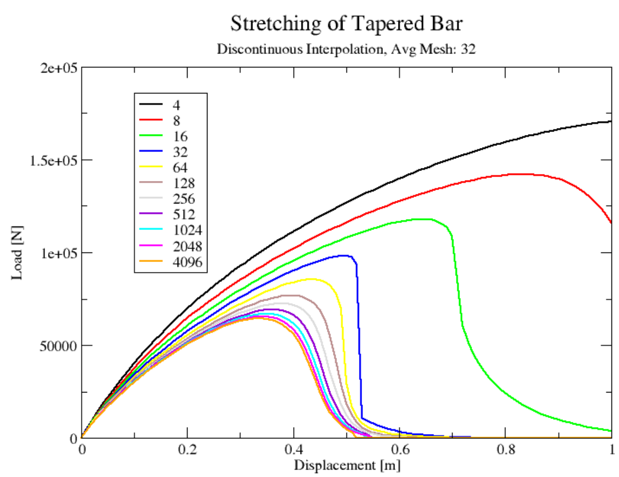
Constant Unit Interpolation

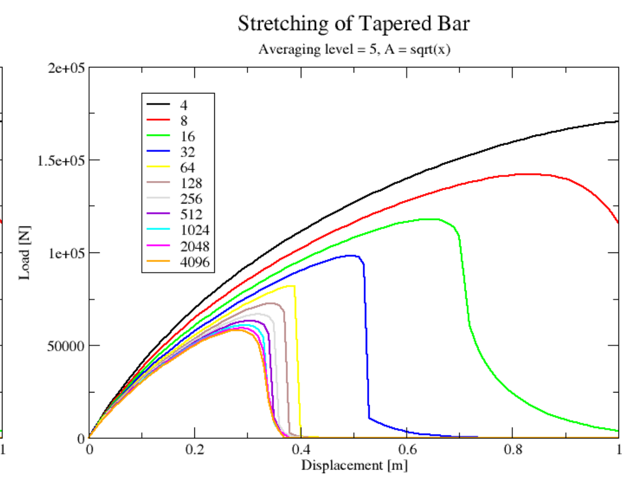












Mesh Dependence

Simple finite-deformation elastic model with damage:

$$W(\boldsymbol{C}, \zeta) = (1-\zeta) W_0(\boldsymbol{C})$$

$$\boldsymbol{\epsilon} = \frac{1}{2}\log(\boldsymbol{C})$$

$$\bar{\boldsymbol{\epsilon}} = \mathrm{dev}(\boldsymbol{\epsilon}), \quad \theta = \mathrm{tr}(\boldsymbol{\epsilon}),$$

$$W_0(\boldsymbol{C}) = W_0^{\mathrm{vol}}(\theta) + W_0^{\mathrm{dev}}(\bar{\boldsymbol{\epsilon}}),$$

$$W_0^{\mathrm{vol}}(\theta) = \frac{\kappa}{4}\left[\exp(2\theta) - 1 - 2\theta\right],$$

$$W_0^{\mathrm{dev}}(\bar{\boldsymbol{\epsilon}}) = \frac{\mu}{2}\left[\mathrm{tr}(\exp\bar{\boldsymbol{\epsilon}}) - 3\right].$$

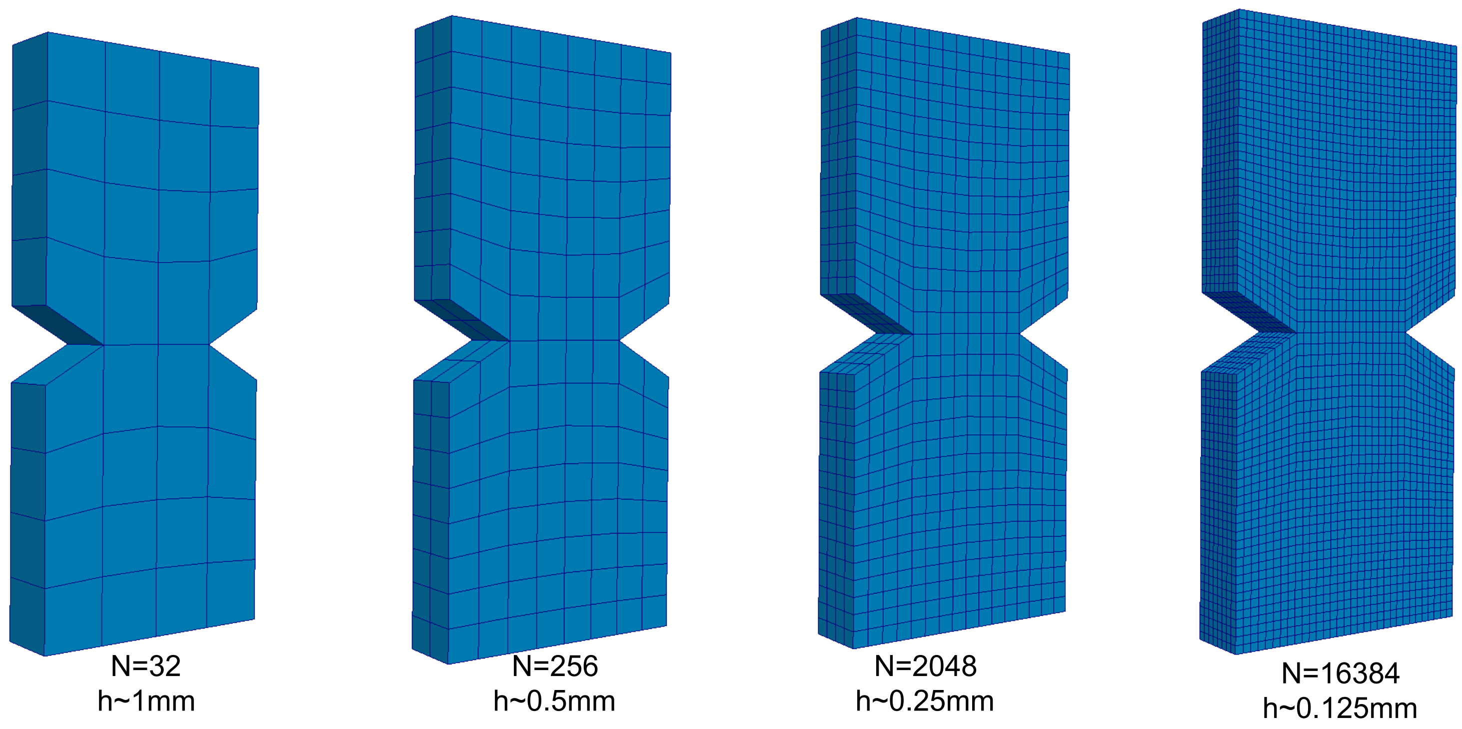
$$\zeta(\alpha) := \zeta_\infty[1 - \exp(-\alpha/\iota)]$$

