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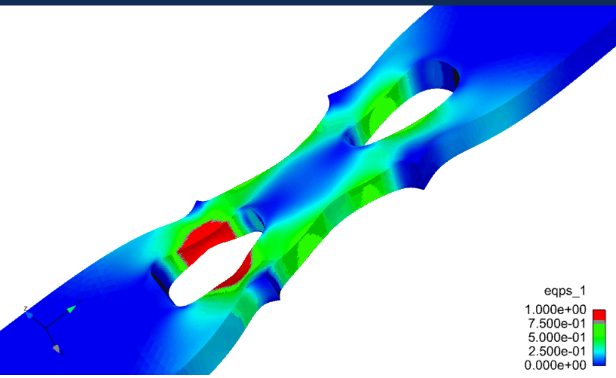

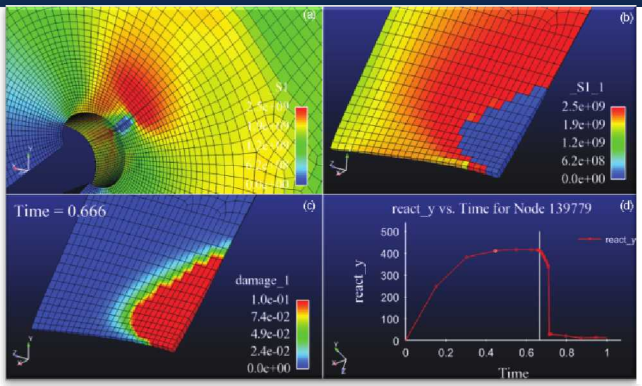

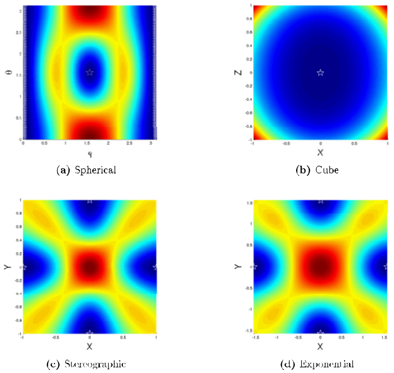

Computational Mechanics Efforts in the Multiscale Description of Material Fracture and Failure

Jakob T. Ostien, James W. Foulk III, Alejandro Mota, Qiushi Chen, WaiChing Sun

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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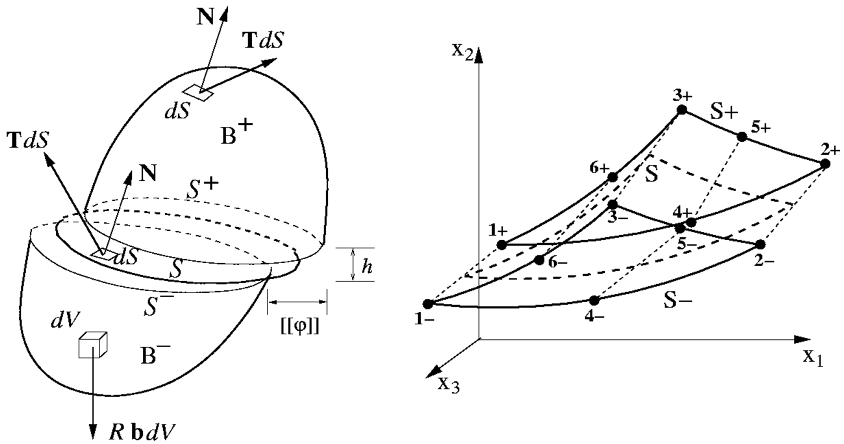
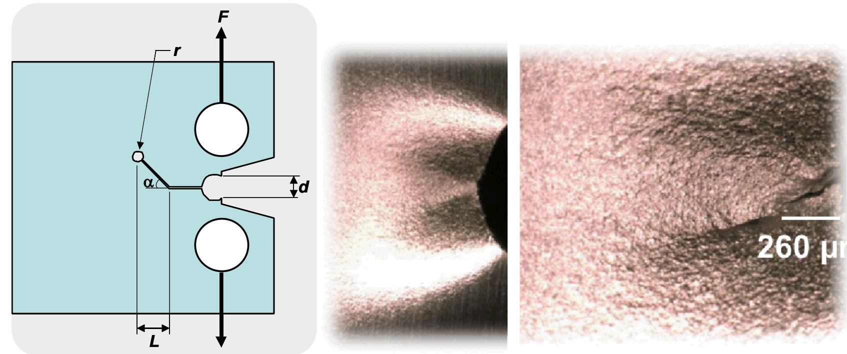
Outline

- Motivating problems in continuum multiscale plasticity
  - Modeling fracture and failure
  - Good finite elements are required to resolve stress states
  - Constitutive models must capture necking and plastic localization (global instabilities)
- Convergent numerical methods for models with local damage require *regularization* → *Nonlocal methods, surface elements*
  - Material (local) instabilities, loss of ellipticity, indicate localization and/or failure
- Continuum-to-Continuum Coupling
- Summary and Conclusions

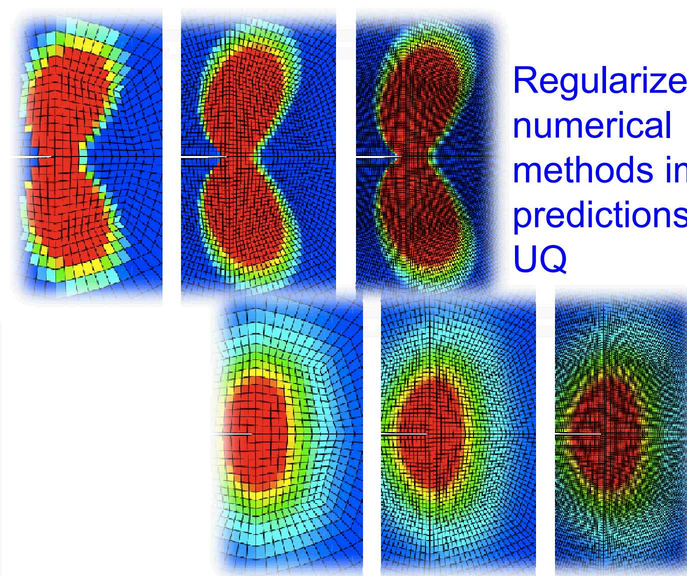
Modeling Fracture and Failure



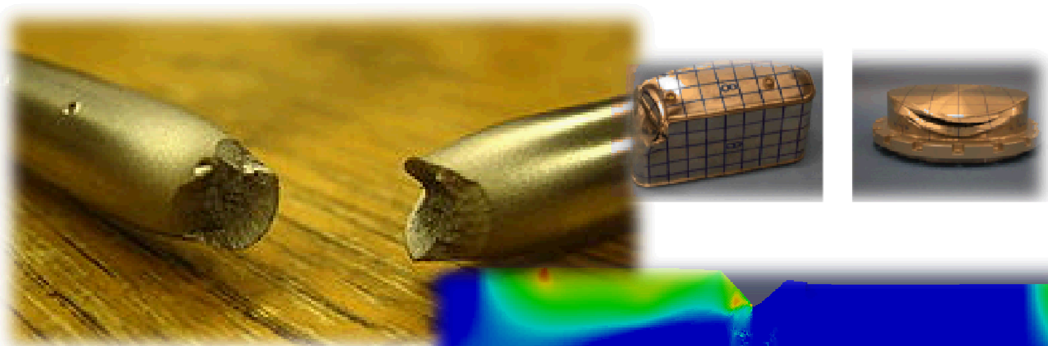
Finite element formulations for localization phenomena

