

# Regularizing damage evolution for ductile fracture using localization elements

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# Issues

## MISSION

Need to predict fracture/failure of critical components loaded in abnormal environments – crack initiation and propagation

## MATERIALS AND MECHANISMS

Aluminum and steel alloys which can exhibit distributed and localized processes evolving from void nucleation, growth, microinertia, and coalescence. Failure processes are rate and temperature dependent.

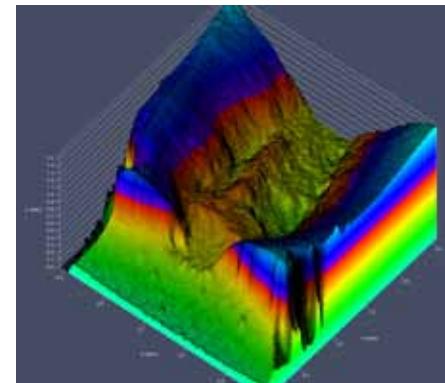
## CURRENT MODELS

*The community has developed plasticity/damage models to address rate dependence, temperature dependence, and void growth. Literature is rich with damage models for metals, polymers, and composites.*

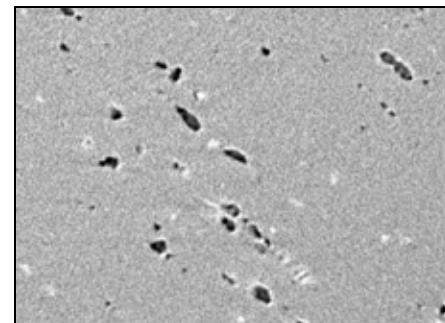
*Glitch – they corrupt the PDE.*

## REGULARIZATION

Our goal is to retain the micromechanics of local damage models and add regularization through multiple methods. *We need to work on the numerics and the physics simultaneously.*



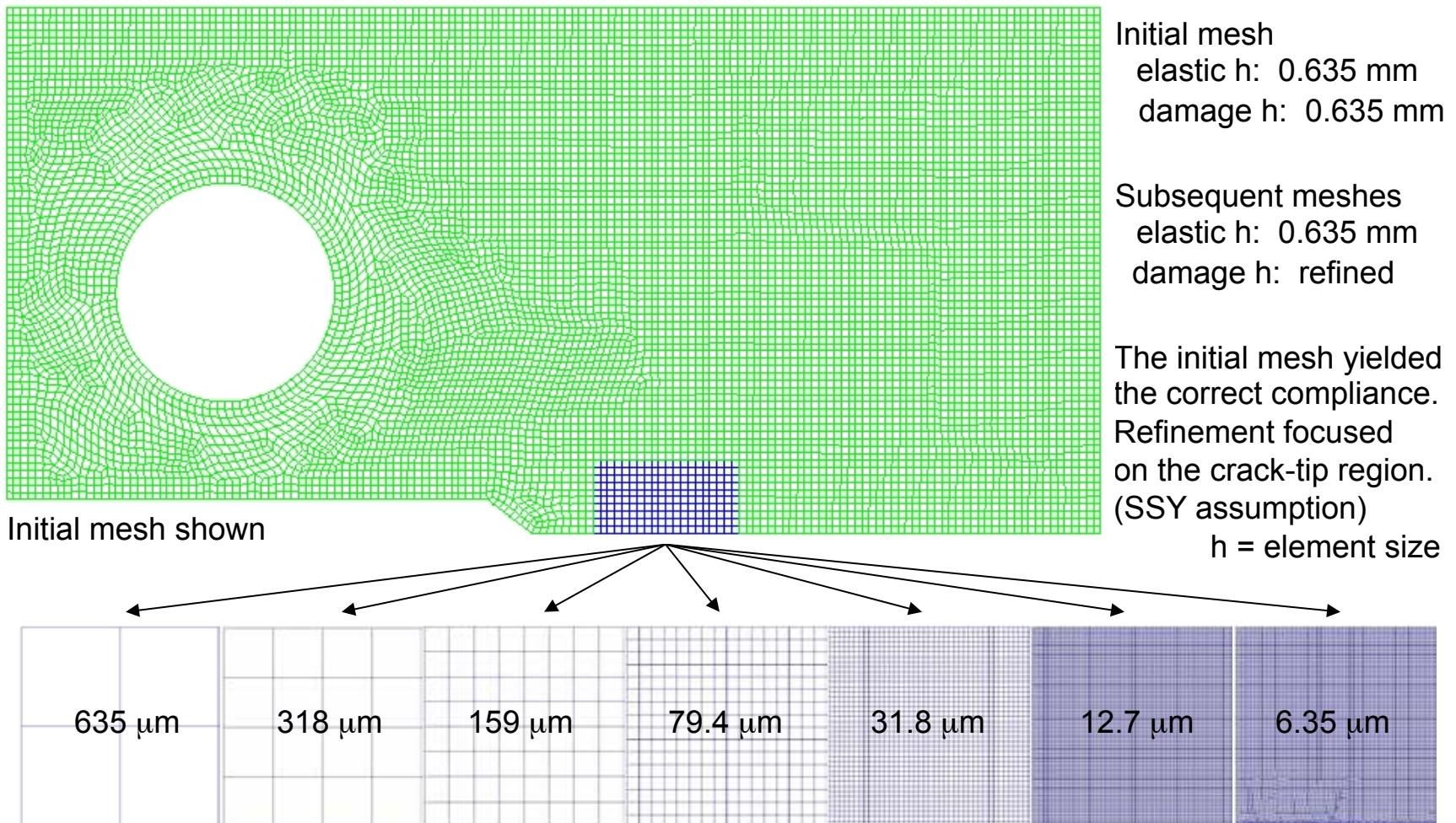
Boyce, PH13-8, H950



ALS, 7075-T7351

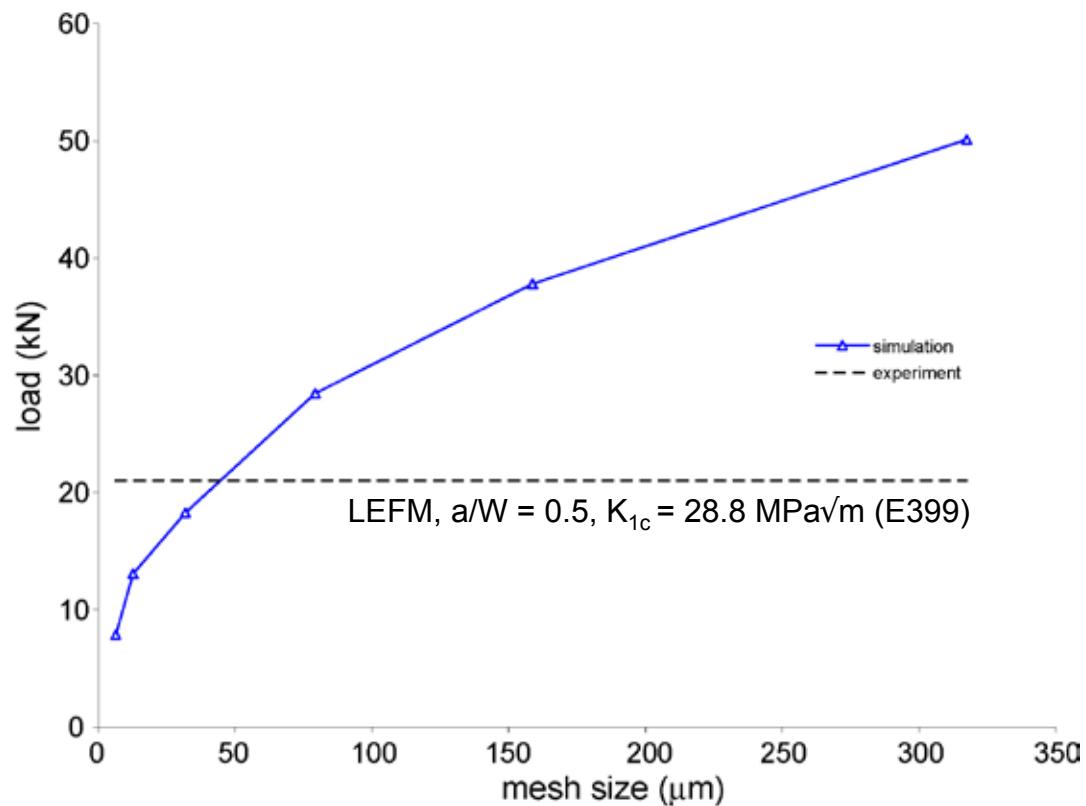
# This could be you...

- Finite elements are only used to solve a partial differential equation
- Any correlation of a finite element with a physical process can be misleading

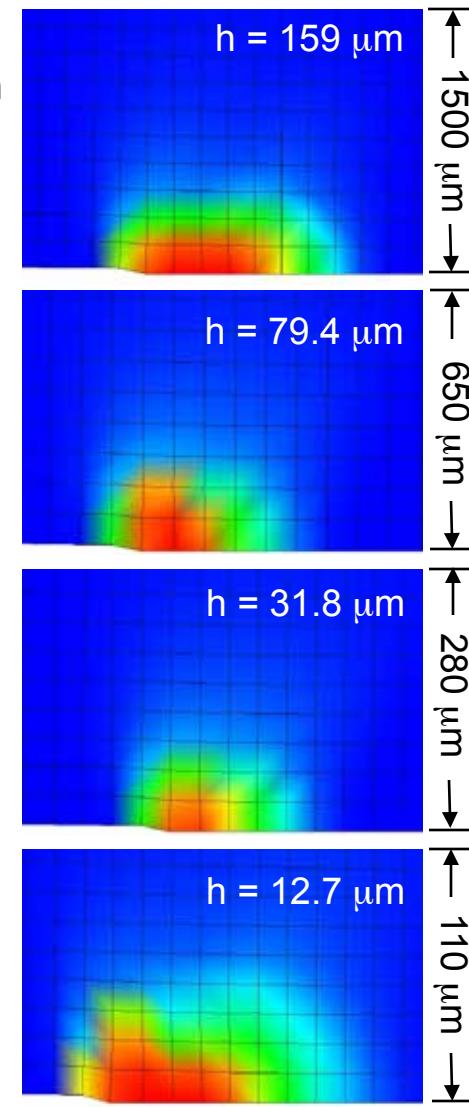


# Seeking a length scale for damage

Snapshots of damage taken at propagation. The process zone scales with the mesh size and the predicted loads span the experimental finding.



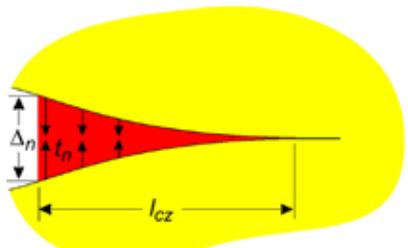
Note: Contours of porosity,  $1.0\text{E-}4$  to 1.0, log scale



# Exploring multiple methods for regularization

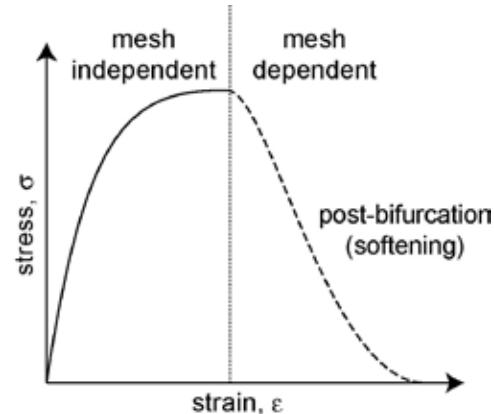
cohesive zone, crack band

*PROBLEMATIC, BUT RICH*

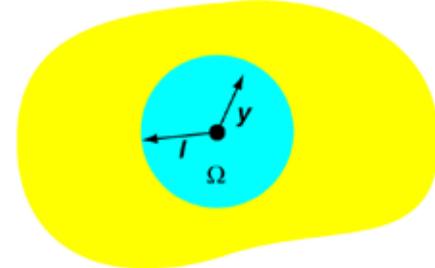


$$t_n = t_n(\sigma_{max}, \phi, \Delta_n/\ell)$$

Adaptive insertion before bifurcation  
Bulk + surface model, mesh topology



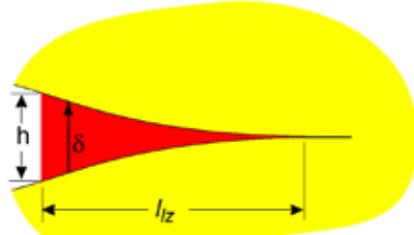
nonlocal



$$\bar{\phi}(x) = \frac{1}{\Psi(x)} \int_{\Omega} \psi(y, x) \dot{\phi}(y) d\Omega(y)$$

Integrate over a ball  
Rescaling at boundaries

*localization elements*

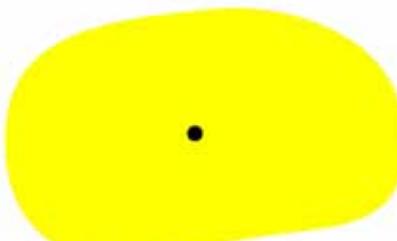


$$\mathbf{F} = \mathbf{F}^{\parallel} \mathbf{F}^{\perp} \quad \mathbf{F}^{\perp} = \mathbf{I} + \frac{\phi}{h} \otimes \mathbf{N}$$

Adaptive insertion before bifurcation  
Restricted path via mesh topology

Mesh adaption needed

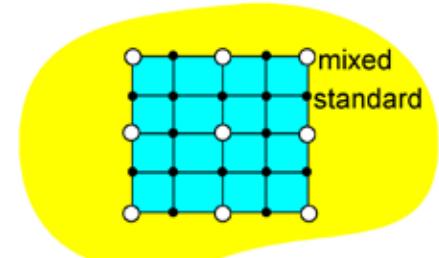
*gradients*



$$\dot{\phi} = f(\sigma, \phi) + \ell \frac{\partial \phi}{\partial x} + \ell^2 \frac{\partial^2 \phi}{\partial x^2}$$