$$\alpha(t) := \max_{s\in[0,t]} W_0(s)$$

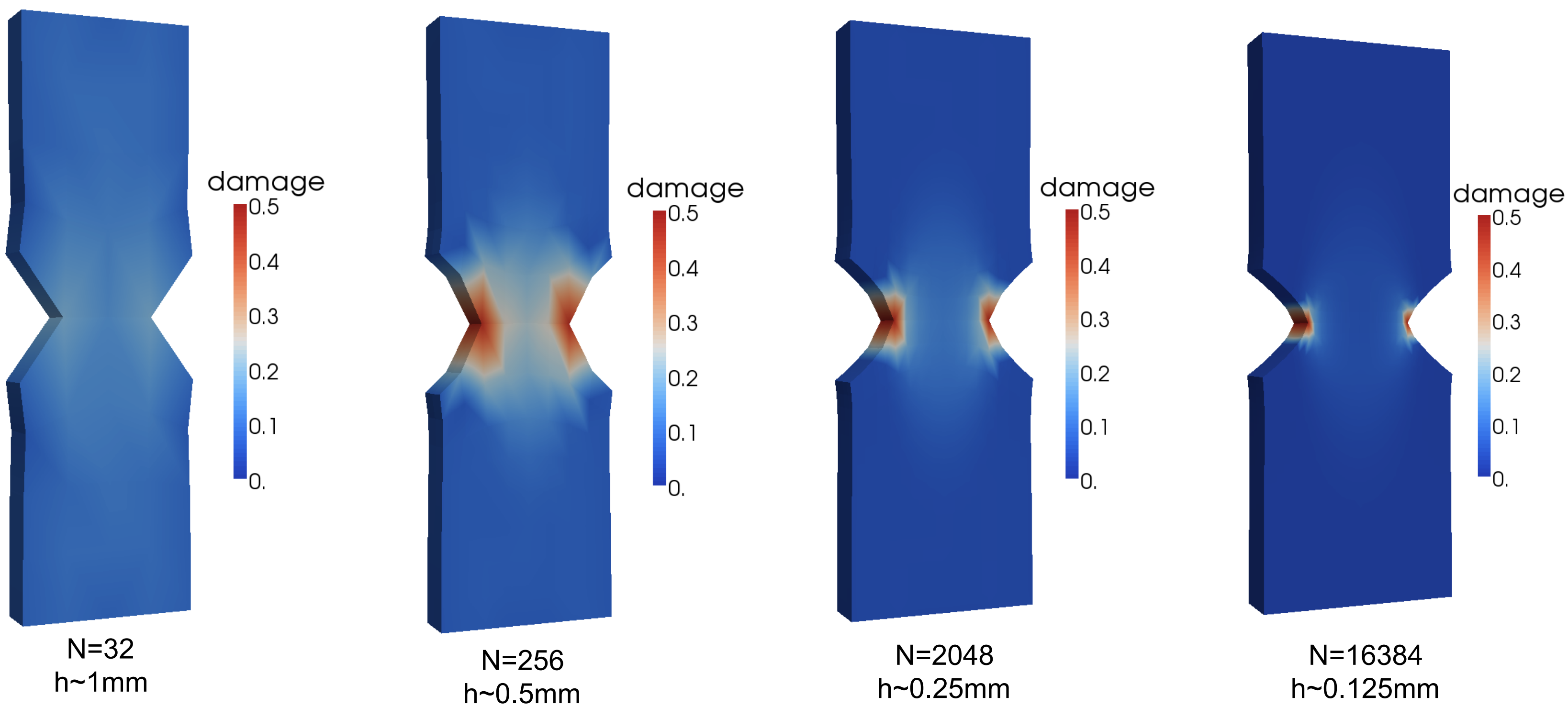
ζ_∞: maximum possible damage

ι: damage saturation parameter

$$E = 200\mathrm{GPa}$$
$$\nu = 0.25$$
$$\kappa = 133\mathrm{GPa}$$
$$\mu = 67\mathrm{GPa}$$
$$\zeta_\infty = 1.0$$
$$\iota = 100\mathrm{GJm}^{-3}$$

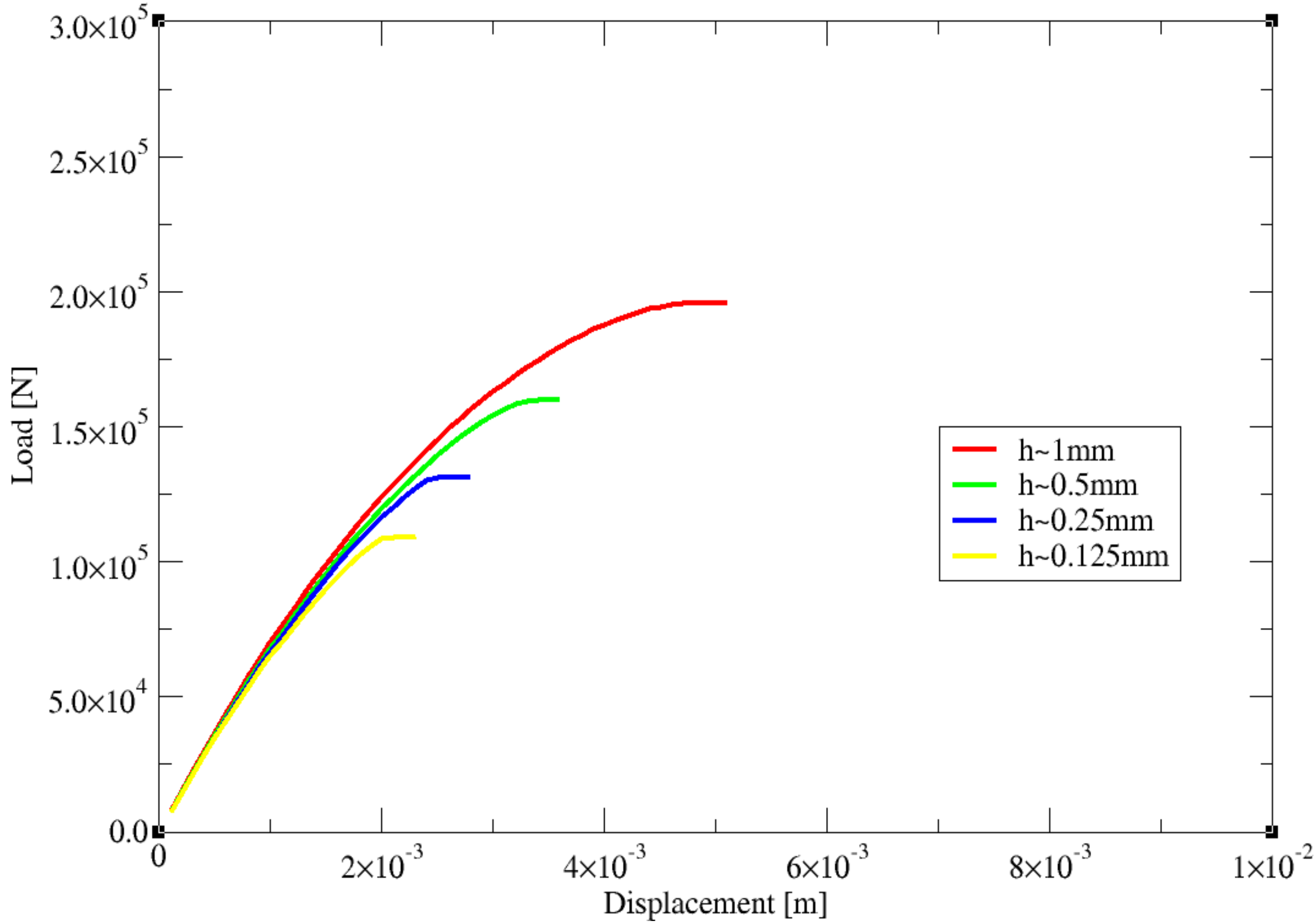


Mesh Dependence



Damage

Mesh Dependence



Load - Displacement

Implementation

$$\bar{\boldsymbol{Y}} = \frac{1}{\mathrm{vol}(D)} \int_D \boldsymbol{Y}\; dV,$$

$$\bar{\boldsymbol{Z}} = \frac{1}{\mathrm{vol}(D)} \int_D \boldsymbol{Z}\; dV,$$

$$\mathrm{vol}(\bullet) := \int_{(\bullet)} dV,$$

Constant interpolation leads to simple averaging:

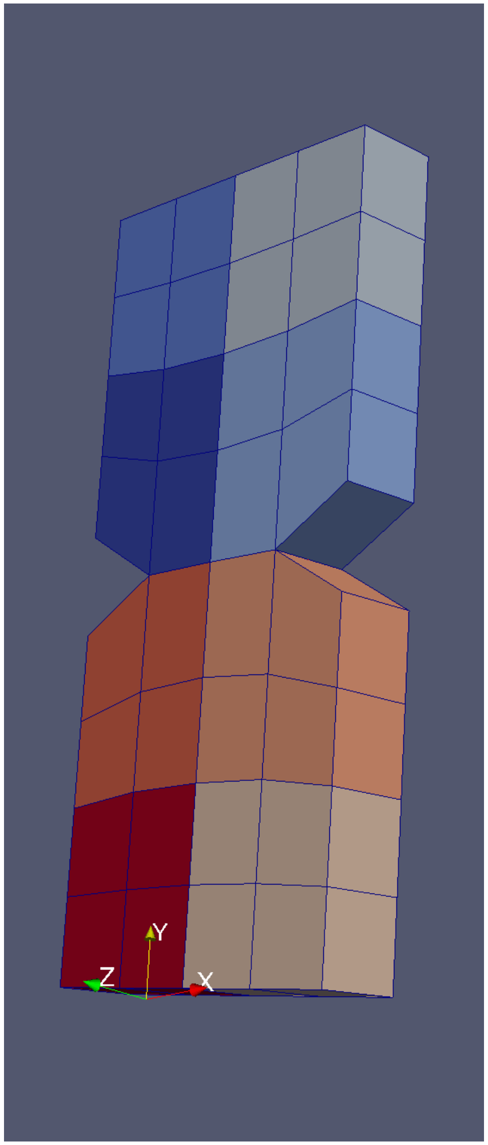
$$\mathrm{vol}(D) = \sum_{i=0}^{n} \mathrm{vol}(E_i),$$

$$\int_D \boldsymbol{Y}\; dV = \sum_{i=0}^{n} \int_{E_i} \boldsymbol{Y}\; dV,$$

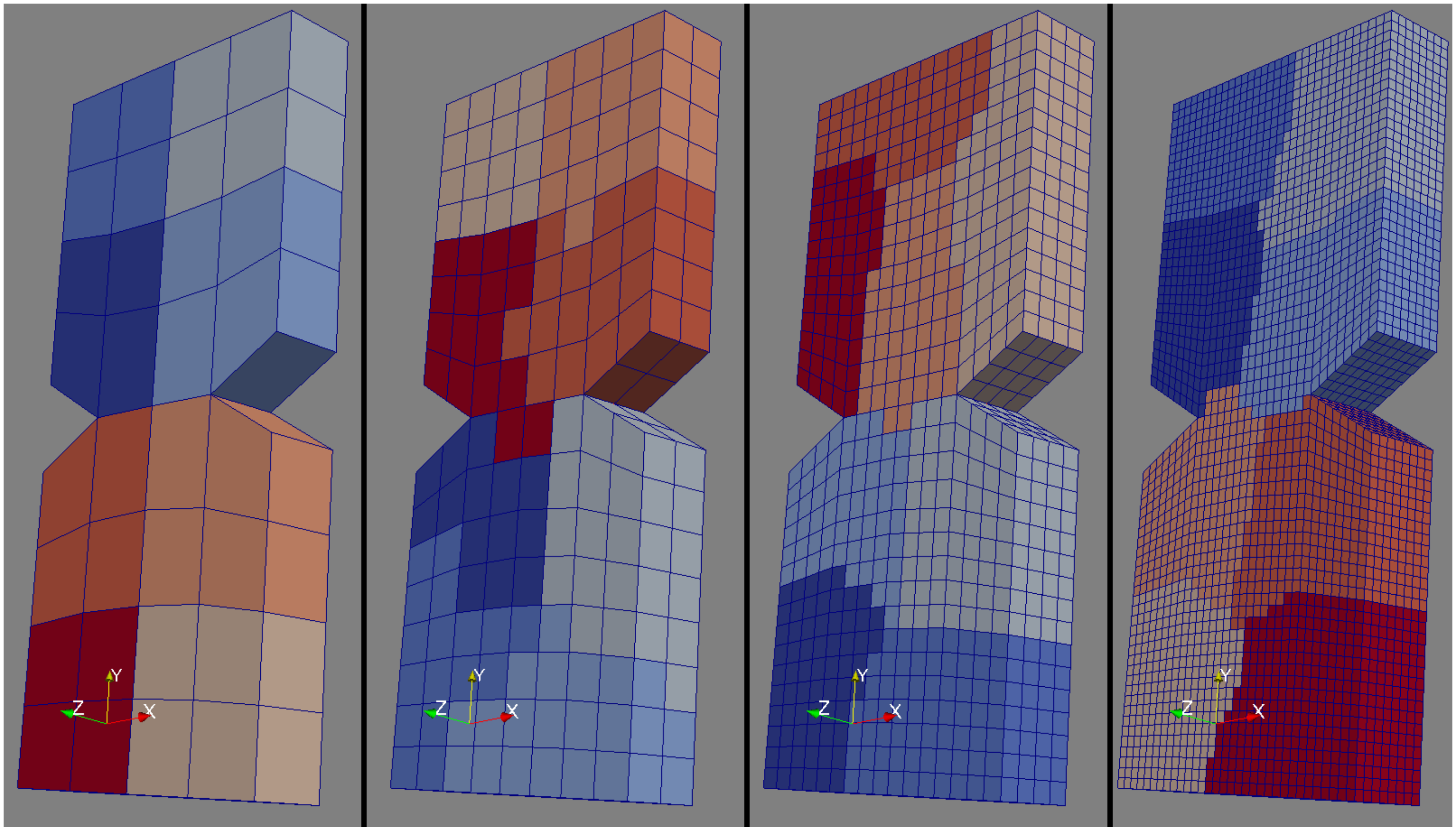
$$\int_D \boldsymbol{Z}\; dV = \sum_{i=0}^{n} \int_{E_i} \boldsymbol{Z}\; dV.$$