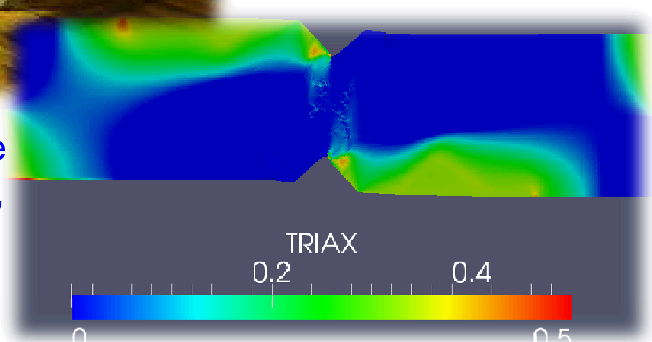


Ductile failure experiments, courtesy Brad Boyce via Sandia X-Prize



Regularized numerical methods improve predictions and UQ

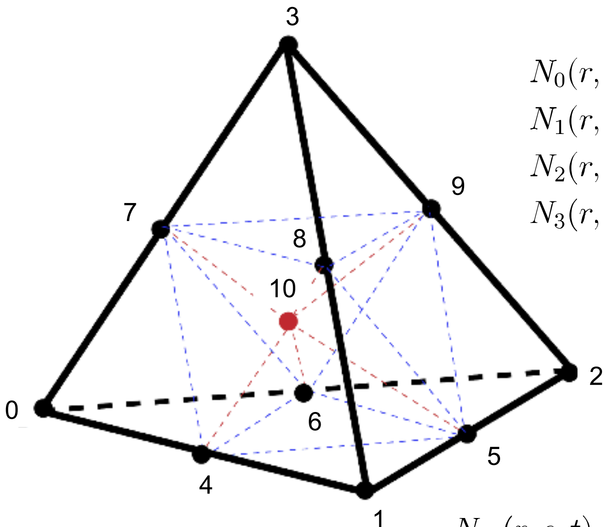




Ductility across a wide range of stress states, triaxialities

Finite Elements

- 10 noded tetrahedral element, Thoutireddy et al 2002.
- Multilinear basis with assumed linear spaces for deformation gradient and stress stemming from a three field Hu-Washizu variational principle



$$N_0(r,s,t) = \{1 - 2(r+s+t) \in E_0$$
$$N_1(r,s,t) = \{2r - 1 \in E_1$$
$$N_2(r,s,t) = \{2s - 1 \in E_2$$
$$N_3(r,s,t) = \{2t - 1 \in E_3$$

$$N_4(r,s,t) = \begin{cases} 2r & \in E_0, \\ 2 - 2(r+s+t) & \in E_1, \\ 1 - 2(s+t) & \in E_4 \cup E_7 \cup E_8 \cup E_{11} \end{cases}$$

$$N_5(r,s,t) = \begin{cases} 2s & \in E_1, \\ 2r & \in E_2 \\ 2(r+s) - 1 & \in E_4 \cup E_5 \cup E_8 \cup E_9 \end{cases}$$

$$N_6(r,s,t) = \begin{cases} 2s & \in E_0, \\ 2 - 2(r+s+t) & \in E_2, \\ 1 - 2(r+t) & \in E_8 \cup E_9 \cup E_{10} \cup E_{11} \end{cases}$$

$$N_7(r,s,t) = \begin{cases} 2t & \in E_0, \\ 2 - 2(r+s+t) & \in E_3, \\ 1 - 2(r+s) & \in E_6 \cup E_7 \cup E_{10} \cup E_{11} \end{cases}$$

$$N_8(r,s,t) = \begin{cases} 2t & \in E_1, \\ 2r & \in E_3, \\ 2(r+t) - 1 & \in E_4 \cup E_5 \cup E_6 \cup E_7 \end{cases}$$

$$N_9(r,s,t) = \begin{cases} 2t & \in E_2, \\ 2s & \in E_3, \\ 2(s+t) - 1 & \in E_5 \cup E_6 \cup E_9 \cup E_{10} \end{cases}$$

$$N_{10}(r,s,t) = \begin{cases} 2 - 4r & \in E_4, \\ 4(r+s+t) - 2 & \in E_5, \\ 2 - 4t & \in E_6, \\ 4s & \in E_7, \\ 4t & \in E_8, \\ 2 - 4s & \in E_9, \\ 4r & \in E_{10}, \\ 4(r+s+t) - 2 & \in E_{11} \end{cases}$$

Constitutive Models

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- Introduce and internal state variable to govern statistically stored dislocations, homogenization of slip system response
- Pose a hardening minus recovery evolution equation for the isotropic hardening variable with a rate and temperature dependent flow rule

$$\dot{\epsilon}_p = f\{\sinh[\frac{\bar{\sigma}}{(1-\phi)(\kappa+Y)} - 1]\}^n$$

$$\dot{\kappa} = [H - R_d\kappa]\dot{\epsilon}_p$$

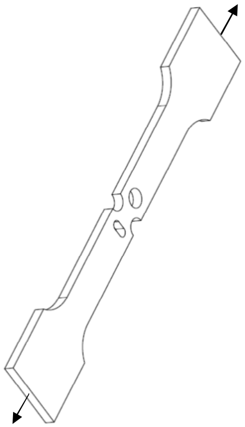
Bammann, Chiesa, Johnson, Regueiro, Marin, Brown, et al

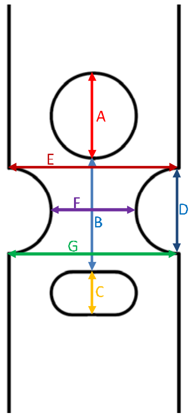
- Add state variables to capture the presence of voids in the matrix, with evolution equations for the size of the voids at a material point

$$\dot{\phi} = \{\frac{1}{(1-\phi)^m} - 1\}\sinh[\frac{2(2m-1)}{2m+1}\frac{<p>}{\bar{\sigma}}]$$