Solve additional pde(s)  
Specify boundary conditions

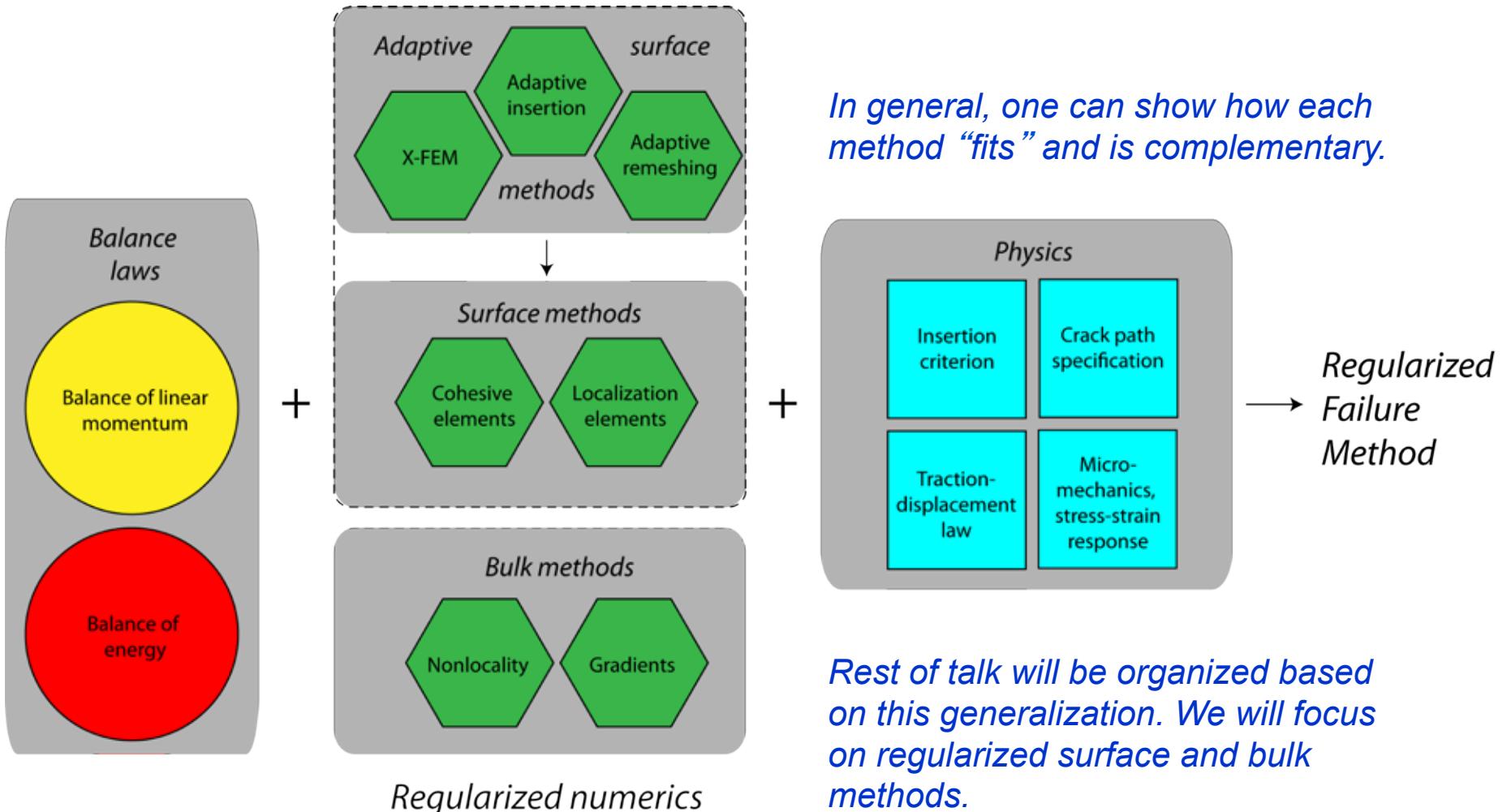
*variational nonlocal*



$$\bar{\mathbf{Z}} = \frac{1}{\text{vol}(D)} \int_D \mathbf{Z} dV$$

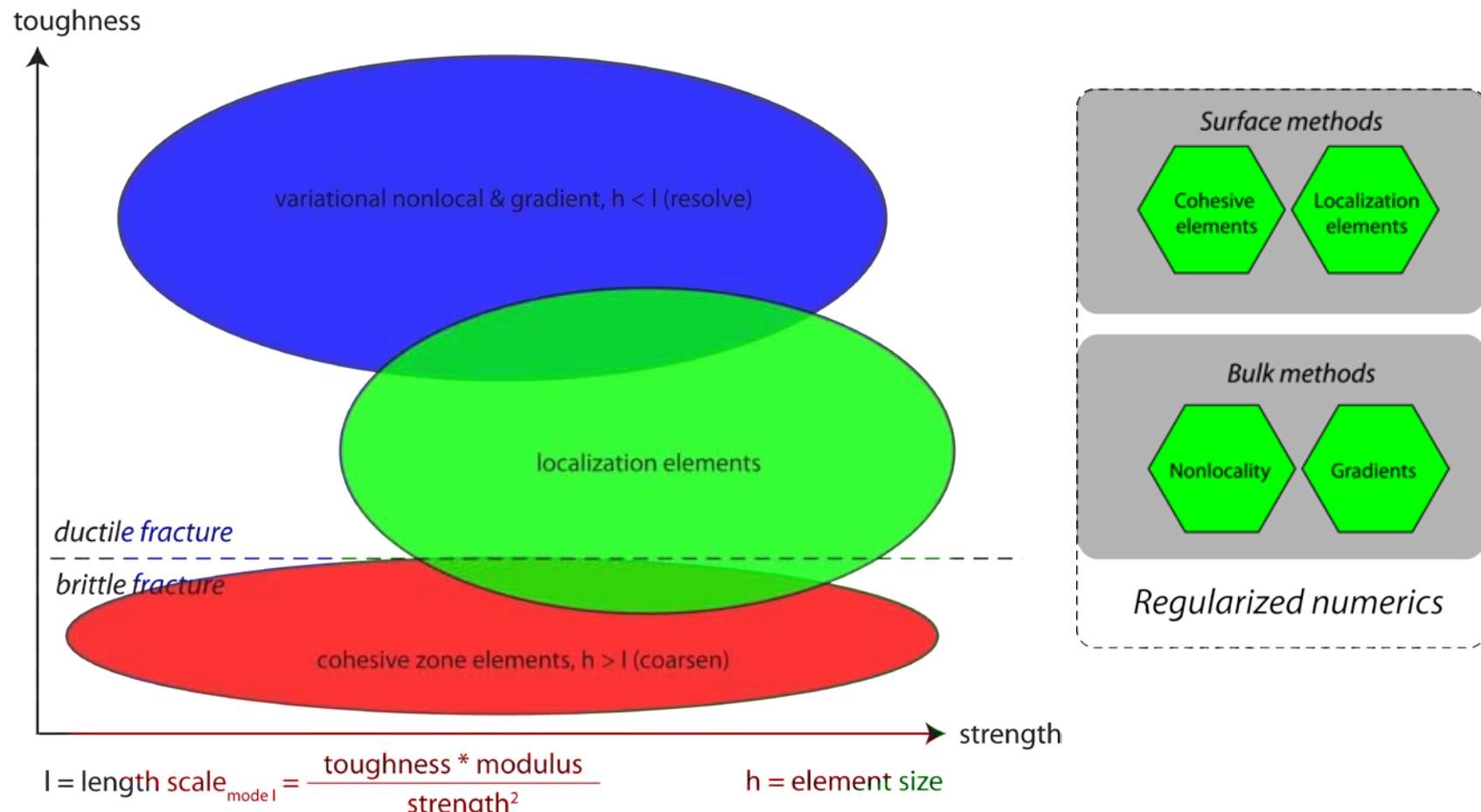
Volume averaging on coarse domain

# Generalizing methods



# Multiple approaches needed for components

- Each method has a region of applicability defined by strength and toughness
- Analysts need a toolbox to span aluminum to stainless steel alloys

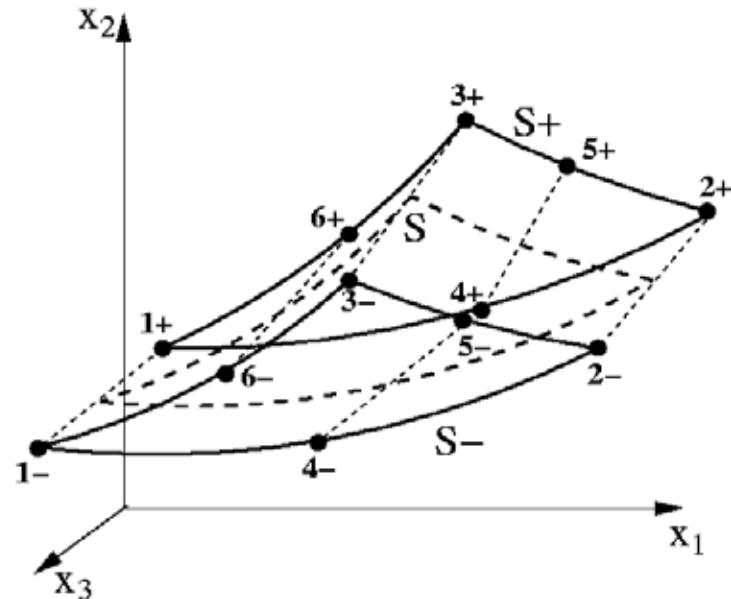
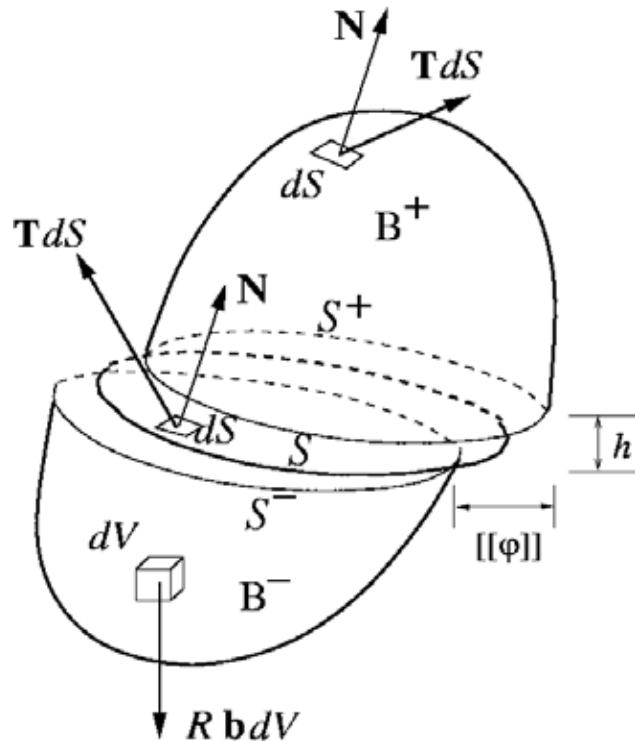
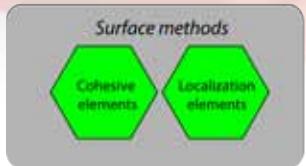




# Localization elements

- Kinematic assumptions
- Improving/simplifying the formulation
- Test case
  - Fitting parameters (smooth tension, K-field)
  - X-prize geometry
- Addressing membrane forces
- Part of a family of methods for regularization

# Kinematic assumptions



- Finite-deformation kinematics.
- Simulation of strain localization.
- No additional constitutive assumptions

$$\mathbf{F}^{\perp} = \mathbf{I} + \frac{[\![\varphi]\!]}{h} \otimes \mathbf{N} \quad \mathbf{F}^{\parallel} = \mathbf{g}_i \otimes \mathbf{G}^i$$

$$\mathbf{F} = \mathbf{F}^{\parallel} \mathbf{F}^{\perp}$$

Yang, Mota and Ortiz, IJNME, 2005



# Issues to remedy

$$\mathbf{F} = \mathbf{F}^{\parallel} + \frac{\mathbf{F}^{\parallel} \llbracket \varphi \rrbracket}{h} \otimes \mathbf{N}$$

*Configuration*

$$\begin{aligned} P^D &= \sum_{\pm} \int_{B_0^{\pm}} \mathbf{P} \cdot \dot{\mathbf{F}} dV + \int_{S_0} \mathbf{P} \cdot \dot{\mathbf{F}} h dS \\ &= \sum_{\pm} \int_{B_0^{\pm}} \mathbf{P} \cdot \dot{\mathbf{F}} dV + \int_{S_0} \mathbf{P} \cdot \left[ \dot{\mathbf{F}}^{\parallel} \mathbf{F}^{\perp} + \mathbf{F}^{\parallel} \dot{\mathbf{F}}^{\perp} \right] h dS \\ &= \sum_{\pm} \int_{B_0^{\pm}} \mathbf{P} \cdot \dot{\mathbf{F}} dV + \int_{S_0} \left[ h \mathbf{P} (\mathbf{F}^{\perp})^T \cdot \dot{\mathbf{F}}^{\parallel} + (\mathbf{F}^{\parallel})^T \mathbf{P} \mathbf{N} \cdot \llbracket \dot{\varphi} \rrbracket \right] dS \end{aligned}$$

*Conjugacy*

$$\mathbf{x}^+ = \mathbf{Q} \mathbf{x} \quad \mathbf{F}^+ = \mathbf{Q} \mathbf{F} \quad \mathbf{g}_i^+ = \mathbf{Q} \mathbf{g}_i \quad \llbracket \varphi \rrbracket^+ = \mathbf{Q} \llbracket \varphi \rrbracket$$