Use Zoltan to create domains *D*

vol(*D*)=(lengh scale)^3=(1.6mm)^3



Partitions



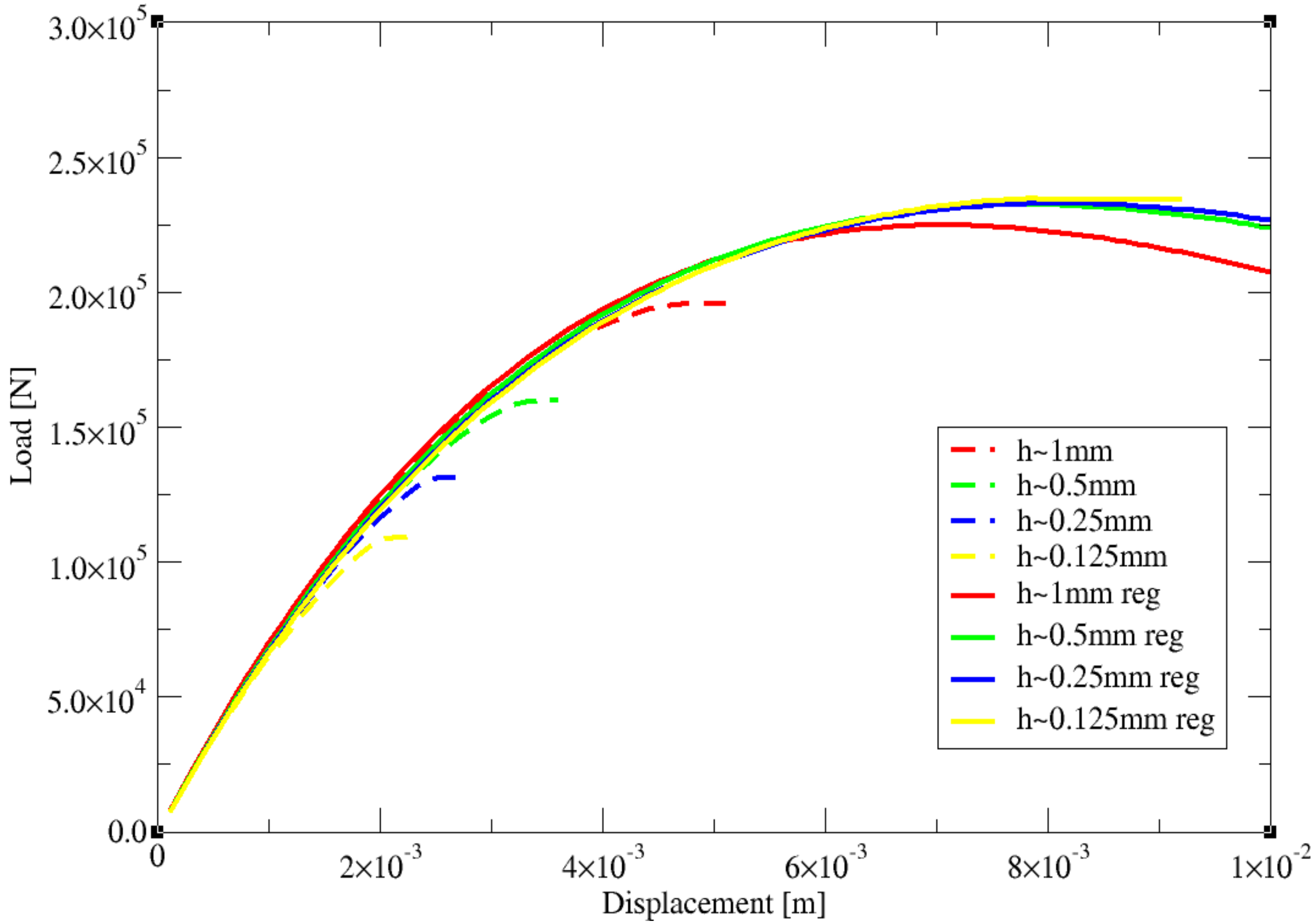
N=32
h~1mm

N=256
h~0.5mm

N=2048
h~0.25mm

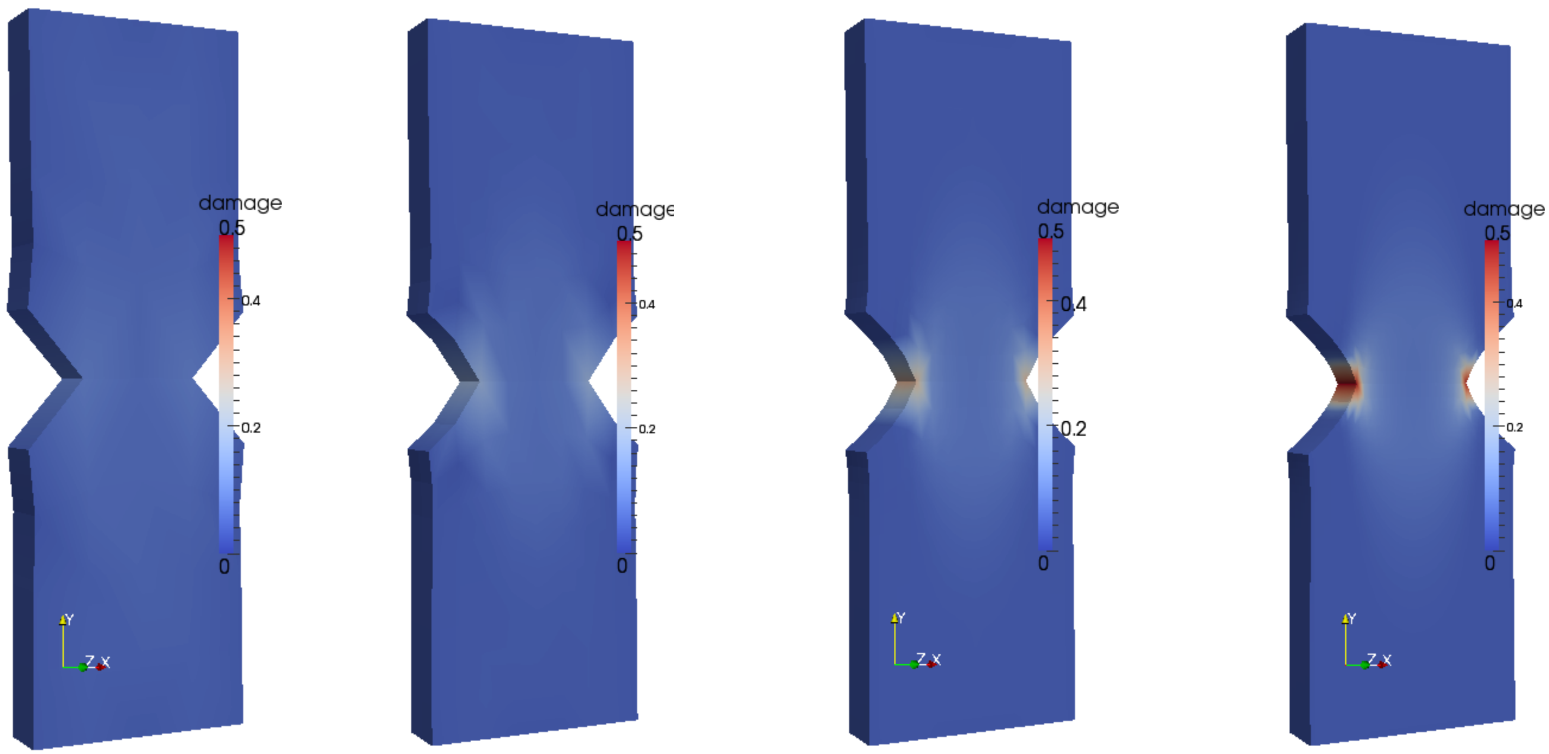
N=16384
