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Verification and Validation of a Variational Cohesive Phase-Field Fracture Model

Andrew Stershic, Kyle Karlson, Brandon Talamini*

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onal Nuclear Security Administration under contract DE-NA0003525.

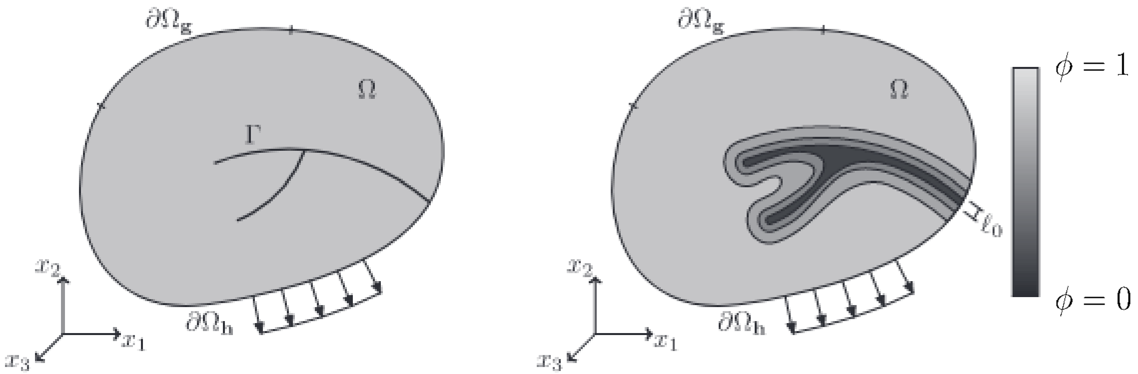
Presentation Overview

- Phase Field Fracture Model
- Characterization Data
- Calibration Strategy
- Validation Problem
- Preliminary Results
- Next Steps

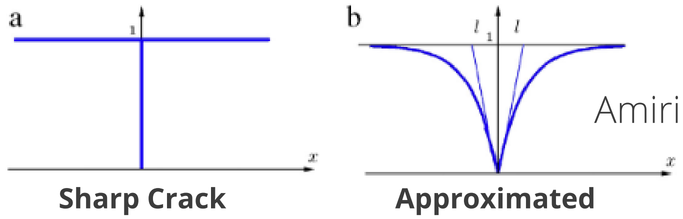
Phase field model for fracture

Concept:

- Derived from Griffith brittle fracture, G_c
- Represent discrete cracks as "smeared" continuum damage fields
- Inject length scale: infinitesimal → finite-width
- Variational: minimize energy functional
- Reformulate fracture problem as a coupled system of PDEs, greatly simplifying solving
- Inherently captures crack nucleation, propagation, bifurcation; mesh-independent
- Approximates fracture for length scale $\ell_0 \rightarrow 0^+$



Borden *et al.* (2014)



Amiri *et al.* (2016)

$$\hat{\psi}^* = \min_{u,z}\left(\int_\Omega \hat{\psi}_{\text{mech}}(u, z)\,d\Omega + \int_\Gamma G_c\,d\Gamma\right)$$

$$\downarrow$$

$$\hat{\psi}^* = \min_{u,z,\phi}\left(\int_\Omega \hat{\psi}_{\text{mech}}(u, z, \phi) + \hat{\psi}_{\text{frac}}(G_c, \phi, \nabla\phi)\,d\Omega\right)$$

Phase Field models from literature

Classical model / AT-2

Total Energy Functional:

$$\hat{\psi}^* = \min_{u,z,\phi} \left(\int_\Omega \hat{\psi}_{\text{mech}}(u, z, \phi) + \hat{\psi}_{\text{frac}}(G_c, \phi, \boldsymbol{\nabla}\phi) \, d\Omega \right)$$

Euler-Lagrange Equations:

$$\boldsymbol{\nabla} \cdot \frac{\partial \psi}{\partial \boldsymbol{\nabla} u} - \frac{\partial \psi}{\partial u} = 0 \qquad \boldsymbol{\nabla} \cdot \frac{\partial \psi}{\partial z} - \frac{\partial \psi}{\partial z} = 0$$

$$\boldsymbol{\nabla} \cdot \frac{\partial \psi}{\partial \boldsymbol{\nabla} \phi} - \frac{\partial \psi}{\partial \phi} = 0$$

Phase-Field Evolution

$$2G_c \ell \Delta\phi - 2\phi(\psi^e + \psi^p) + \frac{G_c}{2\ell}(1 - \phi) = 0$$

Driving Energies & Degradation Functions:

$$\hat{\psi}_{\text{mech}}(u, z, \phi) = g(\phi)\psi^e(u, z) + h(\phi)\psi^p(z)$$

$$g(\phi) = h(\phi) = \phi^2$$

Fracture Energy Approximation Functional:

$$\hat{\psi}_{\text{frac}}(G_c, \phi, \boldsymbol{\nabla}\phi) = G_c \frac{1}{4\ell} \left((1 - \phi)^2 + 4\ell^2 \boldsymbol{\nabla}\phi \cdot \boldsymbol{\nabla}\phi \right)$$

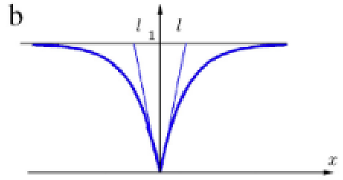
$$\updownarrow$$

$$1 - \phi + 4\ell^2 \Delta\phi = 0$$

$$\updownarrow$$

$$\phi(x) = 1 - \exp\left(\frac{|x|}{2\ell} \right)$$

Amiri *et al.* (2016)