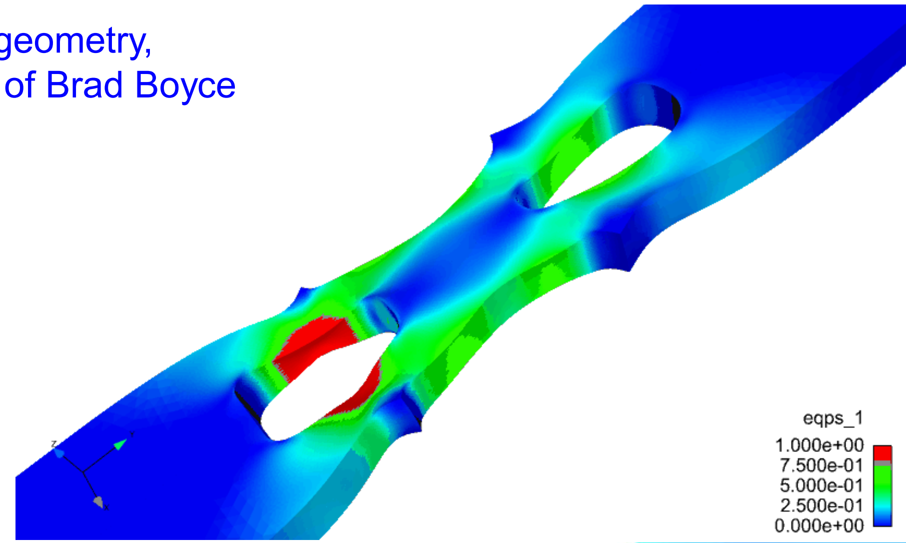
Cocks and Ashby, 1980

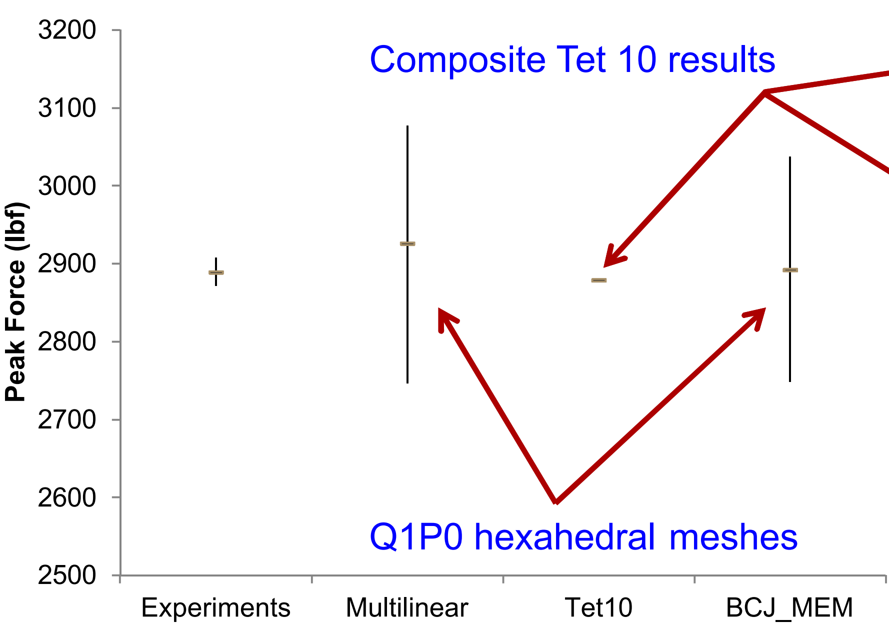
Representative Results

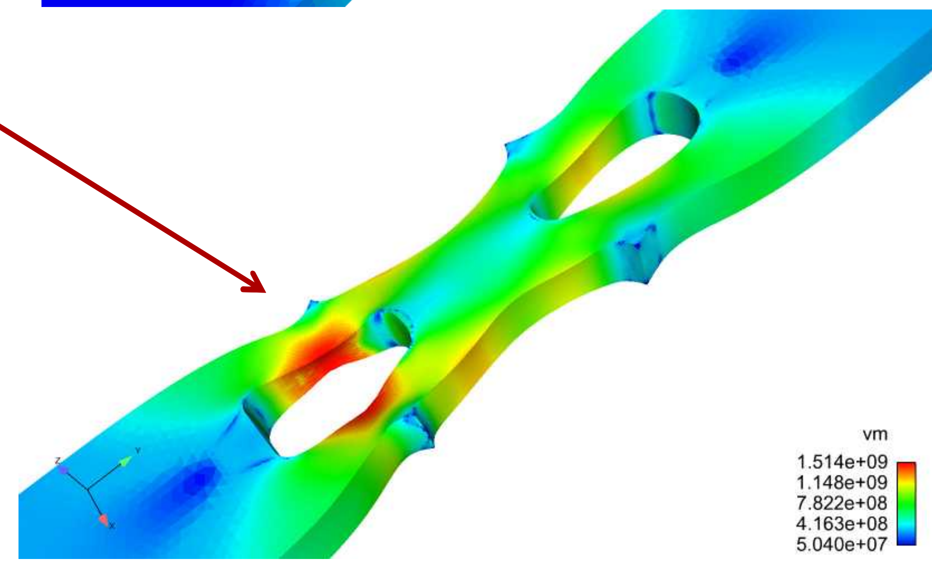




Sandia X-Prize geometry, results courtesy of Brad Boyce







Regularization

- Nonlocal methods

Nonlocal volumes created on processor

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

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

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

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

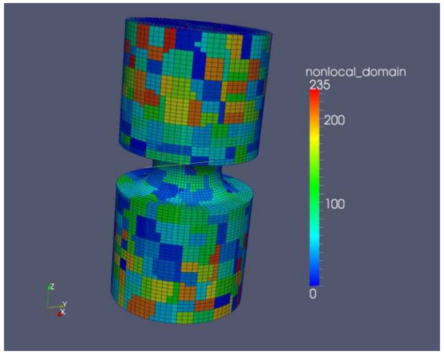
Euler-Lagrange equations

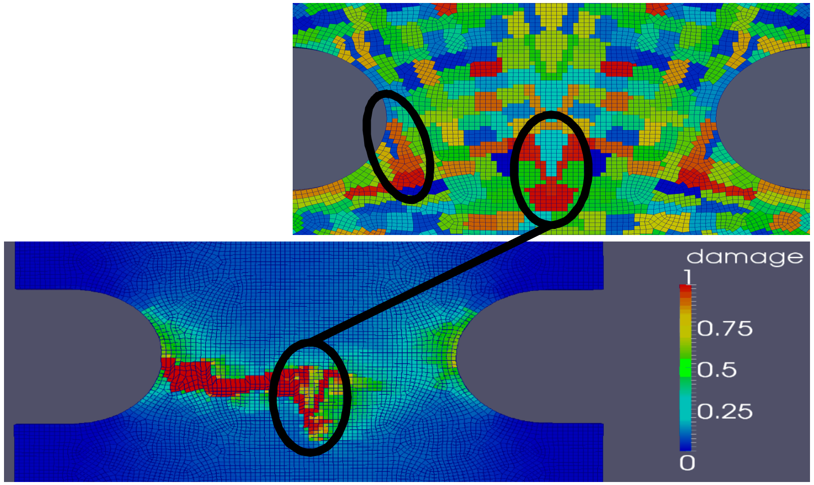
$$\bar{\boldsymbol{Y}} = \frac{1}{\operatorname{vol}(D)} \int_D \boldsymbol{Y}\, dV,$$