h~0.125mm

Regularized Solution



Load - Displacement

Regularized Solution



N=32
h~1mm

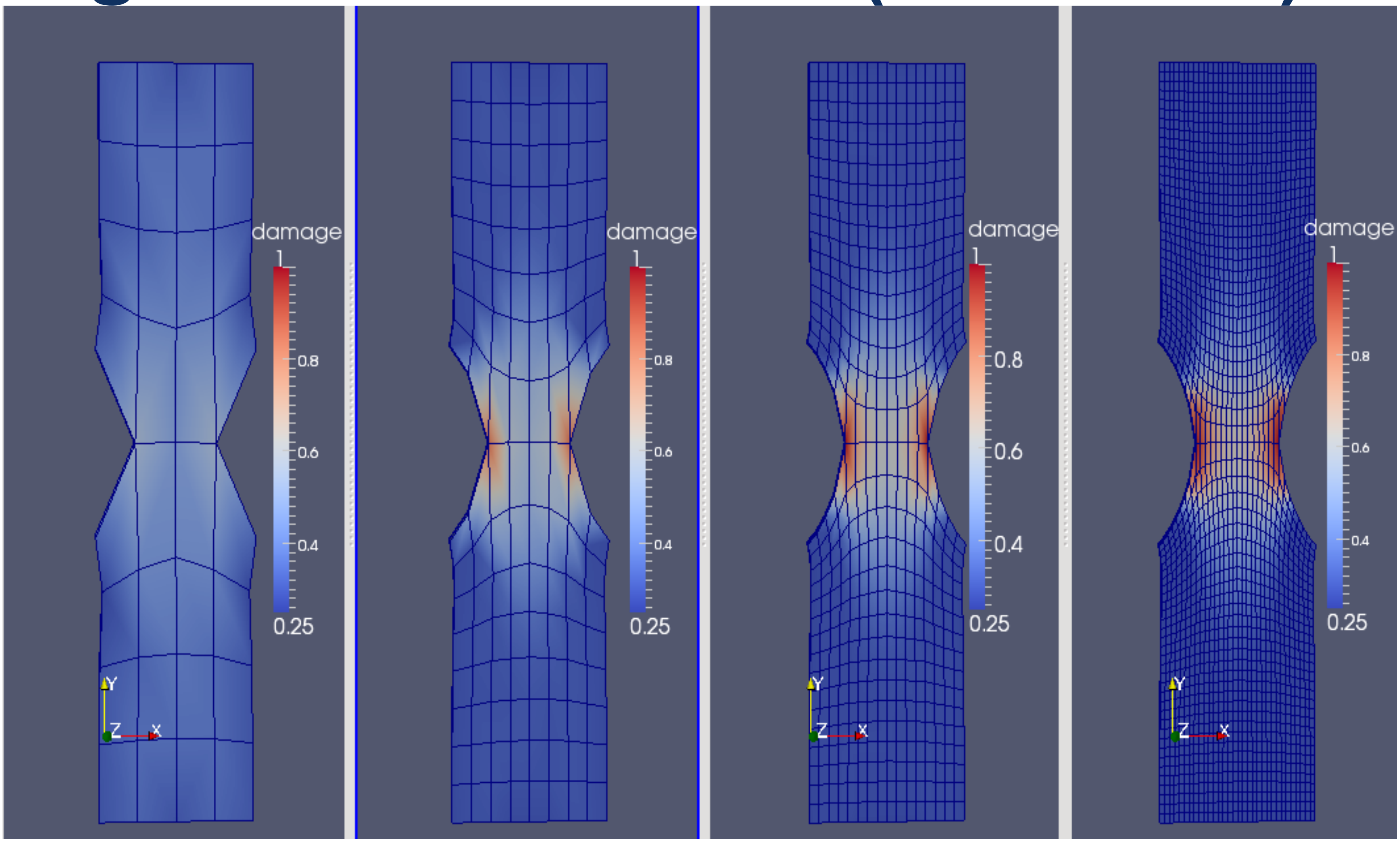
N=256
h~0.5mm

N=2048
h~0.25mm

N=16384
h~0.125mm

Damage

Regularized Solution (deformed)