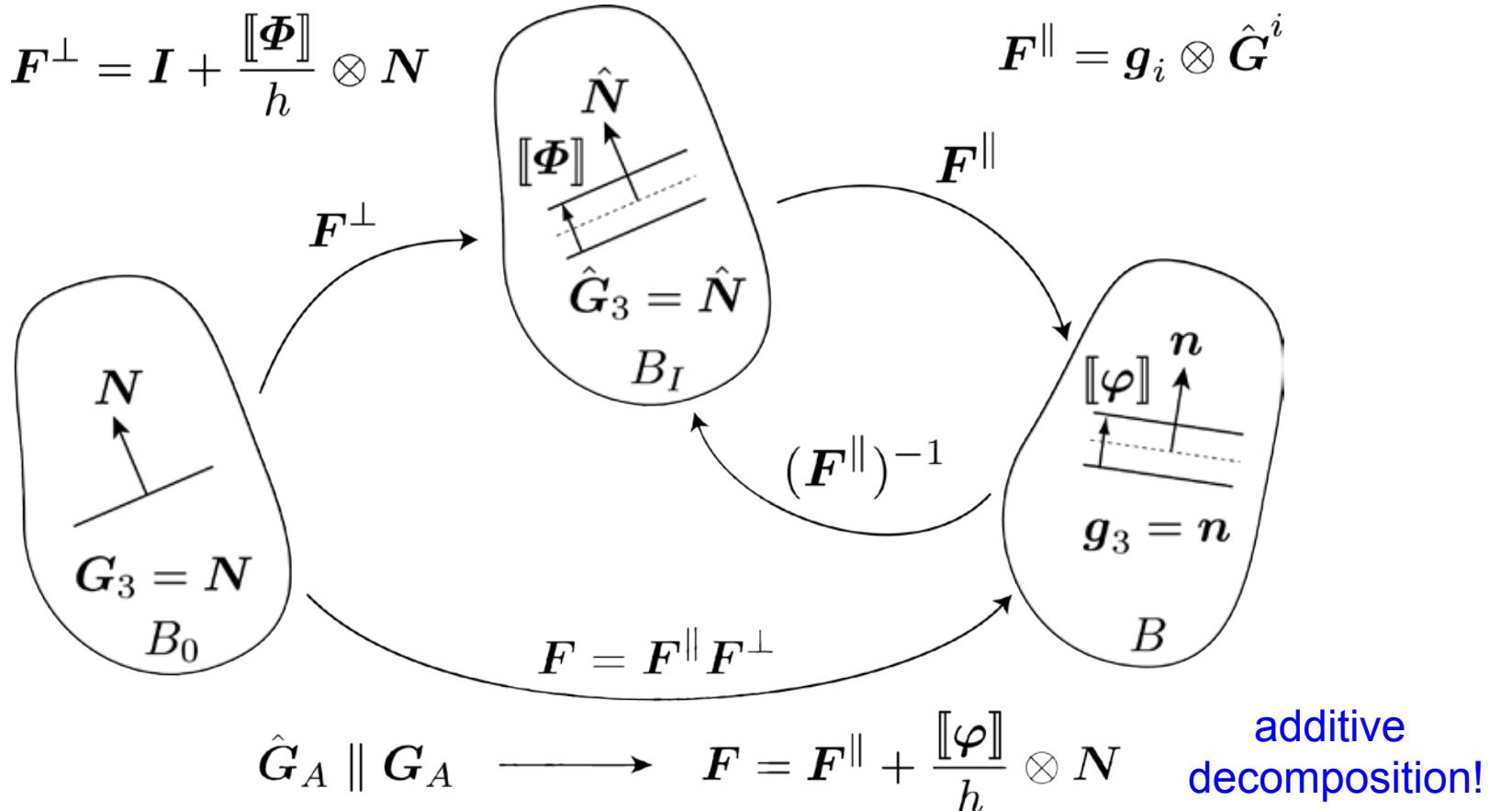
$$(\mathbf{F}^{\perp})^+ = \mathbf{I} + \frac{\mathbf{Q} \llbracket \varphi \rrbracket}{h} \otimes \mathbf{N} \quad (\mathbf{F}^{\parallel})^+ = \mathbf{g}_i^+ \otimes \mathbf{G}^i = \mathbf{Q} \mathbf{F}^{\parallel}$$

*Objectivity*

$$(\mathbf{F})^+ = \mathbf{Q} \mathbf{F}^{\parallel} + \frac{\mathbf{Q} \mathbf{F}^{\parallel} \mathbf{Q} \llbracket \varphi \rrbracket}{h} \otimes \mathbf{N}$$

# An intermediate configuration

$$\mathbf{F}^\perp = \mathbf{I} + \frac{[\![\Phi]\!]}{h} \otimes \mathbf{N}$$



The jump is pushed backwards

$$[\![\Phi]\!] = (\mathbf{F}^\parallel)^{-1} [\![\varphi]\!]$$

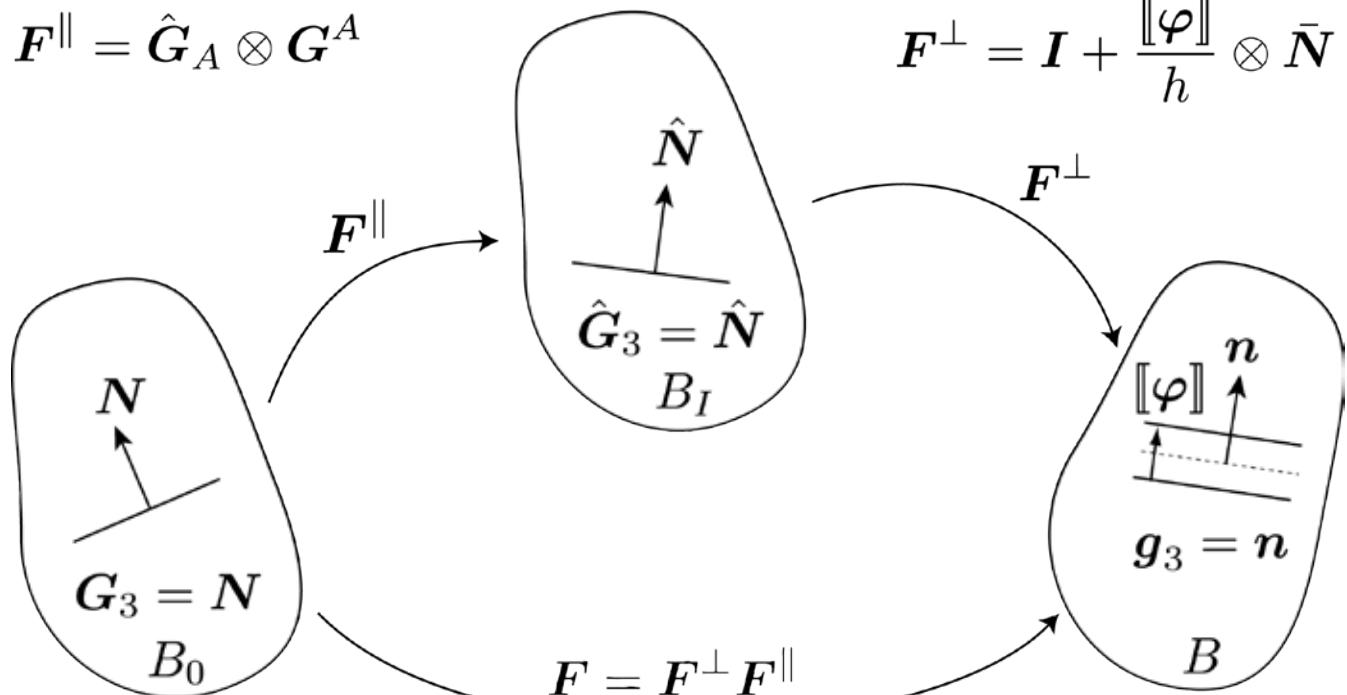
Retain definition of membrane def. grad.

$$\mathbf{F}^\parallel = \mathbf{g}_i \otimes \mathbf{G}^i$$

# The order is not unique

$$\mathbf{F}^{\parallel} = \hat{\mathbf{G}}_A \otimes \mathbf{G}^A$$

$$\mathbf{F}^{\perp} = \mathbf{I} + \frac{[\![\varphi]\!]}{h} \otimes \bar{\mathbf{N}}$$



$$\bar{\mathbf{N}} = \hat{\mathbf{N}} \frac{d\hat{A}}{\hat{J} dA}$$

$$\mathbf{g}_i \parallel \hat{\mathbf{G}}_i$$

$$\mathbf{F} = \mathbf{F}^{\parallel} + \frac{[\![\varphi]\!]}{h} \otimes \bar{\mathbf{N}}$$

additive decomposition!

The normal used for construction

$$\bar{\mathbf{N}} = (\mathbf{F}^{\parallel})^{-T} \mathbf{N}$$

Retain definition of membrane def. grad.

$$\mathbf{F}^{\parallel} = \mathbf{g}_i \otimes \mathbf{G}^i$$



# Benefits of minor change in the kinematics

$$\mathbf{F} = \mathbf{F}^{\parallel} + \frac{[\![\varphi]\!]}{h} \otimes \mathbf{N}$$

*Configuration, Additive decomposition*

$$\begin{aligned} P^D &= \sum_{\pm} \int_{B_0^{\pm}} \mathbf{P} \cdot \dot{\mathbf{F}} dV + \int_{S_0} \mathbf{P} \cdot \dot{\mathbf{F}} h dS \\ &= \sum_{\pm} \int_{B_0^{\pm}} \mathbf{P} \cdot \dot{\mathbf{F}} dV + \int_{S_0} \mathbf{P} \cdot [\dot{\mathbf{F}}^{\parallel} + \dot{\mathbf{F}}^{\perp}] h dS && \text{Conjugacy} \\ &= \sum_{\pm} \int_{B_0^{\pm}} \mathbf{P} \cdot \dot{\mathbf{F}} dV + \int_{S_0} [h \mathbf{P} \cdot \dot{\mathbf{F}}^{\parallel} + \mathbf{P} \mathbf{N} \cdot [\![\dot{\varphi}]\!]] dS \end{aligned}$$

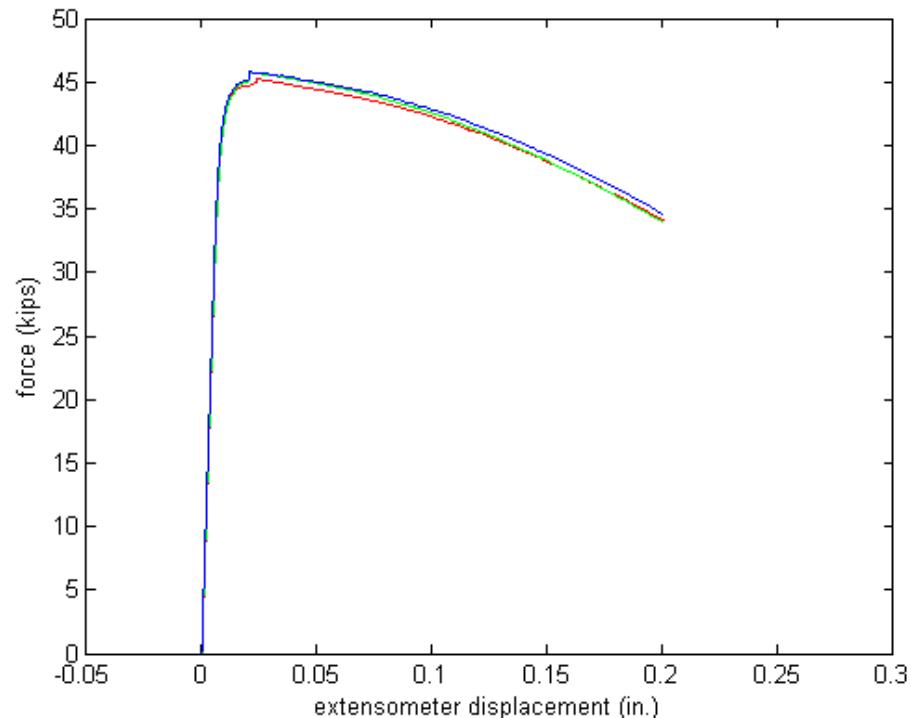
$$\mathbf{x}^+ = \mathbf{Q} \mathbf{x} \quad \mathbf{F}^+ = \mathbf{Q} \mathbf{F} \quad \mathbf{g}_i^+ = \mathbf{Q} \mathbf{g}_i \quad [\![\varphi]\!]^+ = \mathbf{Q} [\![\varphi]\!]$$

$$(\mathbf{F}^{\parallel})^+ = \mathbf{g}_i^+ \otimes \mathbf{G}^i = \mathbf{Q} \mathbf{F}^{\parallel} && \text{Objectivity}$$

$$(\mathbf{F})^+ = \mathbf{Q} \mathbf{F}^{\parallel} + \frac{\mathbf{Q} [\![\varphi]\!]}{h} \otimes \mathbf{N} = \mathbf{Q} \mathbf{F}$$

# Case study for PH 13-8 H950

We obtained a data point from a PH 13-8 H977 test in which they used Bridgman correction factors (knowing the notch dimensions) to infer that the stress at a true strain of 0.316 was 1750 MPa.



$f$	$4.52 \times 10^4$
$Y$	1600 MPa
$n$	0.386
$H$	492 MPa
$R_d$	$1.0 \times 10^{-4}$

In this model, there is no recovery. Because  $f$  is big and  $n$  small, they do not affect the response. Hence, we really only fit two parameters, the yield stress,  $Y$ , and the hardening,  $H$ . Can two parameters get us there?

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

NOTE: For ease, the constitutive behavior is assumed to be isotropic, linear hardening.