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

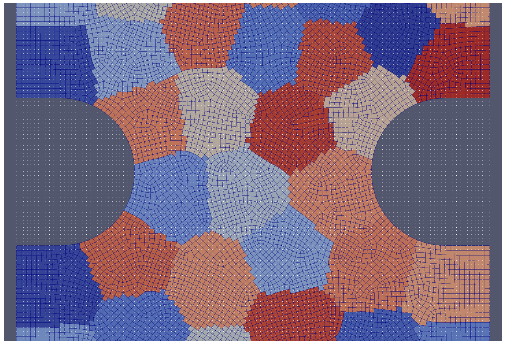
$$\operatorname{vol}(\bullet) := \int_{(\bullet)} dV,$$

Length scale comes form the nonlocal volume





Domain decomposition algorithms can give poorly shaped volumes (left), a solution may be centroidal Voronoi tesselation (right)

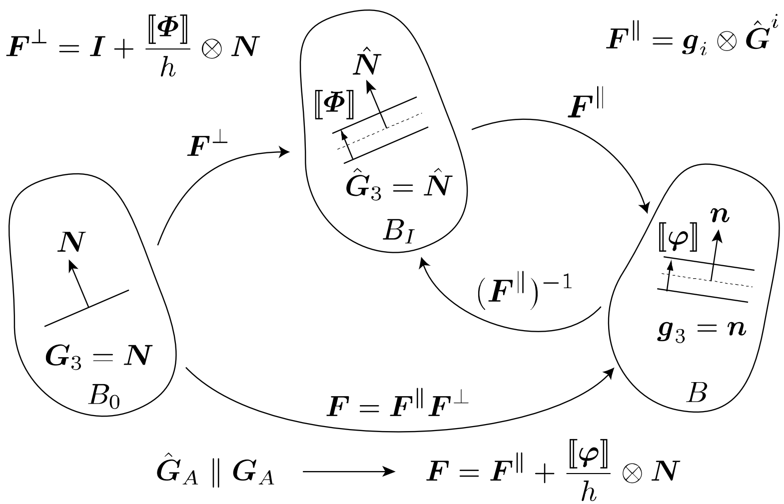


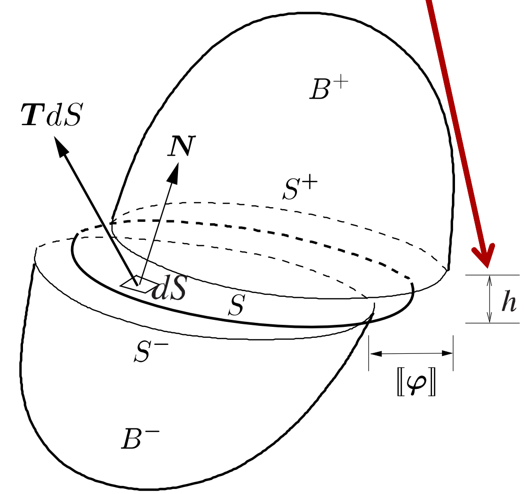
Foulk, Mota, Ostien, Variational Nonlocal Regularization, *in prep*

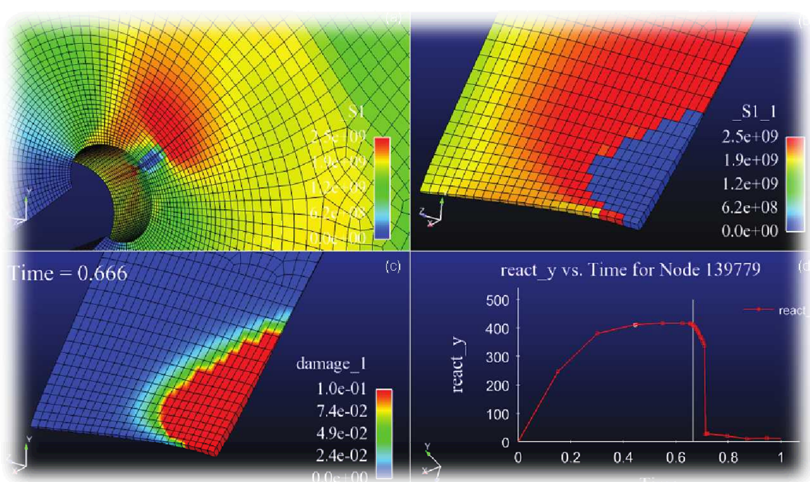
Regularization

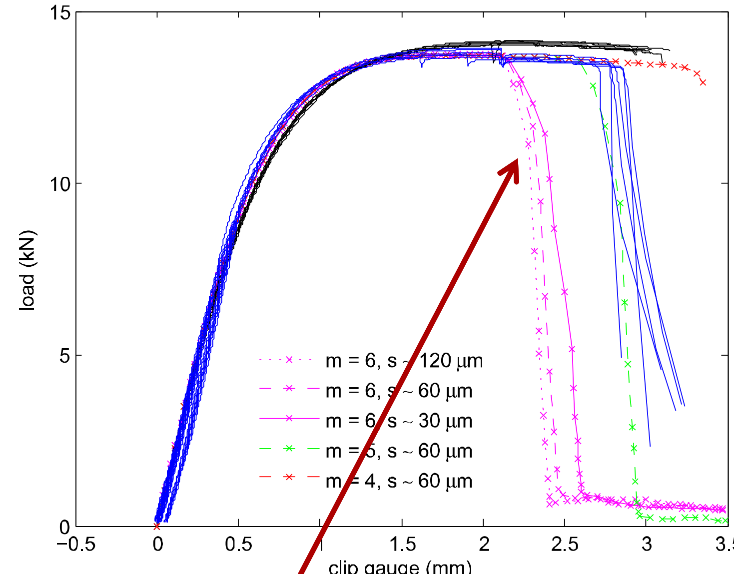
Length scale comes from thickness parameter

- Surface elements





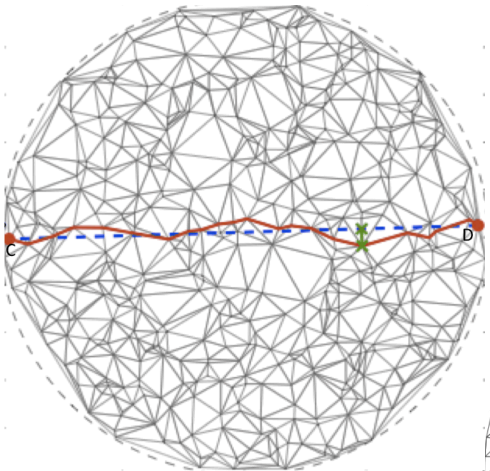




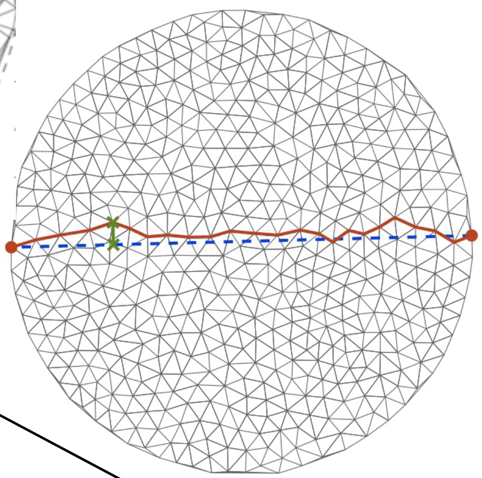
Foulk, Emery, Mota, Lindblad, Ostien, Brown, Boyce, The formulation and application of strain localization elements to ductile fracture, *in prep*