N=32
h~1mm

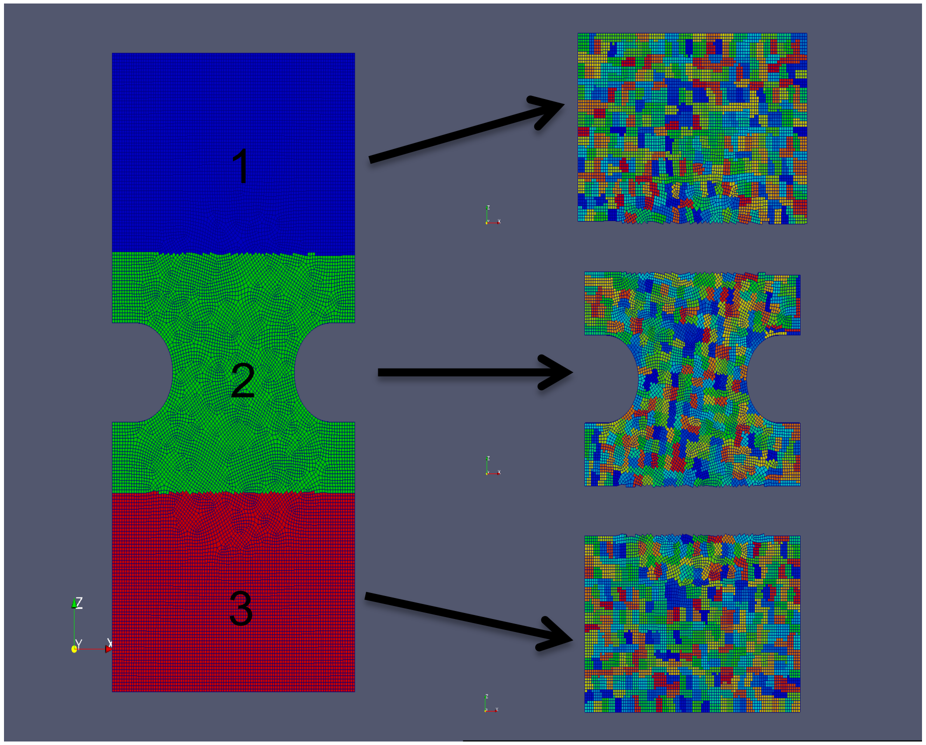
N=256
h~0.5mm

N=2048
h~0.25mm

N=16384
h~0.125mm

3D Implementation

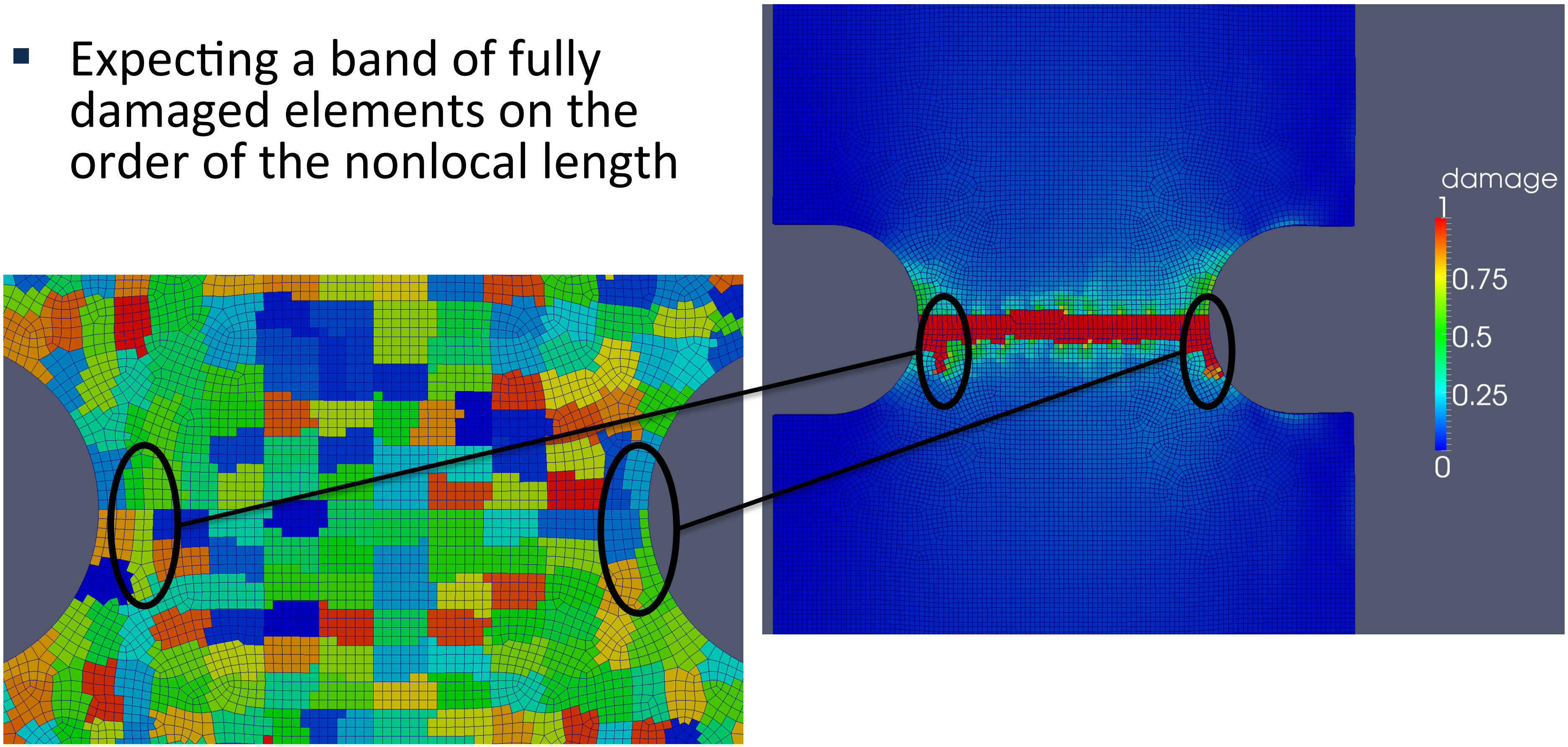
- Sierra Mechanics implementation
  - Regularization parameter and length scale
    - Nonlocal volume
    - Influenced by material (e.g. process zone)
  - Nonlocal partitioning schemes
    - zoltan_RCB, zoltan_RIB, METIS, zoltan_hypergraph
  - Nonlocal domain partitioning procedure
    1. Domain decomposition for parallel computation
    2. On each processor nonlocal domains are created



Nonlocal domain partitioning procedure

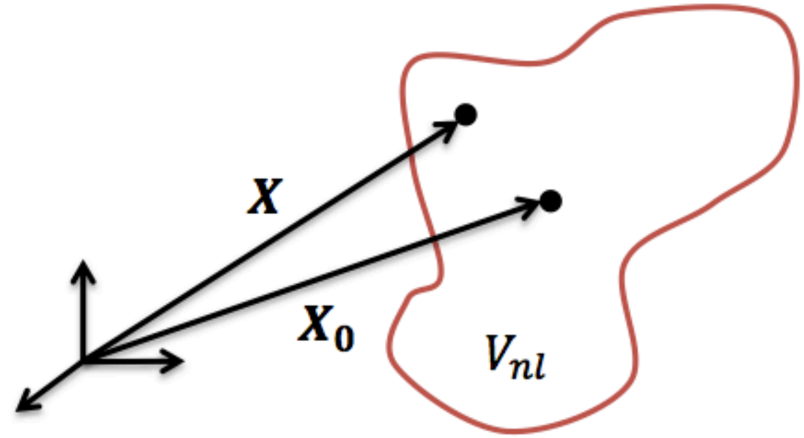
Domain Shape Effect

- Expecting a band of fully damaged elements on the order of the nonlocal length



Domain Shape Quality

- Our current shape quality metric (Aspect Ratio)
  - Division of the largest and smallest eigenvalue of the tensor $H(V_{nl})$
    - $AR = \sqrt{\lambda_{max}/\lambda_{min}}$
  - Script written to calculate AR



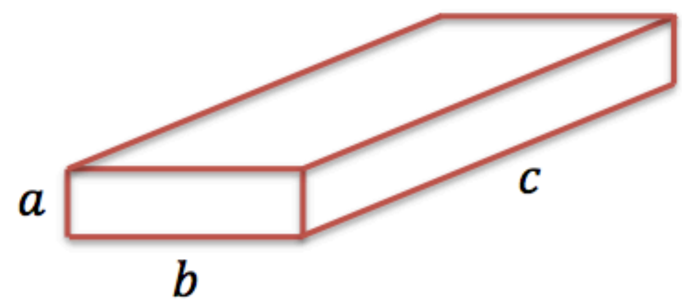
$$H(V_{nl}) = \frac{1}{2V_{nl}} \int (\boldsymbol{X} - \boldsymbol{X_0}) \otimes (\boldsymbol{X} - \boldsymbol{X_0}) dV_{nl}$$