# Damage model and length scale

The only parameters that remain are the damage exponent,  $m$ , in the evolution of damage  $\phi$  and the characteristic length scale  $h$  used to normalize the gap vector  $\delta$  to yield a deformation gradient for the localization element. We lock down  $h$  at 30  $\mu\text{m}$  and fit  $m$  with the plane-strain fracture toughness. For damage to evolve, we must select an initial porosity,  $\phi_0$ . We choose to initialize the porosity to  $1 \times 10^{-4}$ .

$$\dot{\phi} = \left\{ \frac{1}{(1-\phi)^m} - (1-\phi) \right\} \sinh \left[ \frac{2(2m-1)}{2m+1} \frac{\langle p \rangle}{\bar{\sigma}} \right] \dot{\epsilon}_p \quad \text{Cocks and Ashby, 1980}$$

$\frac{\langle p \rangle}{\bar{\sigma}}$  triaxiality governing void growth

$$\mathbf{F} = \mathbf{F}^{\parallel} \mathbf{F}^{\perp} \quad \mathbf{F}^{\perp} = \mathbf{I} + \frac{\phi}{h} \otimes \mathbf{N} \quad \text{Yang, Mota, Ortiz, 2005}$$

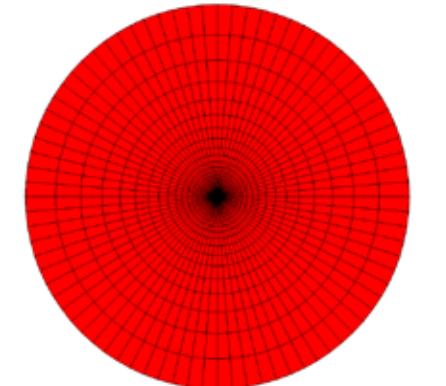
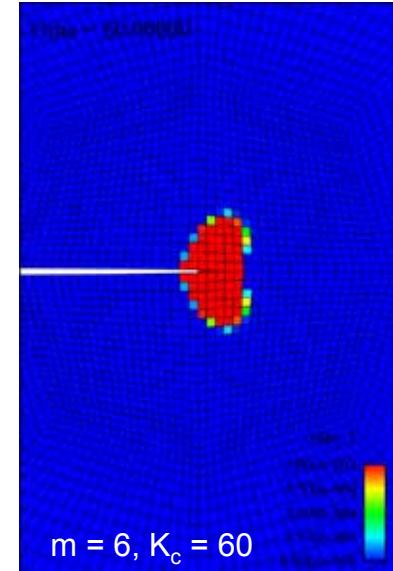
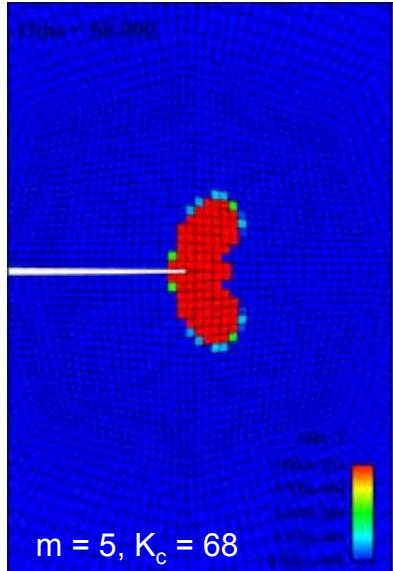
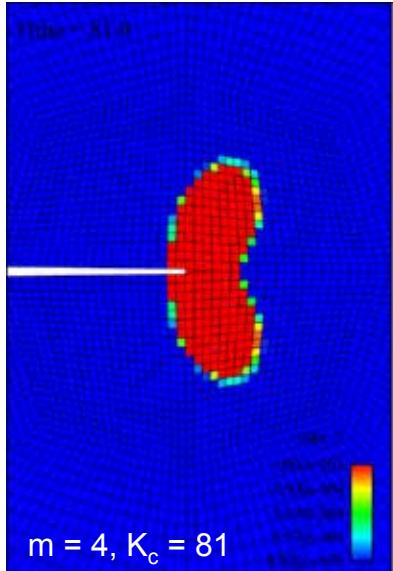
$\phi$  gap vector for surface separation

$\mathbf{N}$  normal to mid-plane in the reference configuration

$h$  characteristic length scale - 30  $\mu\text{m}$

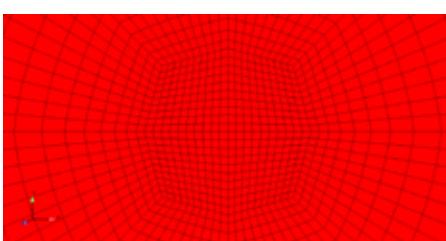
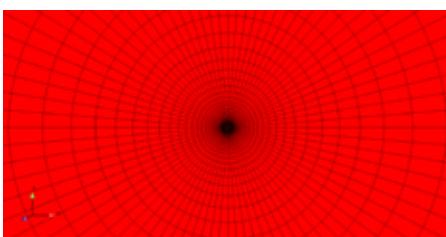
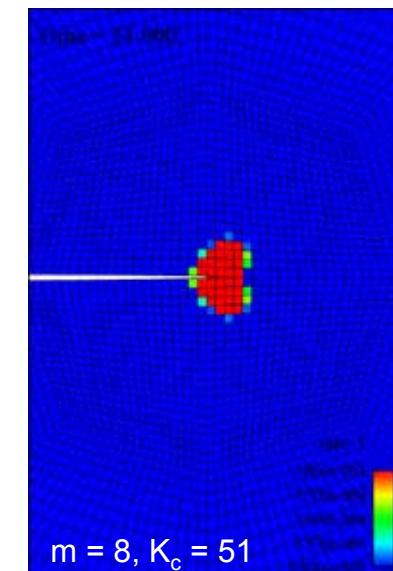
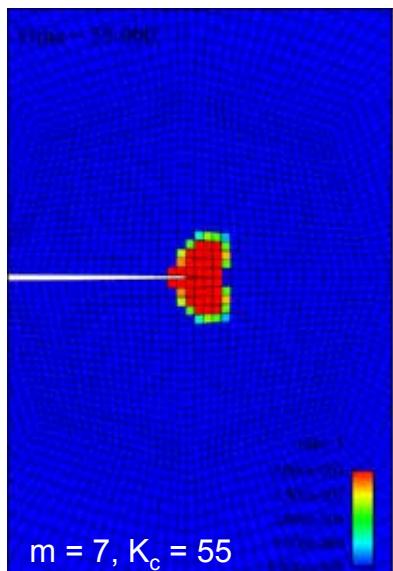
NOTE: In the original work of Cocks and Ashby,  $m$  is the power-law creep exponent. Just as in plasticity, we use the functional form of Cocks and Ashby to “fit”  $m$ .

# Resolution and lumping dissipation



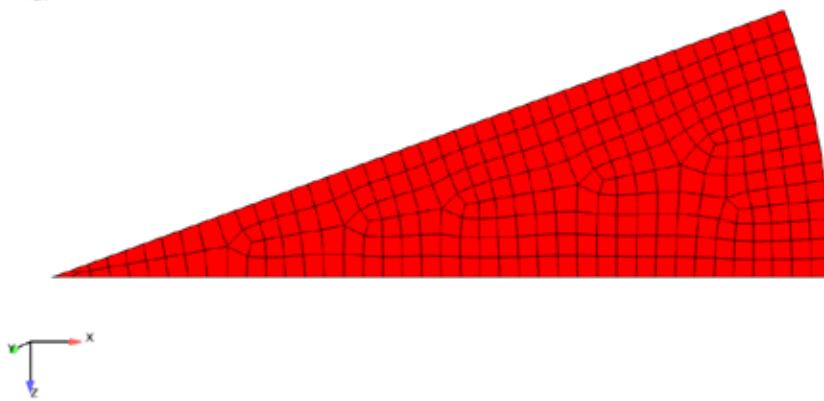
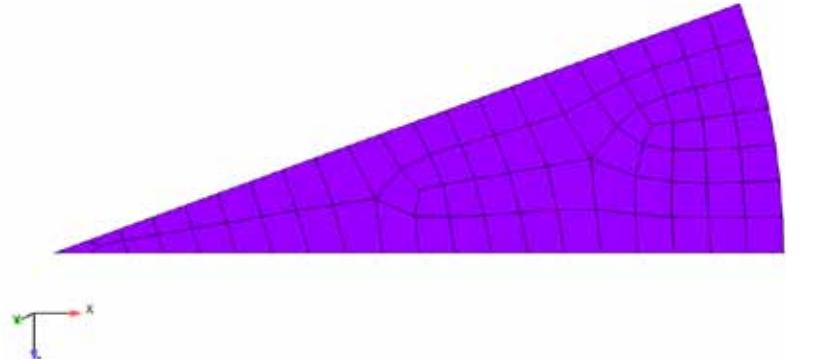
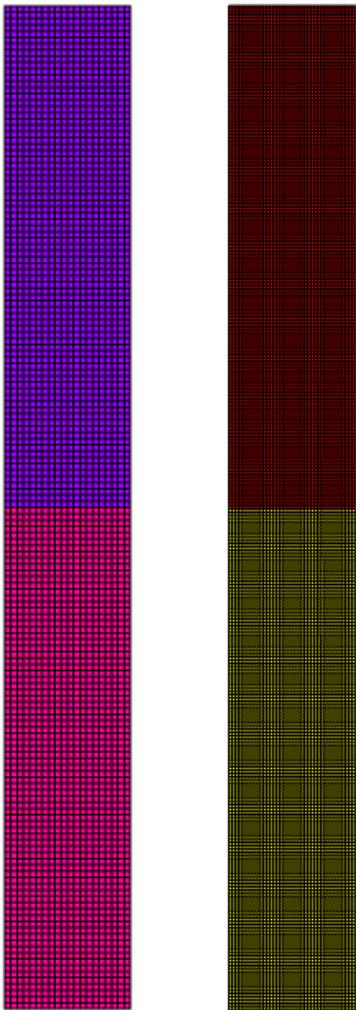
The size of the plastic zone at propagation,  $\Delta a = 60 \mu\text{m}$ ,  $s = 30 \mu\text{m}$ .  
Coarser meshes do not blunt.

$K_{ic} = 70 \text{ MPa}\text{m}$   
 $h = 30 \mu\text{m}$



*K*-field boundary condition

# Probing properties through tensile necking

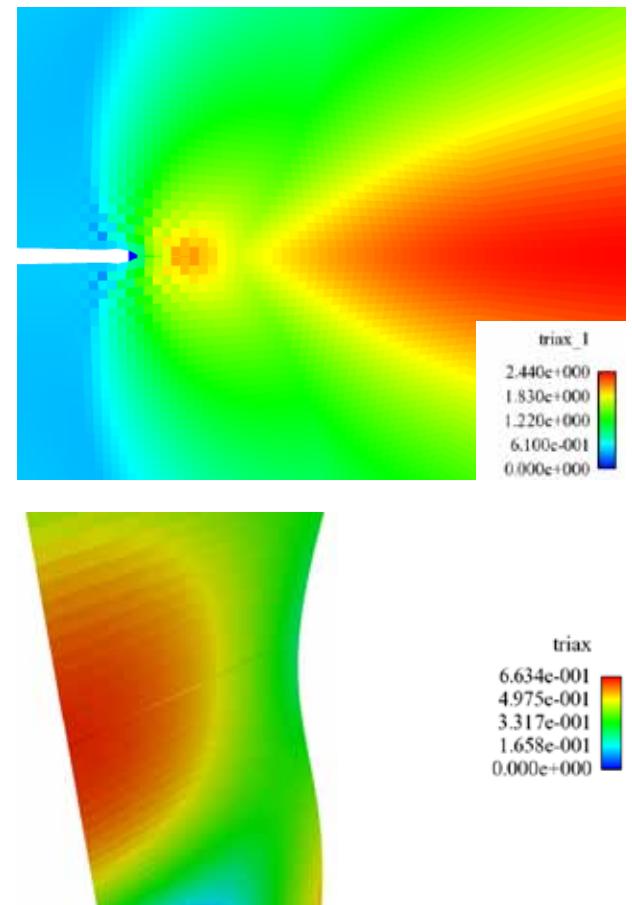
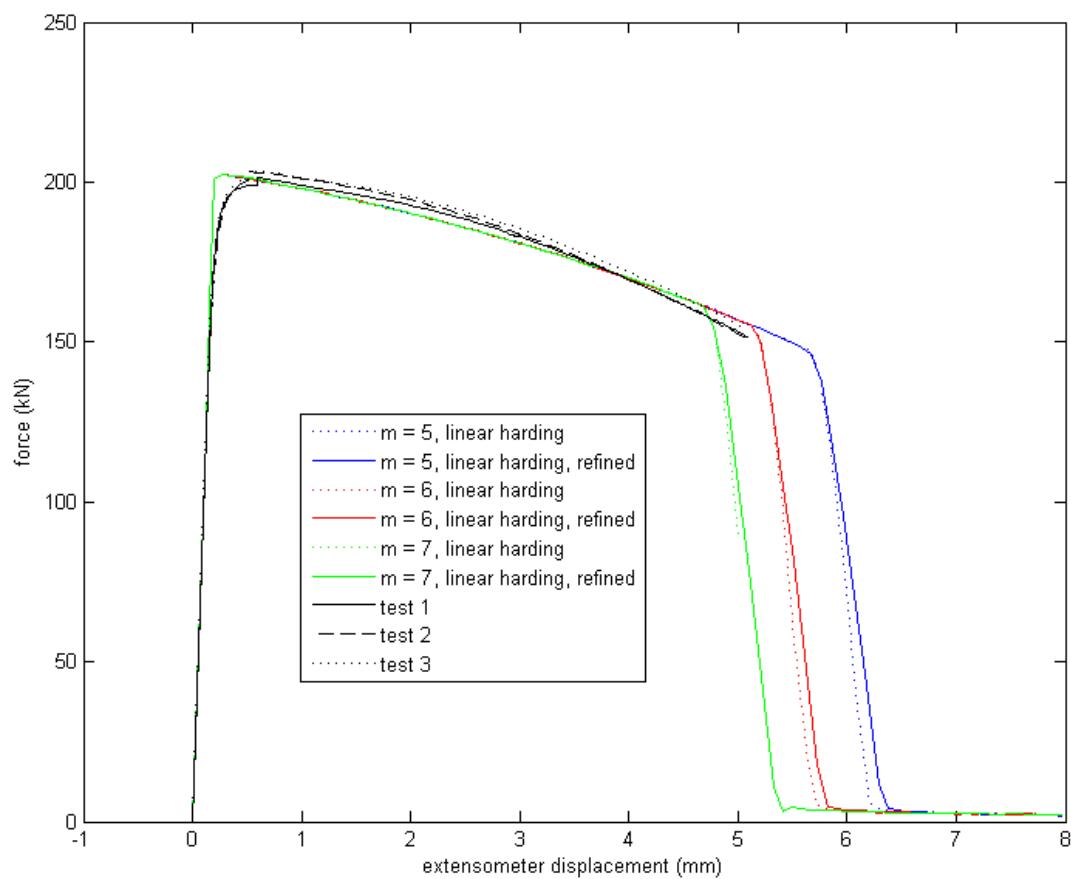


Bar radius: 12.7 mm  
Bar length: 50.8 mm  
Gauge section: 25.4 mm  
Coarse element size  $\sim$  635  $\mu\text{m}$   
Finer element size  $\sim$  318  $\mu\text{m}$

NOTE: A 2.54  $\mu\text{m}$  taper is enforced over  $\frac{1}{2}$  the gauge section to control the necking process.