Regularized global solution solution

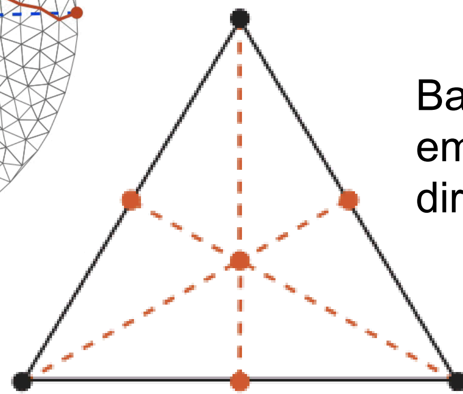
Review of optimal meshes, Rimoli & Rojas



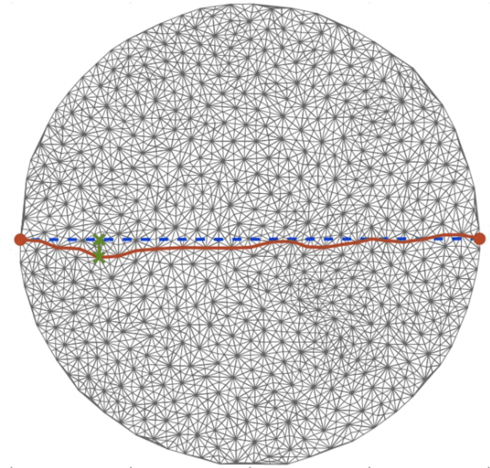
A random mesh is generated by throwing random points and performing Delaunay's triangulation.



A K-means clustering algorithm is used to improve the mesh quality of the random mesh



Barycentric subdivision is employed to add conjugate directions to the mesh



Goal: Minimize error between "true" path and discrete path

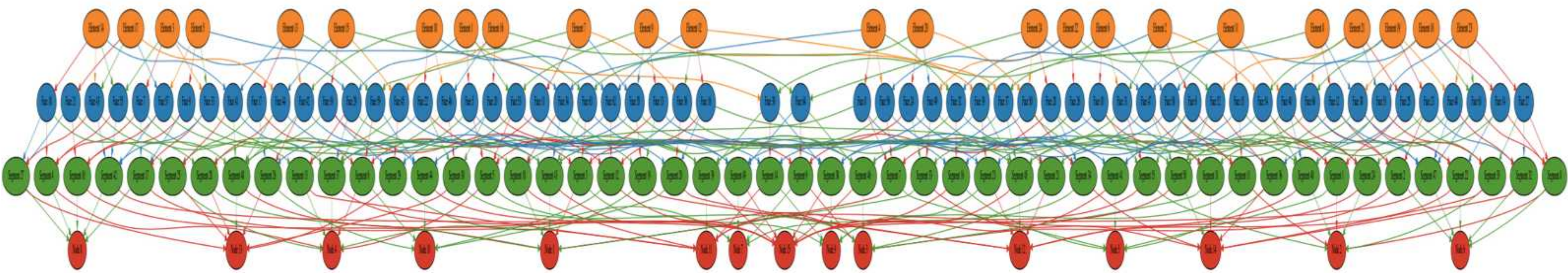
- - - - - - - *"true" path*

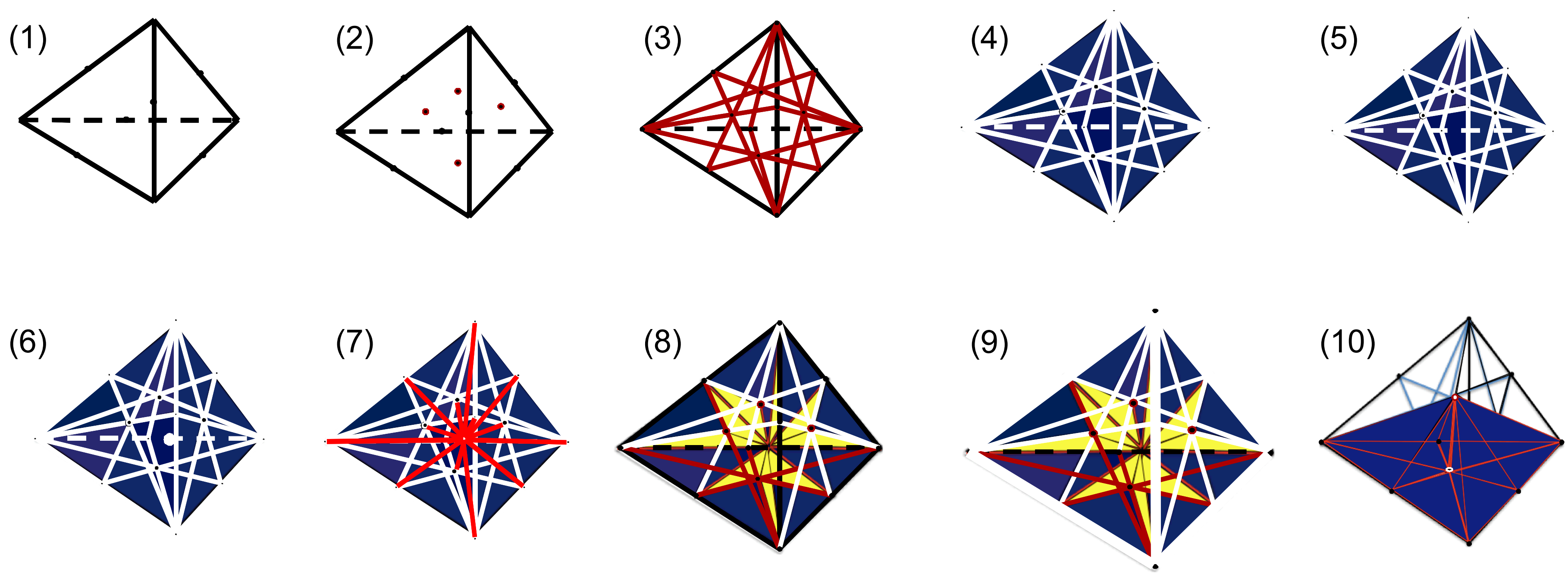
——— *discrete path*

——— *geometric error (Hausdorff distance)*

Evolution of barycentric subdivision in 3-D (10)