- Example: Plate-like geometry

$$AR = \frac{c}{a}$$

- Example: Sphere

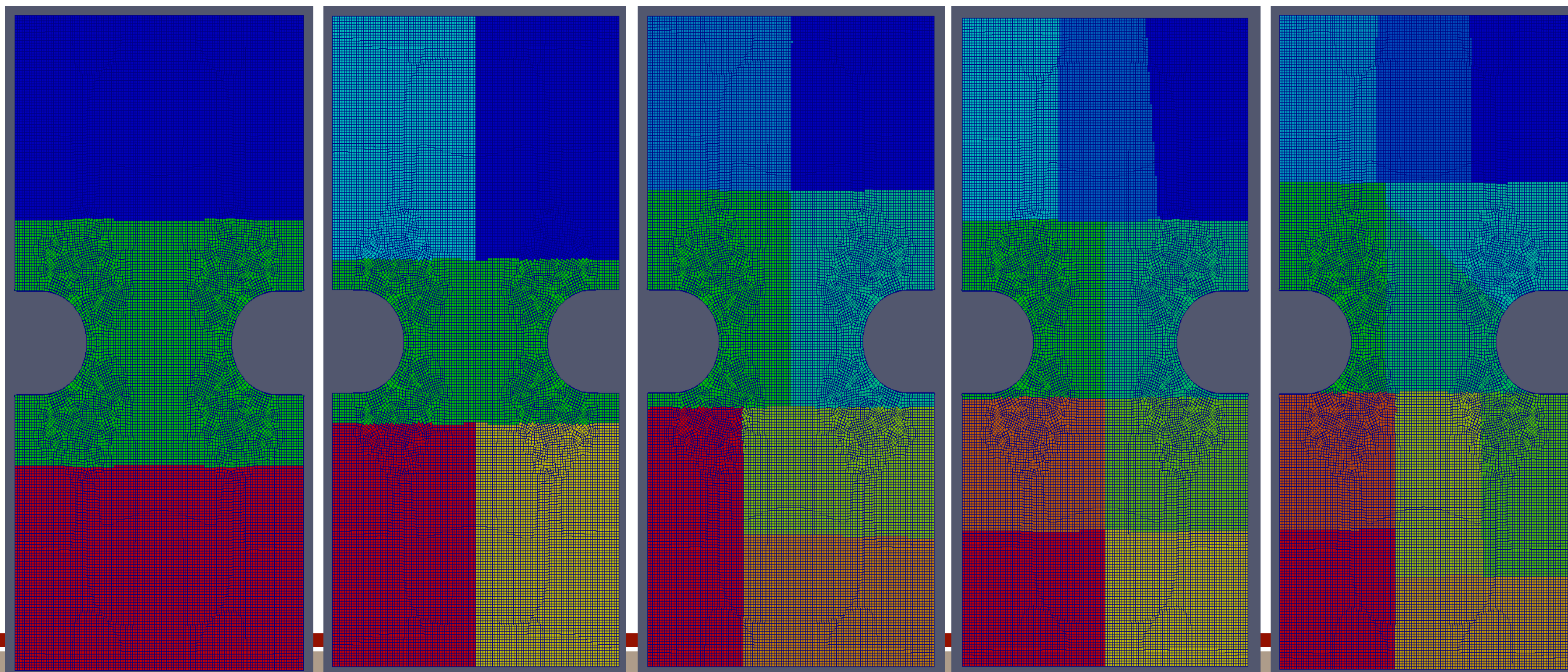
$$AR = 1$$



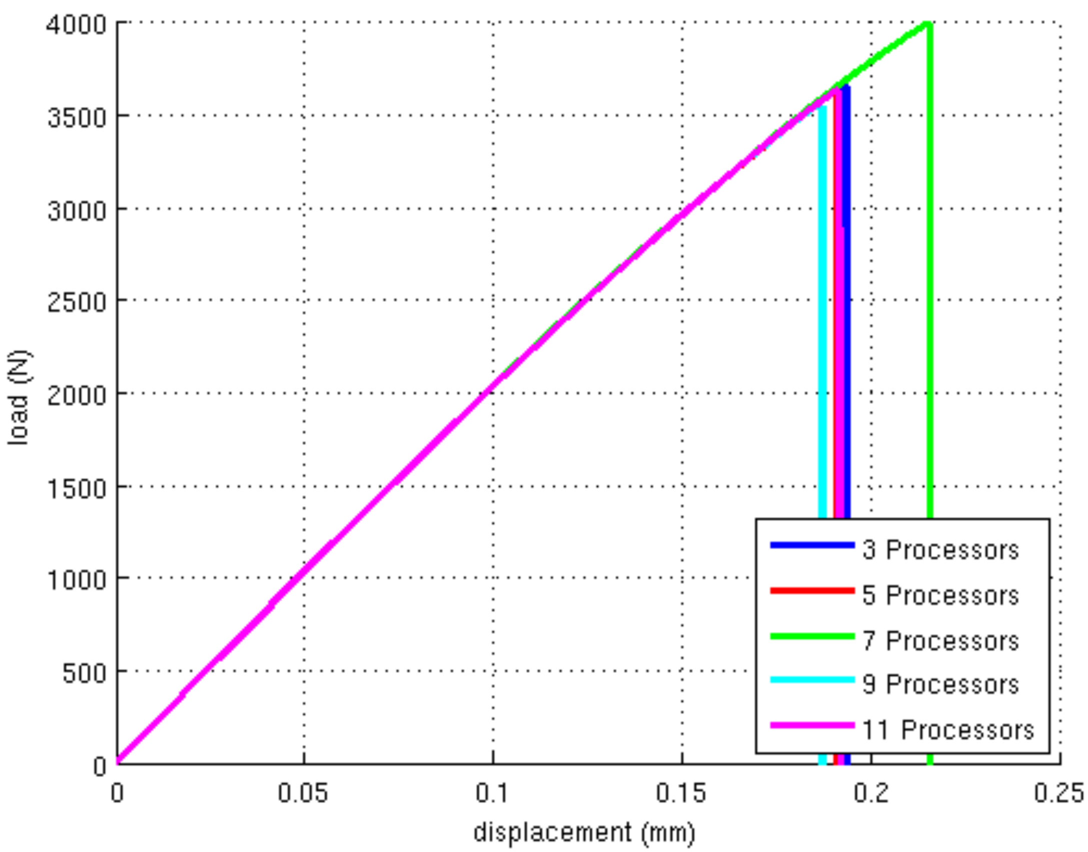
We desire $AR \approx 1$ to ensure the same l_c throughout the domain and good shape quality

Domain Shape Examination

- Domain decomposition for parallel computation
  - 3, 5, 7, 9 and 11 processor runs
- Looking for different nonlocal domain shapes with equivalent volumes



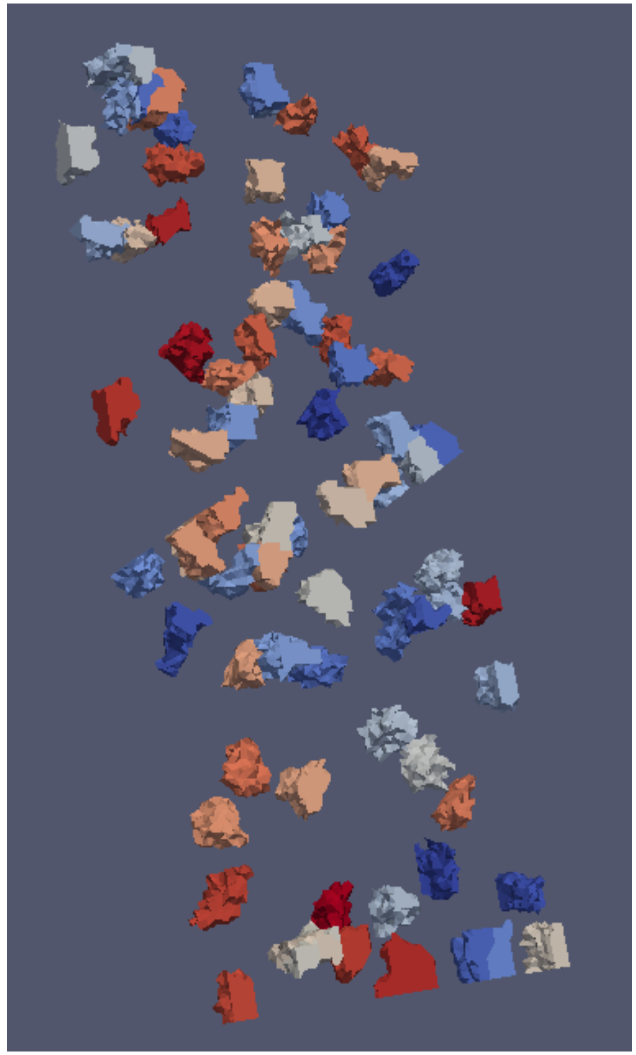
Domain Shape Examination



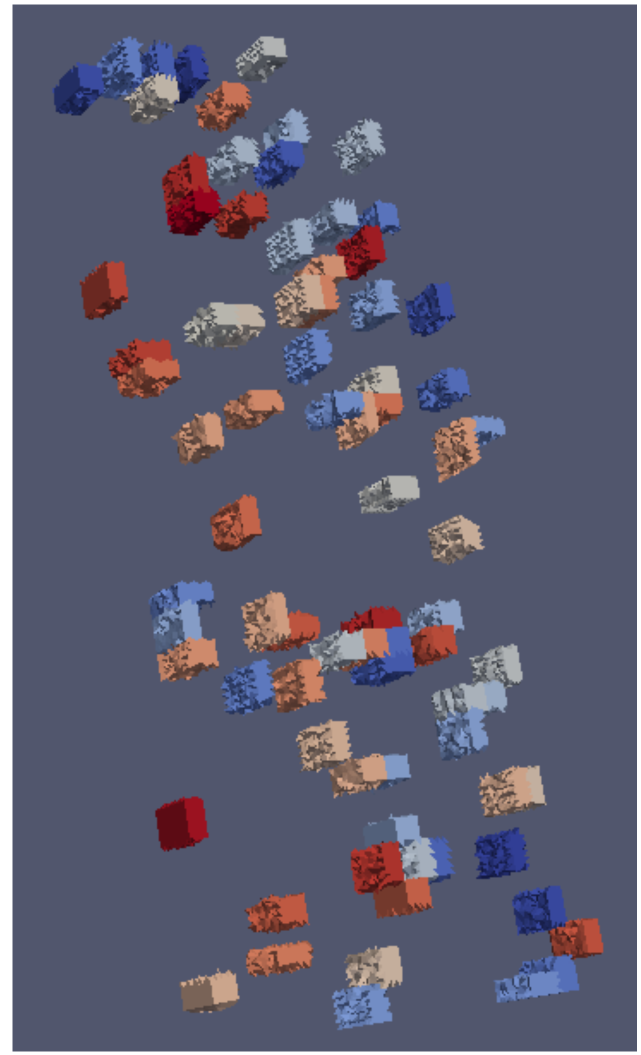
- Effect less pronounced in load displacement curve
- Nonlocal volumes are similar
- Shows importance of shape quality