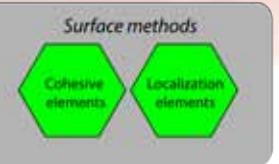
# Global and local information

The simple linear hardening model does quite well to match the slope during the necking process. However, given that we have one curve with no measurements of the neck, this is not too bad. We assert that we did not tune the failure model to the smooth necking simulation.

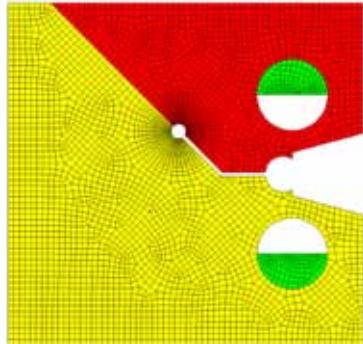


*Load-displacement is convergent*

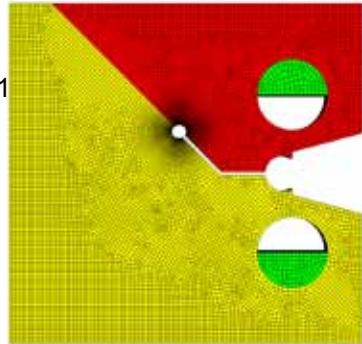
# Damage is convergent



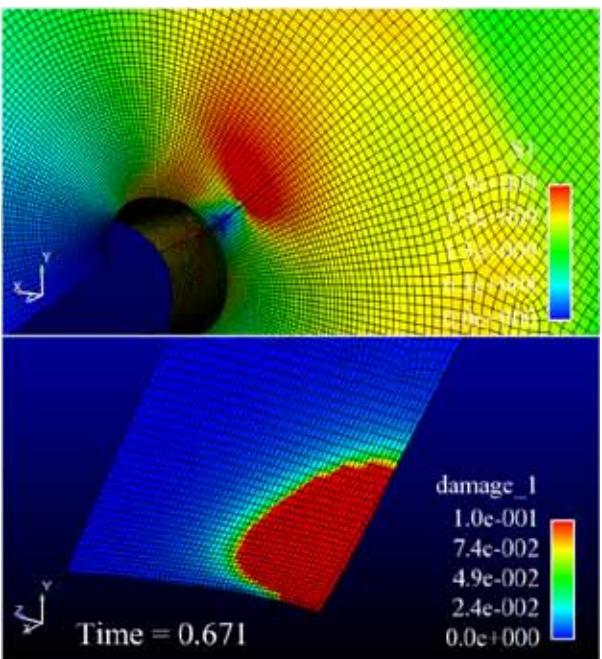
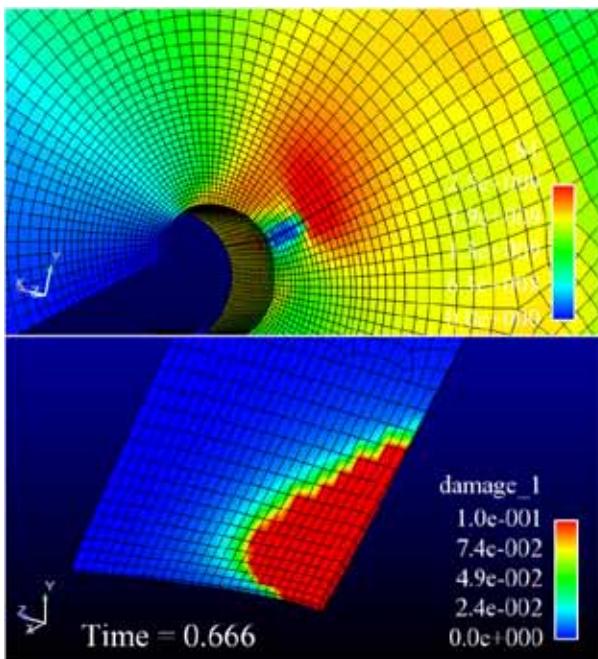
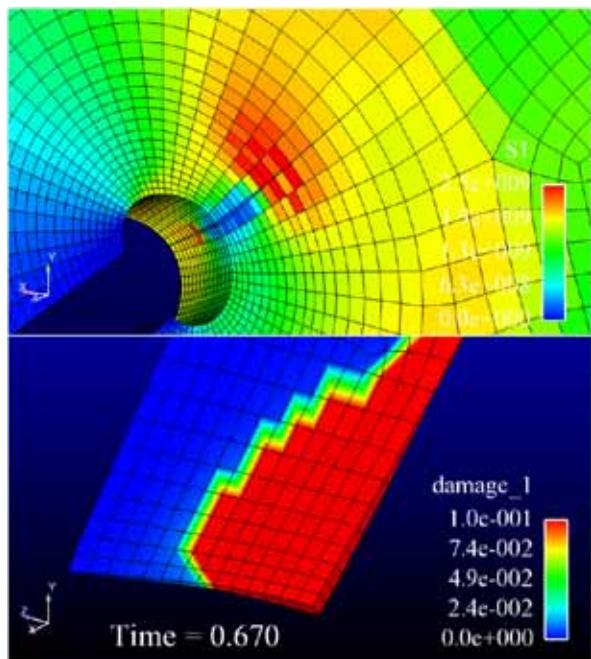
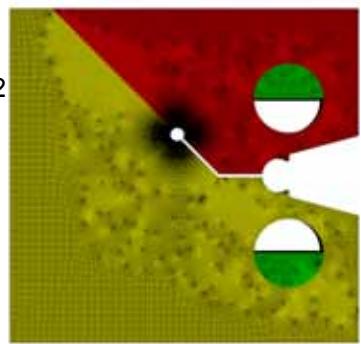
Mesh: 02  
Label: Medium  
Nodes: 29,535  
Elem: 23,673  
 $s \sim 120 \text{ mm}$



Mesh: 03  
Label: Fine  
Nodes: 141,831  
Elem: 125,865  
 $s \sim 60 \mu\text{m}$

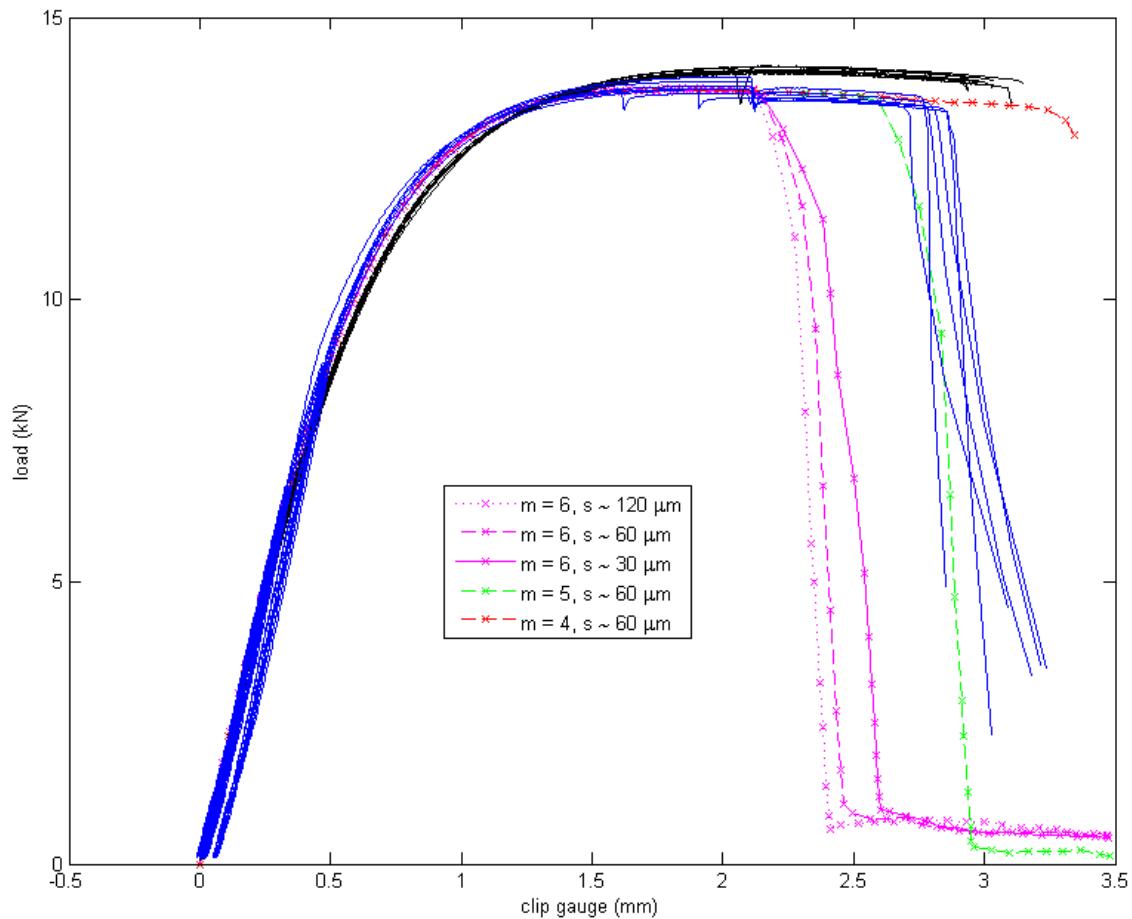
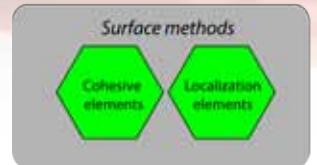


Mesh: 04  
Label: Finest  
Nodes: 1,079,622  
Elem: 1,015,812  
 $s \sim 30 \mu\text{m}$



Although at slightly different times, the evolution of damage is comparable for 03 & 04.

# Load-displacement is convergent



Boyce's lab:

- Load line rate is 0.0127 mm/s

Cordova's lab

- Load line rate before 2.03 mm is 0.0027 mm/s
- Load line rate after 2.03 mm is 0.00025 mm/s

# Element size on the order of $h$

Localization elements with no volume have membrane forces that scale with  $h$ .

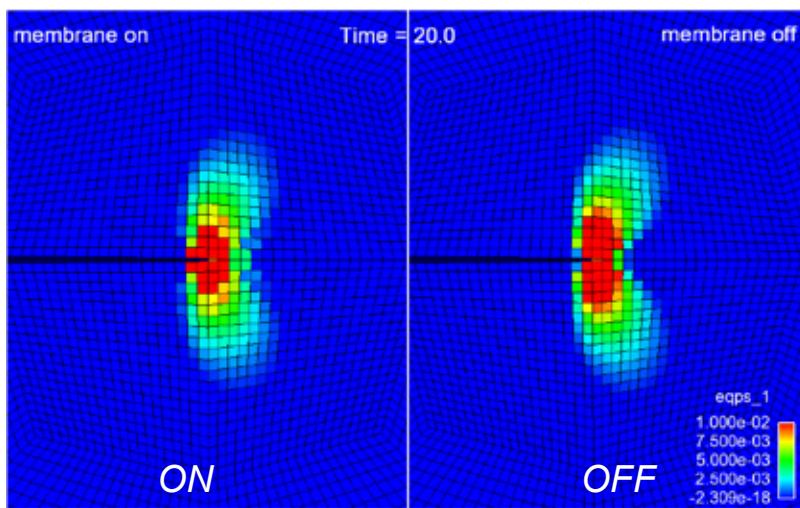
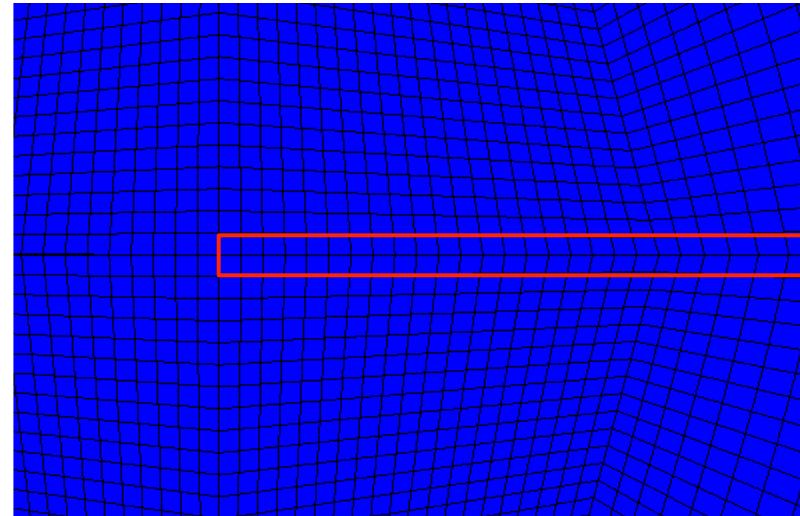
What if the mesh size  $s$  is order  $h$ ?