(10) Add the corresponding new elements





Bifurcation

- Surface insertion criteria evaluated on interior faces

Define the acoustic tensor

$$\boldsymbol{A} := \boldsymbol{n} \cdot \mathbb{C} \cdot \boldsymbol{n}, \quad \boldsymbol{n} \in S^2$$

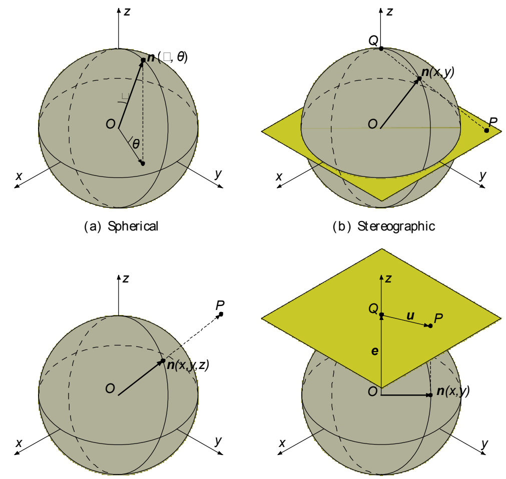
The strong ellipticity condition

$$\boldsymbol{m} \cdot \boldsymbol{A} \cdot \boldsymbol{m} > 0, \quad \boldsymbol{m} \in S^2$$

The bifurcation condition to determine the onset of material failure

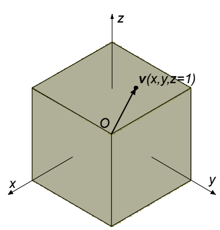
$$\det \boldsymbol{A} > 0$$

Parameterizations of the unit sphere



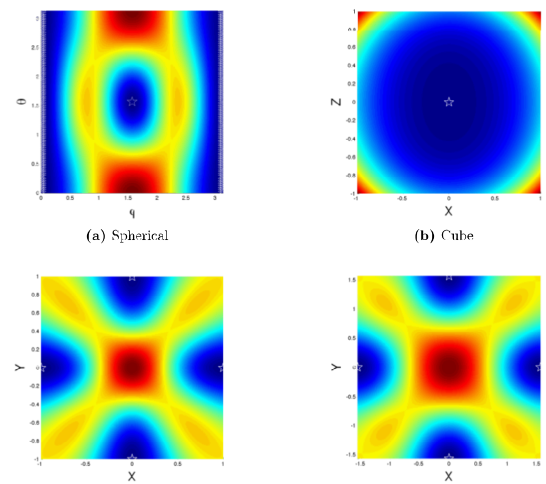
(a) Spherical (b) Stereographic

(c) Projective (d) Tangent



(e) Cartesian

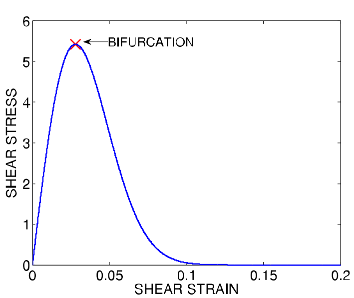
Different landscapes of the determinant emerge as a function of parameterization

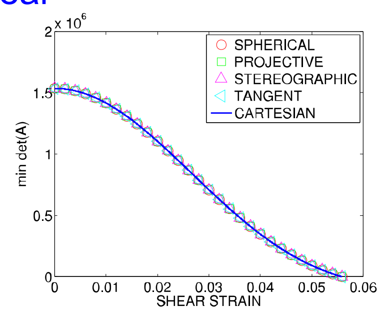


(a) Spherical (b) Cube

(c) Stereographic (d) Exponential

Simple Shear





Evaluate for accuracy, robustness, efficiency

Mota, Chen, Foulk, Ostien, 2012, A Cartesian Parameterization for the Analysis of Material Instability, *in prep.*

Continuum-to-Continuum Coupling

- Methods to couple continuum treatments at different length and time scales
- Two examples
  - Arlequin – Domain coupling via energy partitioning
  - An extension of the variational multiscale method to finite deformation

Energy Partition – method to describe one mechanical response in one domain with two energy functionals

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Partitioned Incremental Energy Functional

$$\Phi[\overline{\varphi}, \varphi', \phi] = \Phi^{\text{int}}[\overline{\varphi}, \varphi'] - \Phi^{\text{ext}}[\overline{\varphi}, \varphi'] + \Lambda[\overline{\varphi}, \varphi', \phi]$$

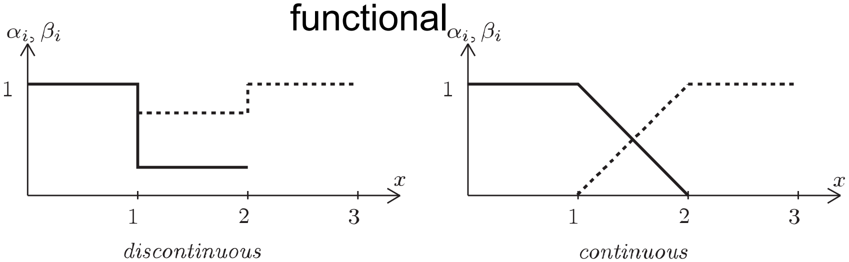
$$\Phi^{\text{int}}[\overline{\varphi}, \varphi'] = \int_{\mathcal{B}} \alpha \overline{W}(\overline{\boldsymbol{F}}, \overline{\boldsymbol{z}}) + (1-\alpha) W'(\boldsymbol{F}', \boldsymbol{z}')\, dV$$

$$\Phi^{\text{ext}}[\overline{\varphi}, \varphi'] = \int_{\mathcal{B}} \beta \overline{\rho_0 \boldsymbol{B}} \cdot \overline{\varphi} + (1-\beta)(\rho_0 \boldsymbol{B})' \cdot \varphi' dV + \int_{\partial_T \mathcal{B}} \beta \overline{\boldsymbol{T}} \cdot \overline{\varphi}\, dS + \int_{\partial_T \mathcal{B}} (1-\beta) \boldsymbol{T}' \cdot \varphi'\, dS$$