Improving Domain Shape

- Element Type
  - Tetrahedrons
- Partitioning scheme
  - Hypergraph
  - RCB



Tets: Hypergraph

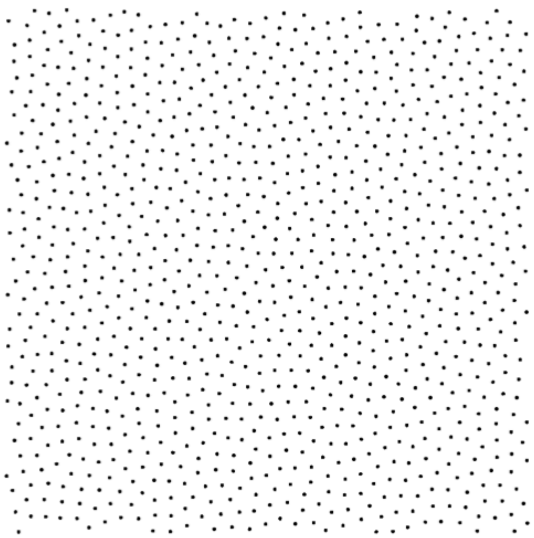


Tets: RCB

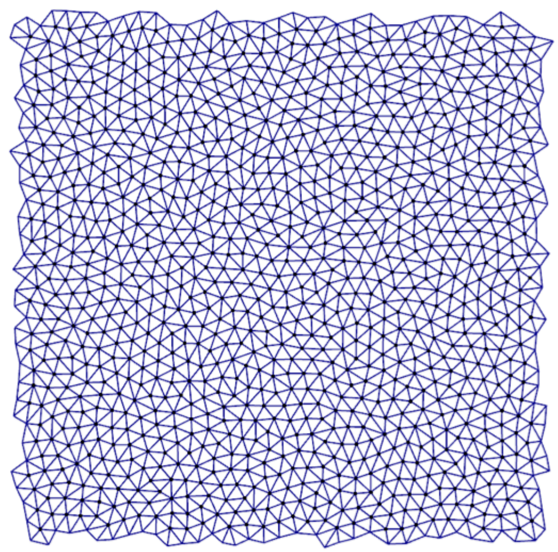
Sandia National Laboratories

Blue Noise

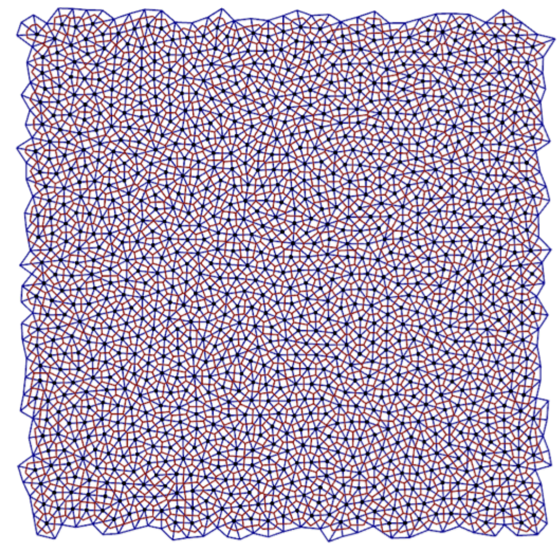
Even, isotropic and unstructured distribution of points (deGoes 2012).



Blue Noise



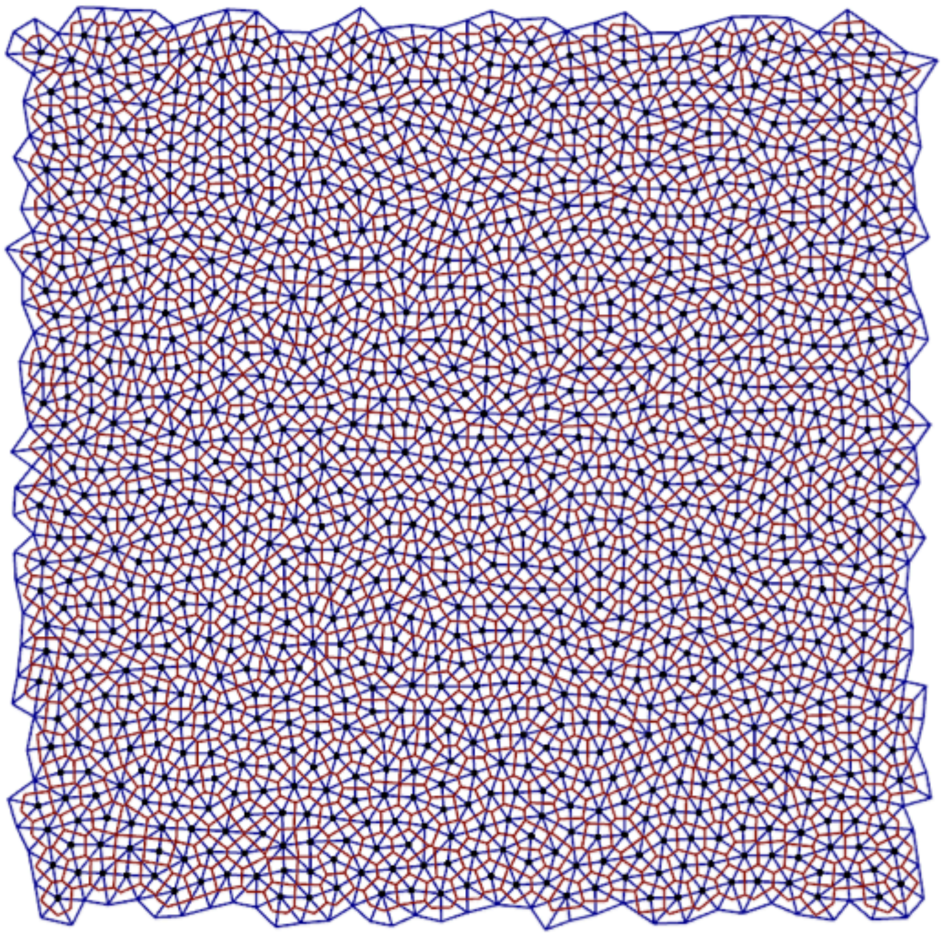
Delauney Mesh



Voronoi Cells

Shape Improved by Blue Noise

Voronoi cells of blue noise are the nonlocal domains.



Conclusions

- Regularization effective.
- Derived naturally from variational principle.
- Strong connection to gradient methods.
- No special boundary considerations.
- Simple form with unit interpolation functions.
- Domain shape is an issue.
- Introduce blue noise for partitioning.