For ductile metals, this is the norm,  
the *plastic zone size*  $\sim$  *process zone size*

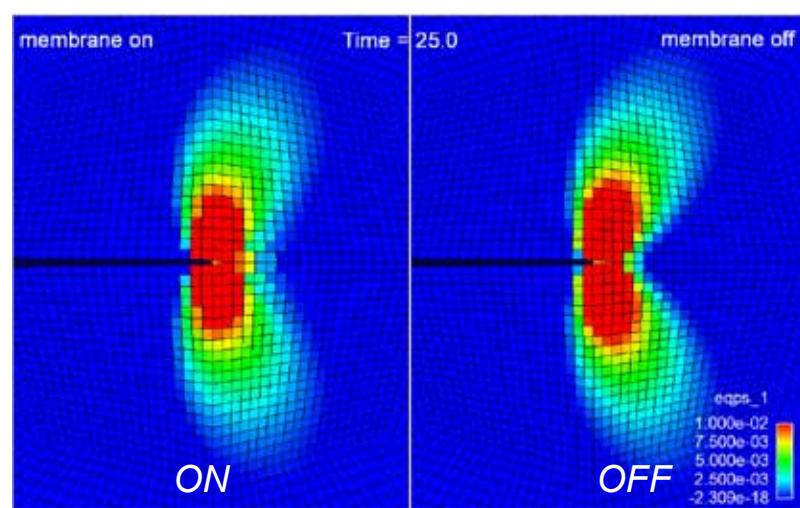
material: 2024-T3

yield stress: 375 MPa,  $K_{lc} \sim 30 \text{ MPa}\sqrt{\text{m}}$

mesh size  $s$ : 30  $\mu\text{m}$ ,  $h = 60 \mu\text{m}$



$$K = 20 \text{ MPa}\sqrt{\text{m}}$$



$$K = 25 \text{ MPa}\sqrt{\text{m}}$$

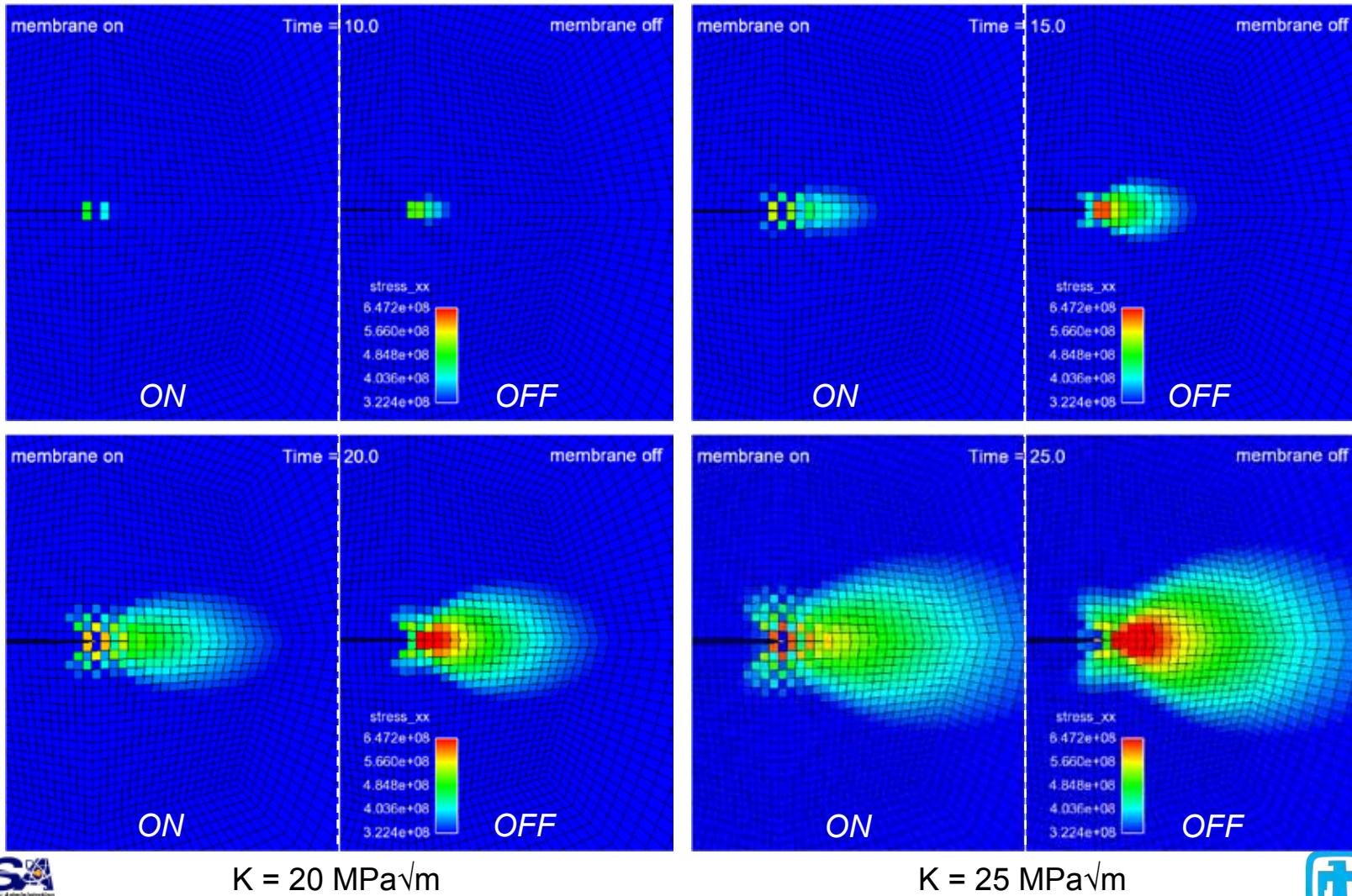
NOTE: The force calculation for membrane forces = off is “cohesive”.

# A case for no membrane forces for $s \sim h$

## *A case for eliminating membrane forces when the mesh size is order $h$*

$$K = 10 \text{ MPa}\sqrt{m}$$

$$K = 15 \text{ MPa}\sqrt{m}$$





# Conclusions

- *Developed methods have broad applicability*
- *Multiple paths towards regularization needed*
- *Localization elements provide regularization*
- *Changes to kinematics remedy issues of configuration, conjugacy, and objectivity*
- *Fitting process extrapolates plane-strain fracture toughness*
- *Case for ignoring membrane forces when element size is on order  $h$*
- *Implemented into Sandia production code, SierraSM*

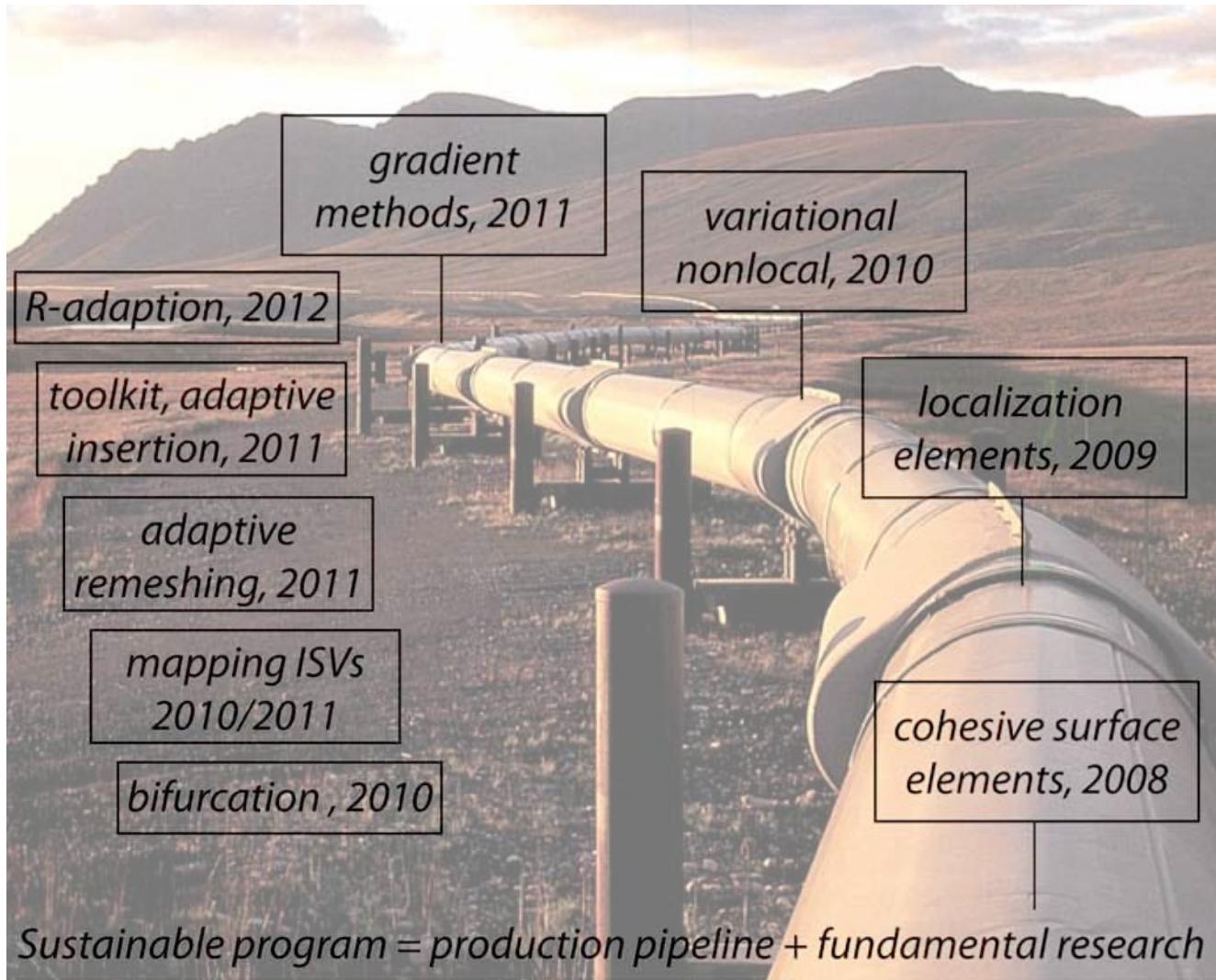
*Acknowledgement: This work was supported in part through the Joint DoD/DOE Munitions Technology Development Program.*



# *Extra Slides*

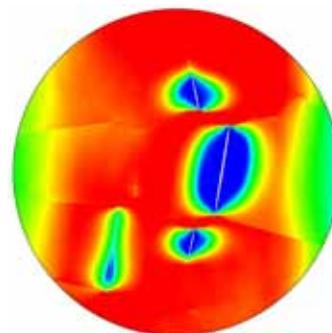
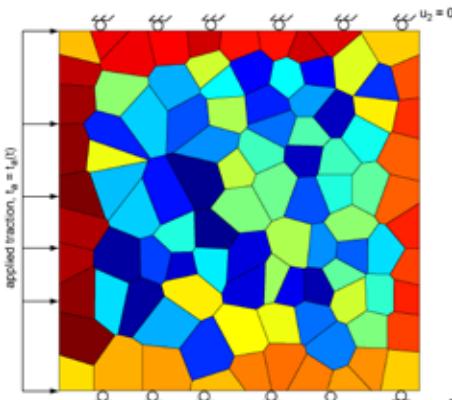
# Methods pipeline for SierraSM

*Basic research in engineering science is earned, not given. Production tools enable research.*

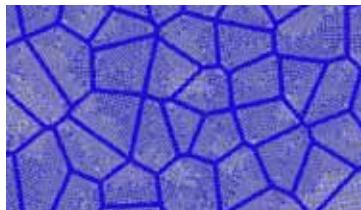


# Cohesive approaches

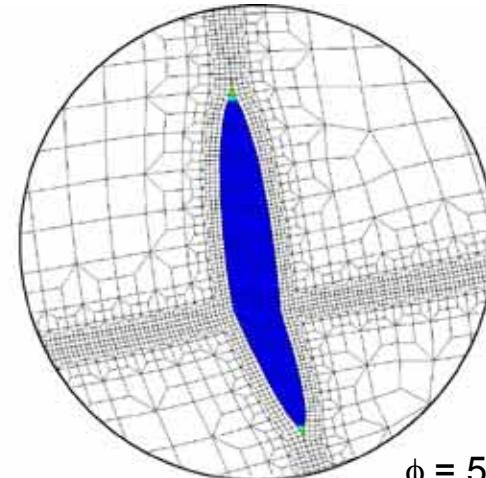
*Cohesive methods work well when we can lump all dissipation into surface separation.  
Ductile fracture challenges this approach (2 model problem, easily incorporating triaxiality)*