Partitioned internal energy

Partitioned external energy

Weighting function partitioned energy functional

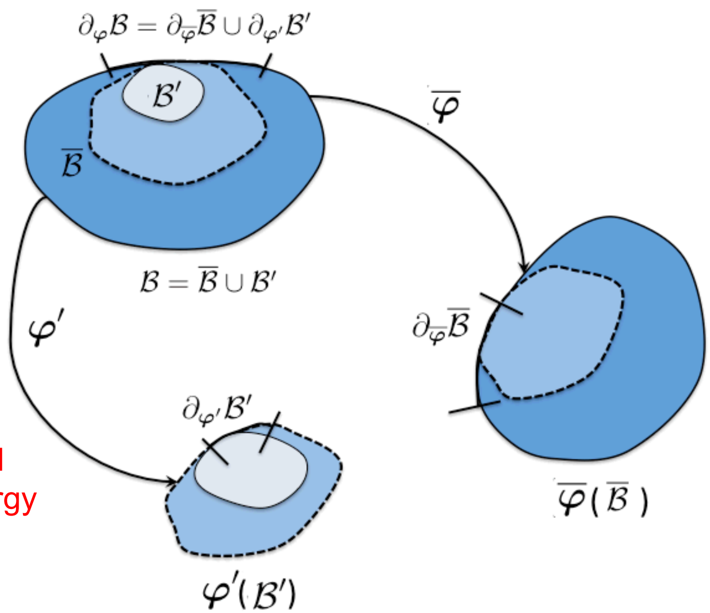


$$\Lambda[\overline{\varphi}, \varphi', \phi] = \int_{\mathcal{B}^c} \phi \cdot (\overline{\varphi} - \varphi') + \kappa l^2\, \text{Grad}\, \overline{\phi} : (\text{Grad}\, \overline{\varphi} - \text{Grad}\, \varphi')\, dV$$

$$\alpha(\boldsymbol{X}) = \beta(\boldsymbol{X}) = \begin{cases} 1 & \boldsymbol{X} \in \overline{\mathcal{B}} \setminus \mathcal{B}^c \\ 0 & \boldsymbol{X} \in \mathcal{B}' \setminus \mathcal{B}^c \end{cases}$$

Partition of unity

Compatibility constraint energy



Partitioned Domain with overlapping region(s)

Sun, Mota, Domain Coupling for Large Deformation Strain Localization, *in prep*

Foulk’s Singular Bar (2008)

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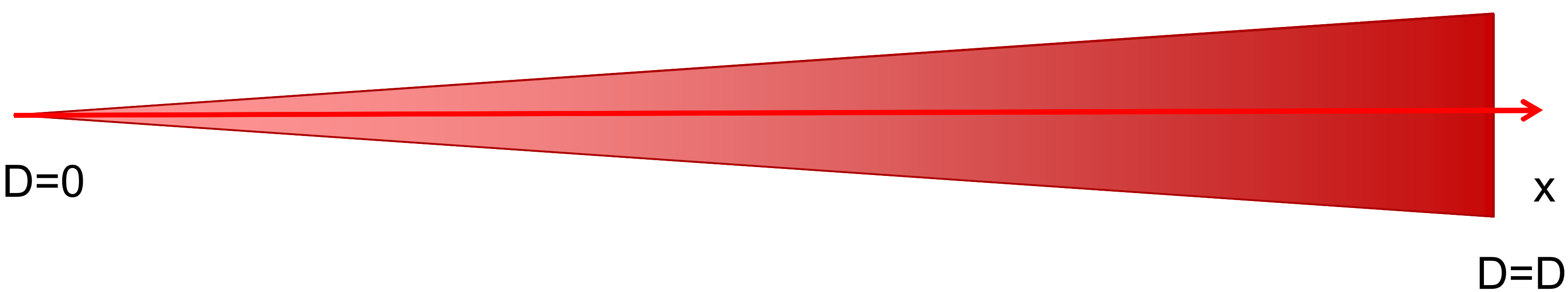
- We use the BVP introduced by James W. Foulk III to test whether regularization procedure is able to regularized the PDE if it is only applied in the fine domain
- Due to the vanishing area, mesh pathology is expected unless length scale is introduced via regularization procedure.

Path dependent damage model

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

$$W_o(\frac{d\varphi}{dX}) = \frac{1}{2}\bar{E}\Big(((\frac{d\varphi}{dX})^{-2} + (\frac{d\varphi}{dX})^{2} - 2\Big)$$

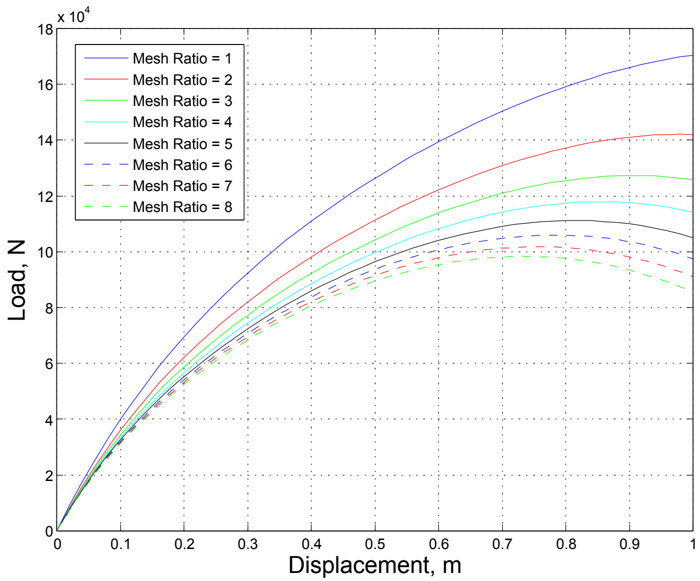
$$\zeta = \zeta(\alpha) = \zeta_\infty[1-\exp(-\alpha/\varsigma)] \quad \alpha(t) = \max_{s\in[0,t]} W_o(s)$$



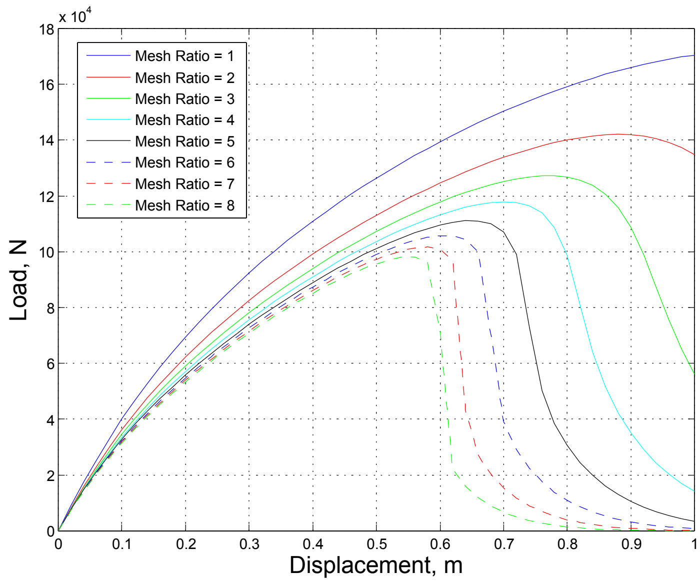
Example 2 Foulk's bar

Regularization in small region

With DOC method, only a small nonlocal domain is required to regularize the PDE. A large portion of the domain is modeled by simpler, cheaper constitutive law with coarser mesh to cut down computational cost.