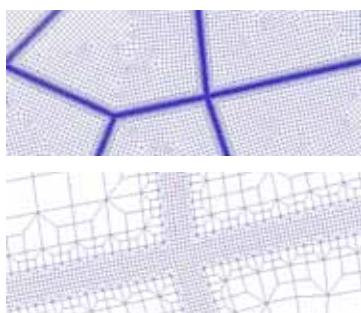
crack initiation



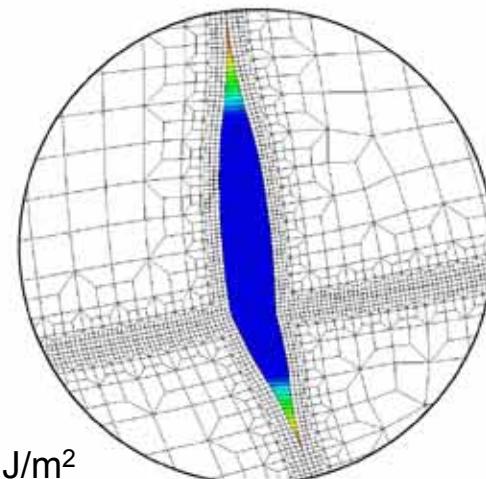
crack propagation



$\phi = 5 \text{ J/m}^2$



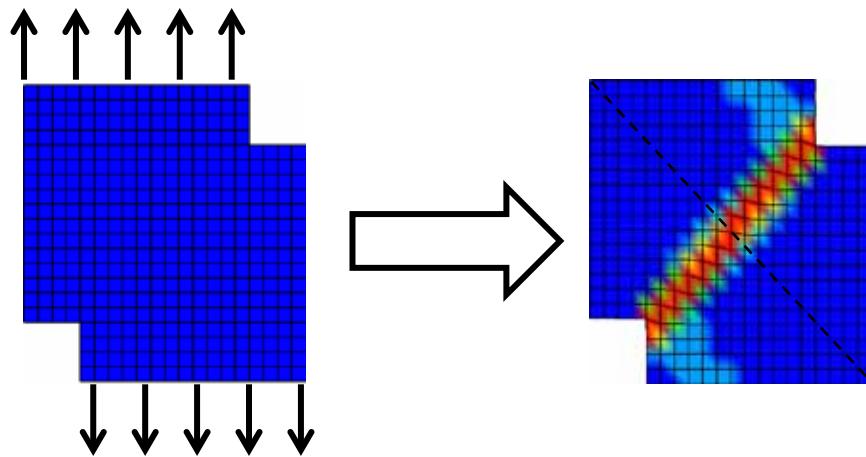
crack interaction



$\phi = 10 \text{ J/m}^2$

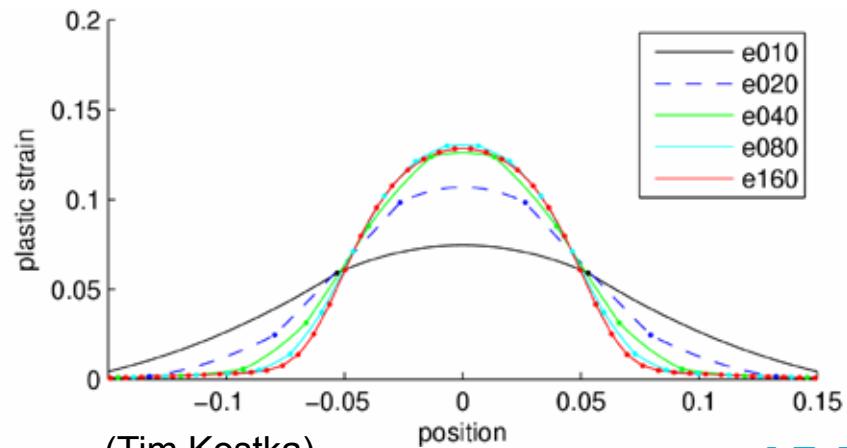
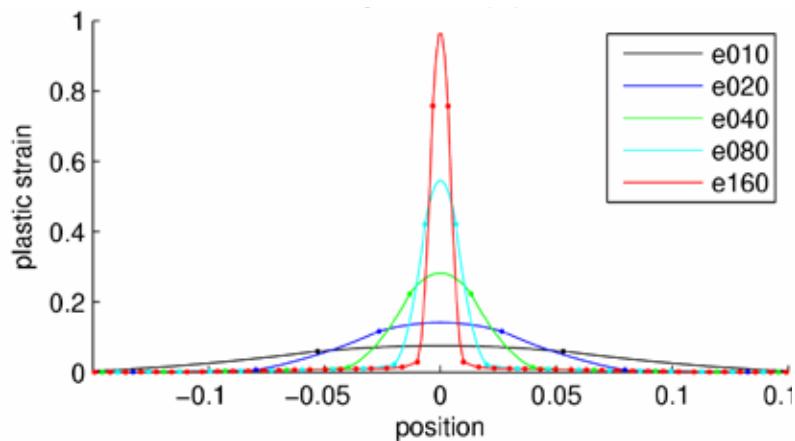
# Nonlocal approaches

*Nonlocality promising but we would like to simplify the numerics, simplify behavior at boundaries, and ensure scalability for massively parallel simulations.*



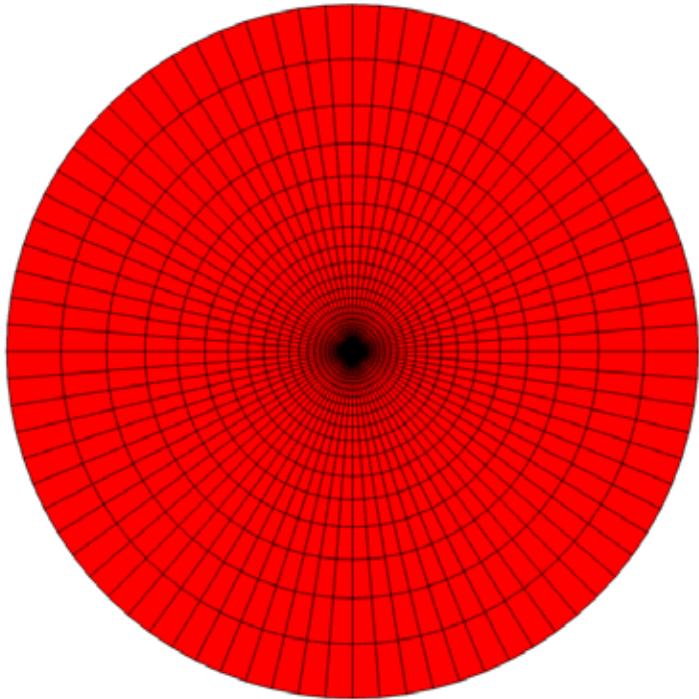
$$\dot{\hat{\varepsilon}}(\underline{x}) = \frac{\sum_{i=1}^N w(|\underline{x}_i - \underline{x}|) \dot{\varepsilon}(\underline{x}_i) V_i}{\sum_{i=1}^N w(|\underline{x}_i - \underline{x}|) V_i}$$
$$w(\rho) = \left[ 1 + \left( \frac{\rho}{L} \right)^p \right]^{-q}$$

(LS-Dyna, single point integration)



(Tim Kostka)

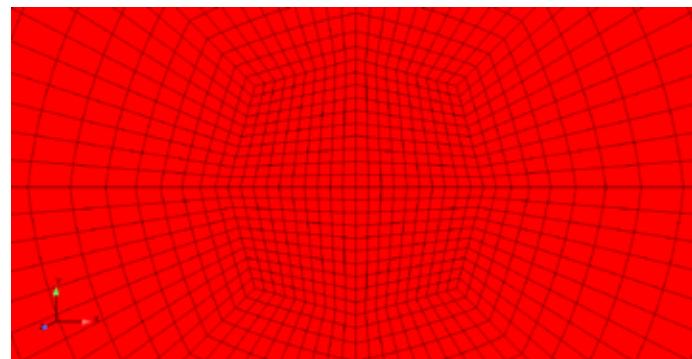
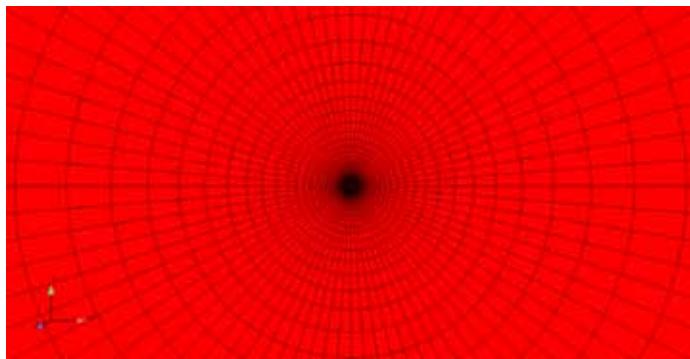
# K-field simulations



Given a node set on the boundary, we can apply a displacement field that enforces mode I,  $K_I$ , and mode II,  $K_{II}$ , stress intensity factors in plane-strain.

$$u_1 = \frac{K_I}{\mu} \sqrt{\frac{r}{2\pi}} \left[ 1 - 2\nu + \sin^2 \frac{\theta}{2} \right] \cos \frac{\theta}{2} + \frac{K_{II}}{\mu} \sqrt{\frac{r}{2\pi}} \left[ 2 - 2\nu + \cos^2 \frac{\theta}{2} \right] \sin \frac{\theta}{2}$$
$$u_2 = \frac{K_I}{\mu} \sqrt{\frac{r}{2\pi}} \left[ 2 - 2\nu - \cos^2 \frac{\theta}{2} \right] \sin \frac{\theta}{2} + \frac{K_{II}}{\mu} \sqrt{\frac{r}{2\pi}} \left[ -1 + 2\nu + \sin^2 \frac{\theta}{2} \right] \cos \frac{\theta}{2}$$

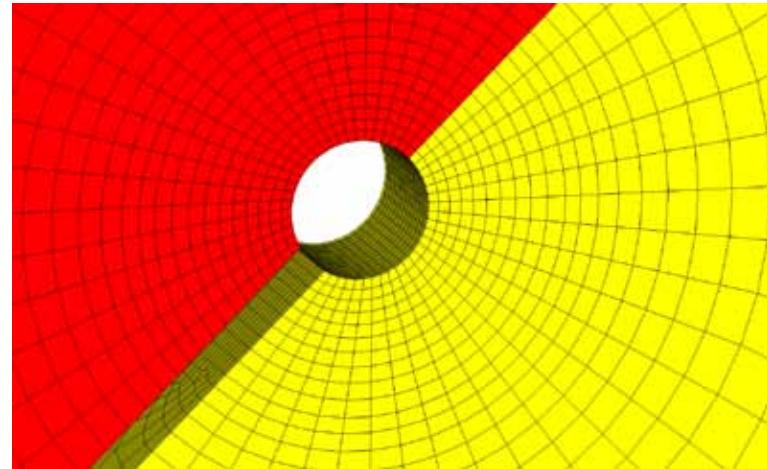
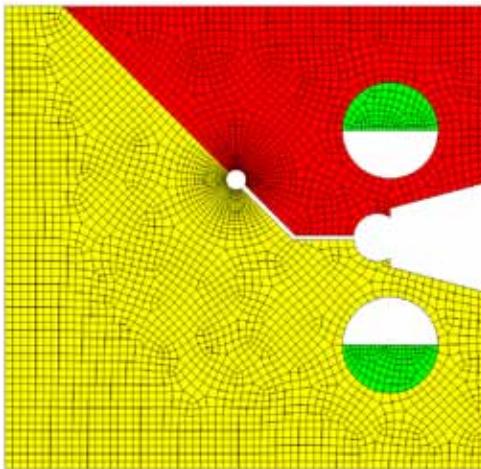
Given  $K_{Ic} = 70 \text{ MPa}\sqrt{\text{m}}$  and  $\sigma_y = 1.25 \text{ GPa}$ , the plastic zone size  $r_p$  is roughly 0.5 mm (500  $\mu\text{m}$ ). We set the radius of the disk  $r_d$  to be 150 mm.  $r_d/r_p \sim 300$ , small-scale yielding. For small-scale yielding, we can use the K-field boundary condition to imply parameters governing the evolution of damage (m).



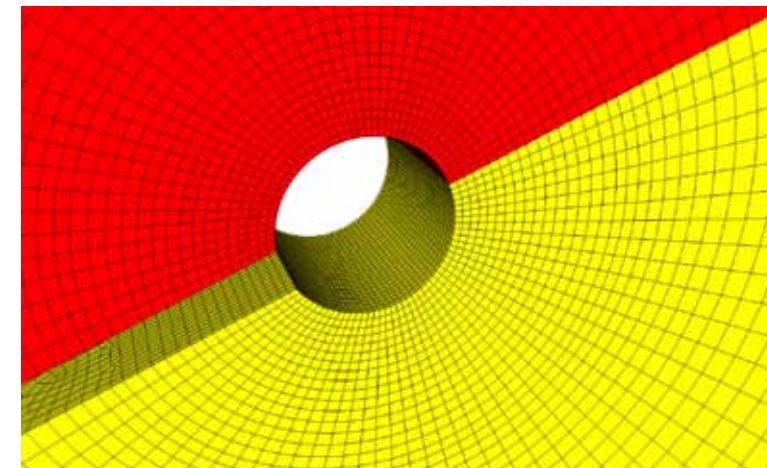
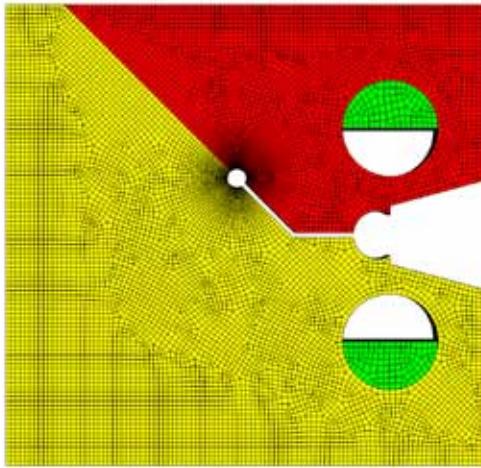
$s = 60 \mu\text{m}$

# Discretization in length and time

Mesh: 02  
Label: Medium  
Nodes: 29,535  
Elements: 23,673  
 $s \sim 120 \mu\text{m}$



Mesh: 03  
Label: Fine  
Nodes: 141,831  
Elements: 125,865  
 $s \sim 60 \mu\text{m}$

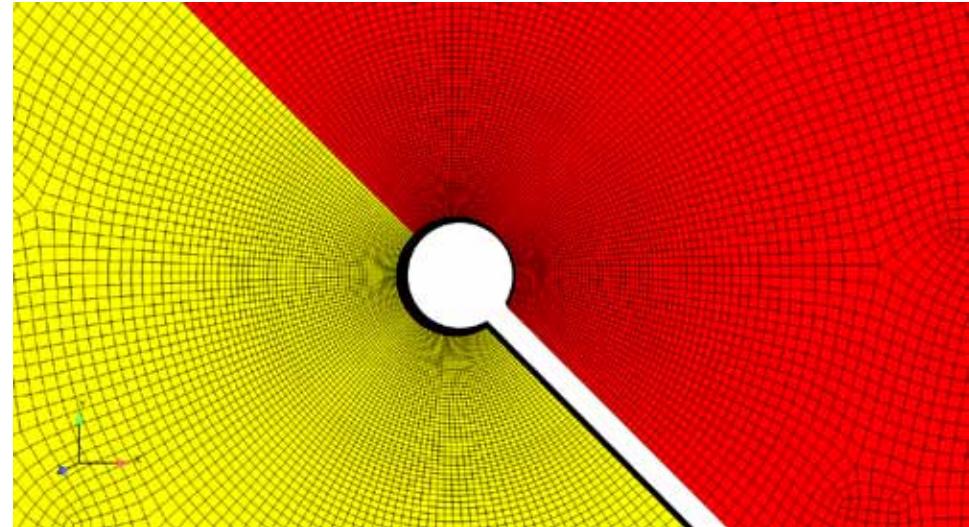
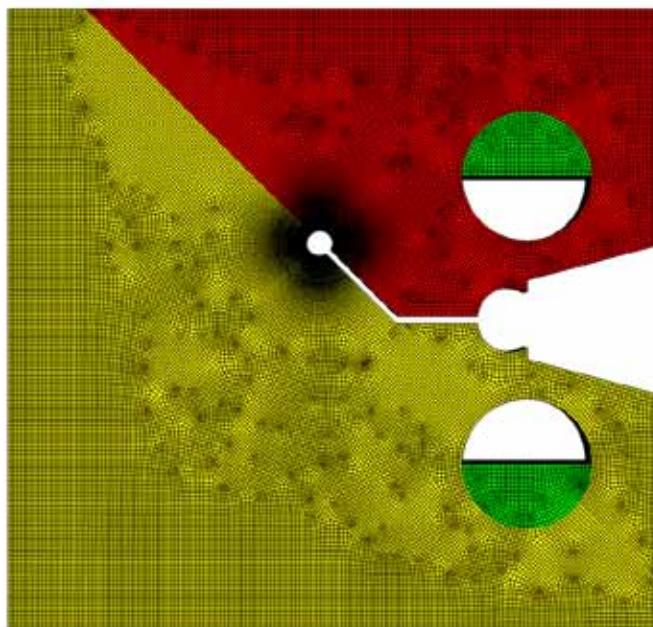


Time discretization: A minimum of 500 time steps were employed with adaptive time stepping (1000 steps specified).