Load-displacement curve with refining nonlocal domain



Load-displacement curve with refining classical domain

Variational Multiscale

a$%' , -. 43''-%7''(')*+, -. *%'1 -EE$%8"

b5 *"34-0' "7')*+, -. *%', -EE$%8"

$$X = \bar{\square}(X), \quad x = \square'(X)$$

b*&0'7')*+, -. *%', -EE$%8"

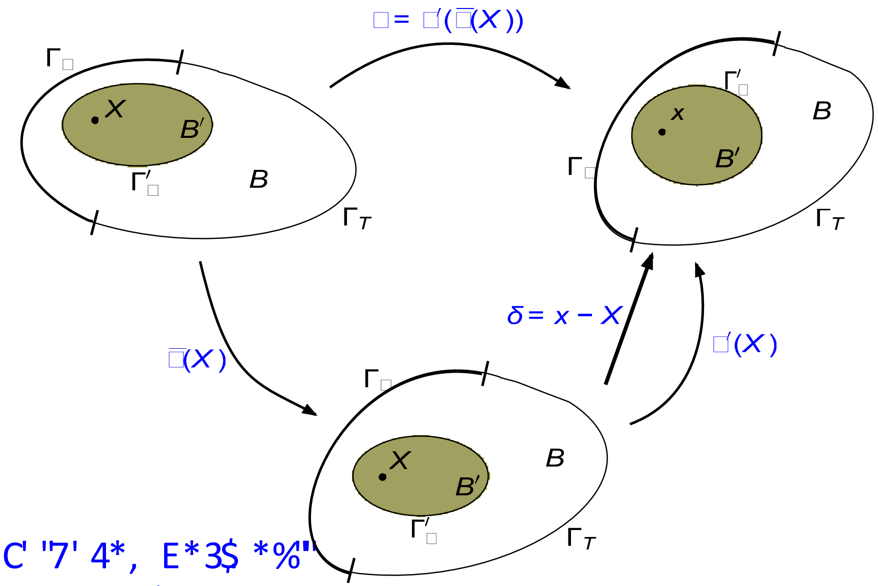
$$\square(X) = \square'(\bar{\square}(X))$$

`%&+*724' "_% "34-0' "_' 07"

$$\delta = x - X$$

$$= \square'(\bar{\square}(X)) - \bar{\square}(X)$$

Decomposition of deformation mapping



! 77$ C' "7' 4*, E*3$ *%' *)"7')*+, -. *%', -EE$%8"

$$\square = \underbrace{\square}_{\text{coarse}} + \underbrace{\delta}_{\text{fine}}$$

1 20 E0$4-. C' "7' 4*, E*3$ *%' *)"7')*+, -. *%'8+-7$ %&'

$$F = \frac{\partial x}{\partial \bar{X}}\frac{\partial \bar{X}}{\partial X} = F'\bar{F}$$

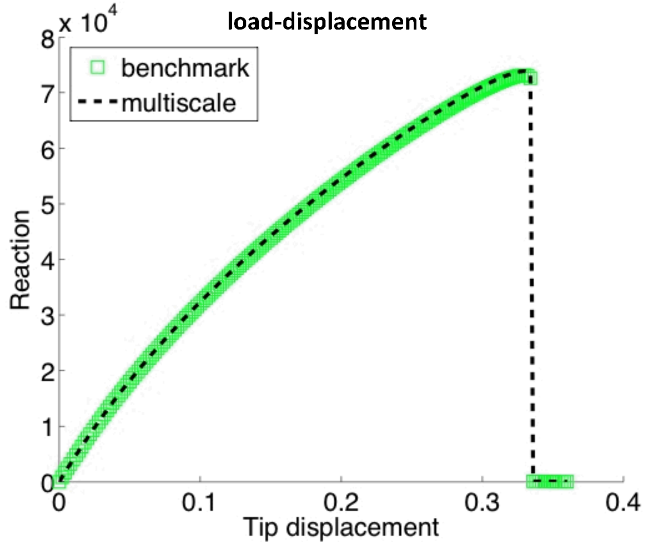
9, -0'3&+-$%'4*%&*2+E-+&'Z-+$6$E-. "-%7"W28=' 3"RMMN?'Z-+6E-. "-%7"W28=' 3"QKKKY"

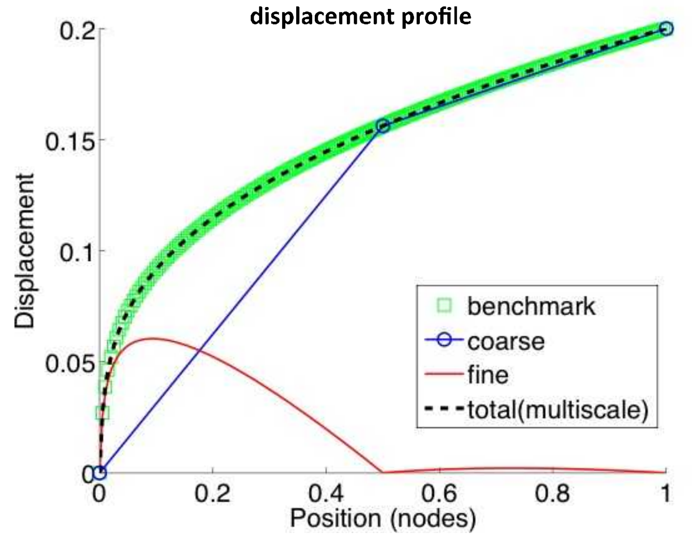
$$u = \bar{u} + u'$$

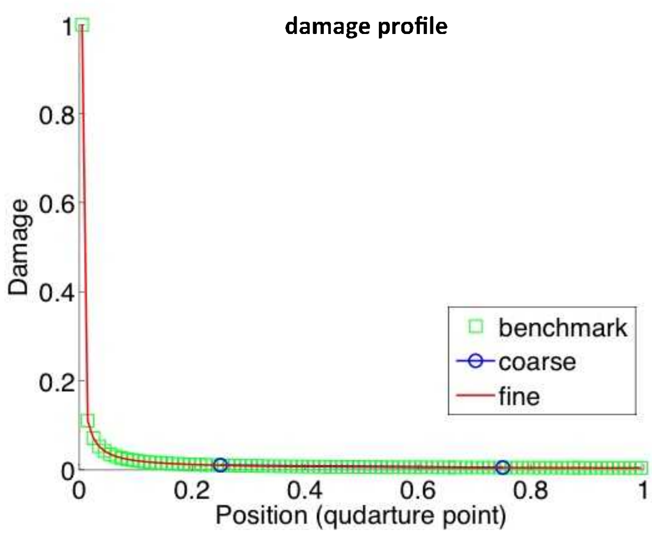
Chen, Mota, *in prep*

Variational Multiscale

Hyper-elasticity with damage







- Benchmark solution by full-single scale computation
- Material properties

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

Computing Environments

- Sandia's production analysis code suite, Sierra and Sierra/Mechanics
  - Surface (localization) elements
  - Active work on the Nonlocal partitioning algorithm
- Research goes into an open source finite element code repository, Albany
  - Coupled physics (not shown)
  - Adaptivity (not shown)

Summary and Conclusions

- Multiple efforts towards modeling ductile material behavior up to and including fracture and failure
- Developing and testing non-standard finite elements and methods
- Relying on regularization methods, introducing length scales, resolving plasticity
- The nature of plasticity and ductile failure requires multiple scales to be resolved