NOTE: Stiff, elastic plugs used to apply the pinned, line load. Contact could be used but typically aids instability during unloading (propagation).

# More refinement

Mesh: 04  
Label: Finest  
Nodes: 1,079,622  
Elements: 1,015,812  
 $s \sim 30 \mu\text{m}$

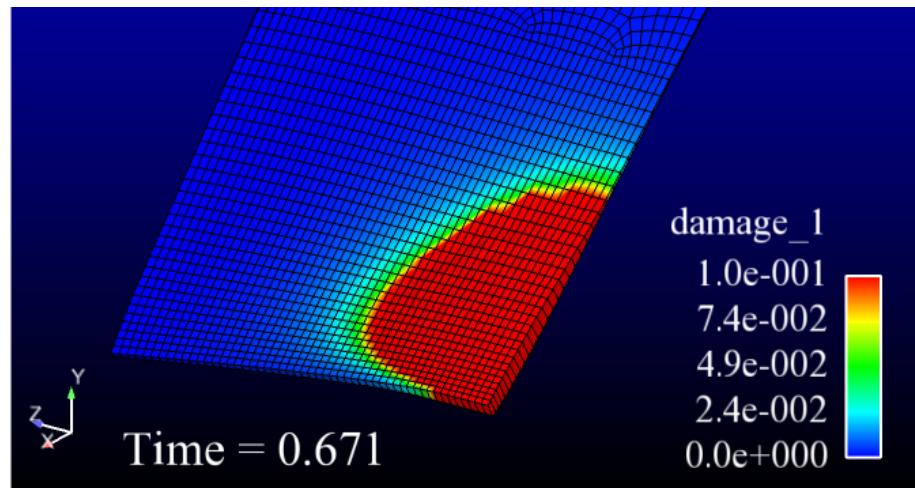




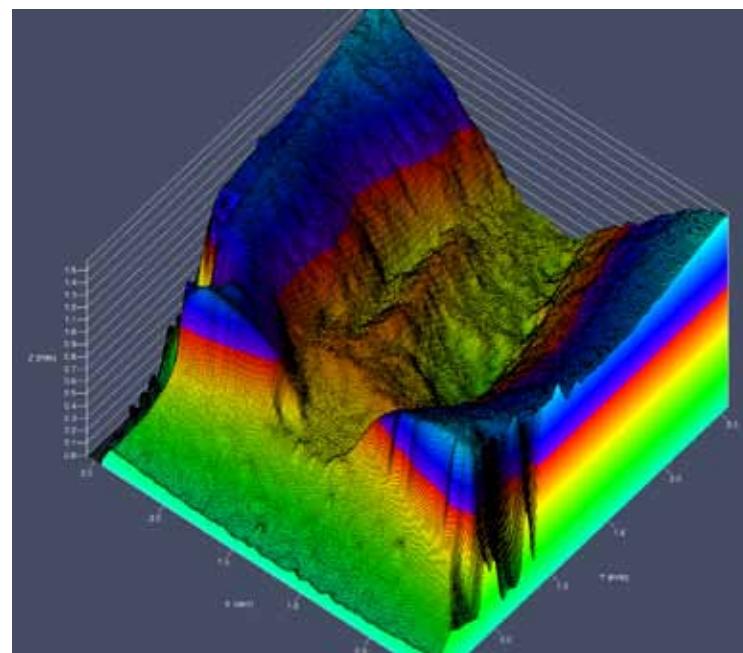
# Life is complicated



(Cordova)



Shear lips, anyone? anyone? Not good.



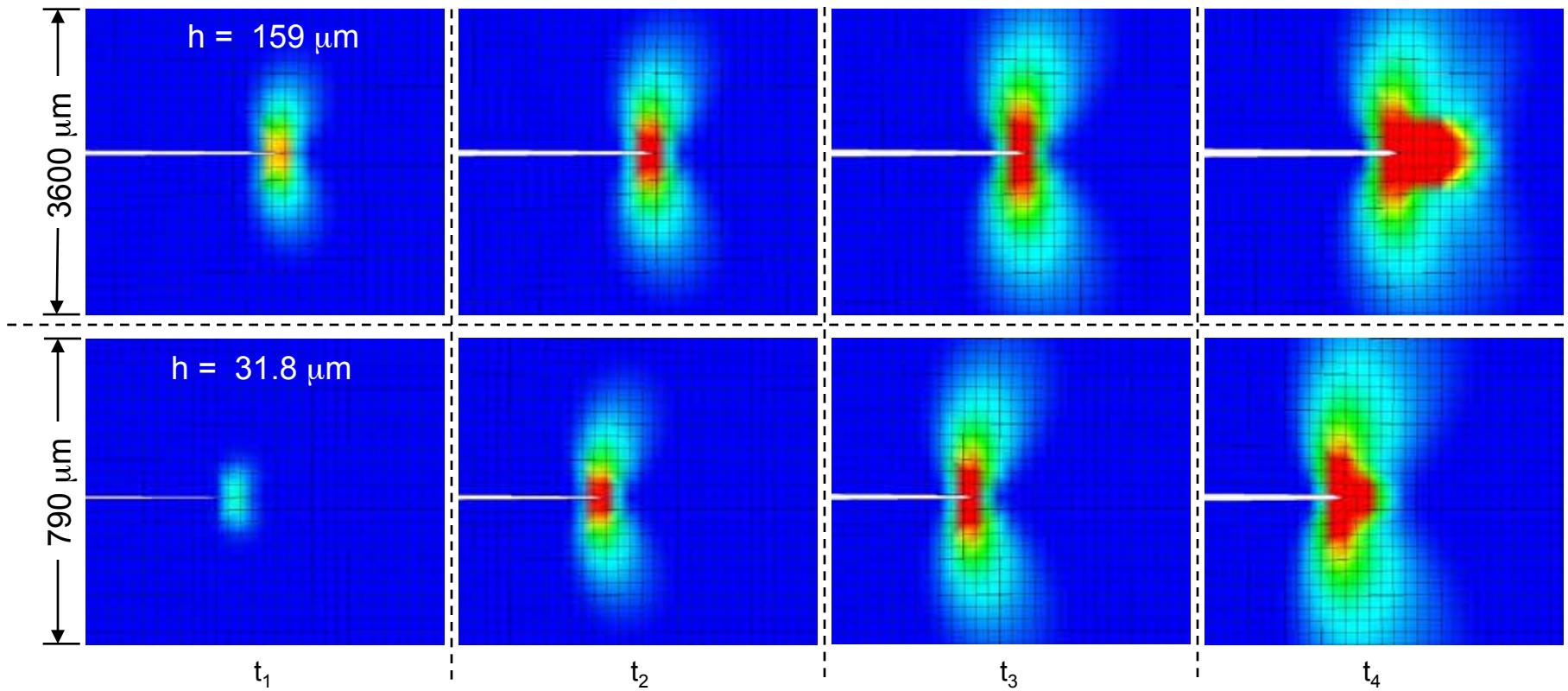


# Planned studies & improvements

- Improvements
  - Revised multiplicative decomposition (implemented)
  - Membrane forces on/off (implemented)
  - Objective velocity gradient update (implemented)
  - Stable time step estimate (to do)
- Planned studies
  - Weld Failure on the W-87 (Kostka, Templeton)
  - Membrane forces on X-Prize (Foulk, Emery, Boyce)
  - Implicit/explicit dynamics V&V study (Dike)
  - Adaptive remeshing (Emery, Veilleux)
  - Applicability to crack-band methods (MLEP-fail) (Veilleux)

# Seeking a length scale for plasticity

Because the plastic zone size is tied to damage, plasticity is also mesh dependent

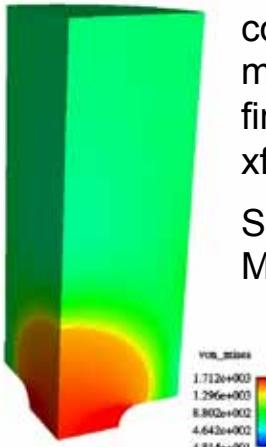
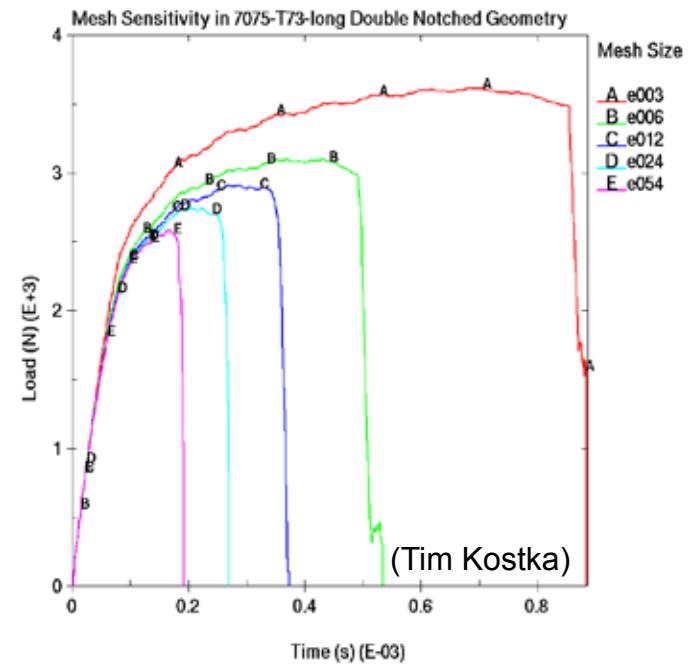
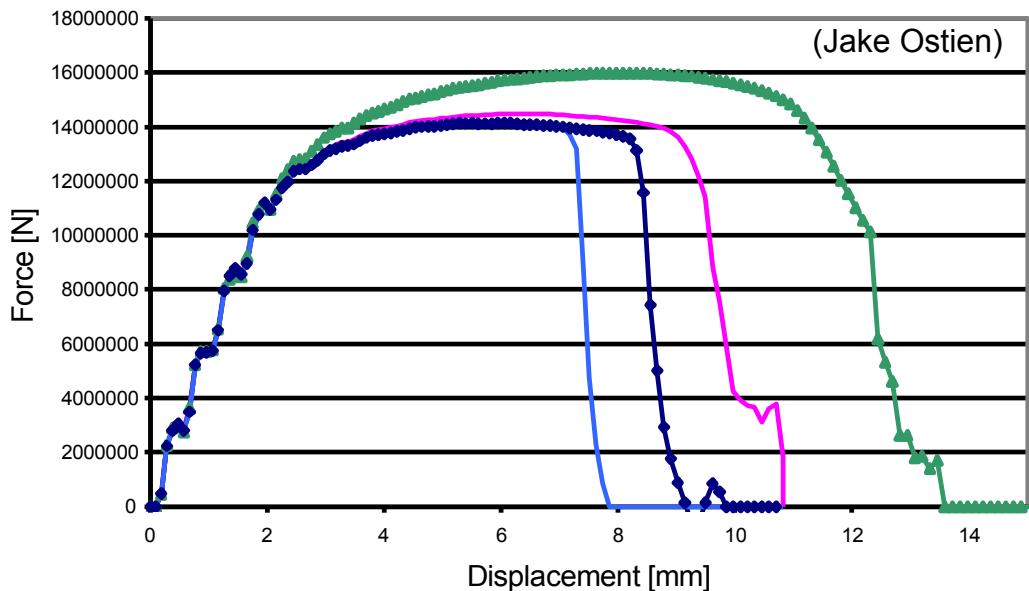


$$r_p = \frac{K^2}{4\pi\sigma_{ys}^2} \left[ \frac{3}{2} + (1 - 2\nu)^2 \right]$$

$$K_{1c} = 28.8 \text{ MPav/m} \text{ (D. Dawson)} \quad r_p = 1390 \text{ } \mu\text{m} \text{ (major axis)}$$

Note: Contours of equivalent plastic strain, 0.0 to 2.0%. Time  $t_4$  taken at propagation.

# Mesh dependence under notched tension



coarse – 752 elements  
med – 6016 elements  
fine – 48128 elements  
xfine – 385024 elements  
Strain rate = 50/s  
Material = A286

- Specimens of various notched radii for “fitting”
- The results depend on the mesh size
- The fitted damage parameters are convoluted
- Goodness of the model is not known
- The issue stems from the governing PDEs

*Finite elements is just a method for solving a partial differential equation. The real issue is that we are using a local model without a length scale to solve a localization problem. It corrupts what we hold sacred...*