Phase Field models from literature

Threshold model / AT-1

Total Energy Functional:

$$\hat{\psi}^* = \min_{u,z,\phi} \left(\int_\Omega \hat{\psi}_{\text{mech}}(u, z, \phi) + \hat{\psi}_{\text{frac}}(G_c, \phi, \boldsymbol{\nabla}\phi) \, d\,\Omega \right)$$

Euler-Lagrange Equations:

$$\boldsymbol{\nabla} \cdot \frac{\partial \psi}{\partial \boldsymbol{\nabla} u} - \frac{\partial \psi}{\partial u} = 0 \qquad \boldsymbol{\nabla} \cdot \frac{\partial \psi}{\partial z} - \frac{\partial \psi}{\partial z} = 0$$

$$\boldsymbol{\nabla} \cdot \frac{\partial \psi}{\partial \boldsymbol{\nabla} \phi} - \frac{\partial \psi}{\partial \phi} = 0$$

Phase-Field Evolution

$$\frac{3G_c\ell}{8}\Delta\phi - 2\phi(\psi^e + \psi^p) + \frac{3G_c\ell}{8} = 0$$

Driving Energies & Degradation Functions:

$$\hat{\psi}_{\text{mech}}(u, z, \phi) = g(\phi)\psi^e(u, z) + h(\phi)\psi^p(z)$$

$$g(\phi) = h(\phi) = \phi^2$$

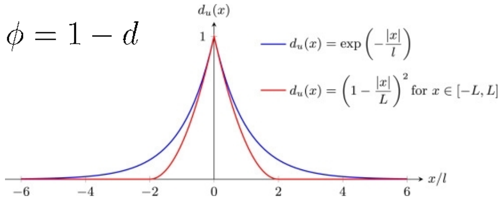
Fracture Energy Approximation Functional:

$$\hat{\psi}_{\text{frac}}(G_c, \phi, \boldsymbol{\nabla}\phi) = G_c \frac{3}{8\ell}\left((1-\phi) + \ell^2 \boldsymbol{\nabla}\phi \cdot \boldsymbol{\nabla}\phi\right)$$

$$1 + 2\ell^2 \Delta\phi = 0$$

$$\phi(x) = 1 - \left(1 - \frac{|x|}{\sqrt{2}\ell}\right)^2$$

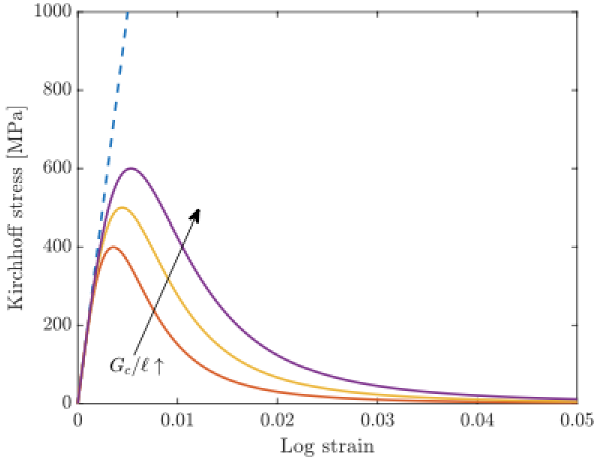
$\phi = 1 - d$



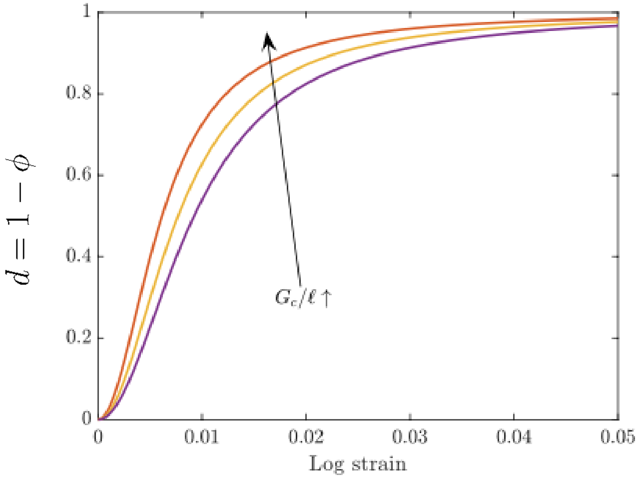
Geelen *et al.* (2016)

Phase Field models from literature

Classical model



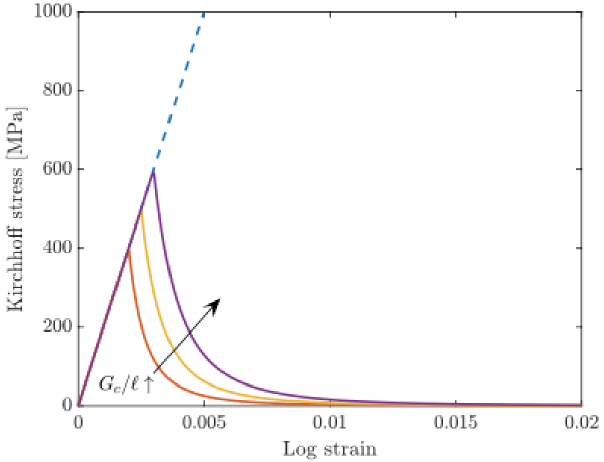
$$\sigma_{max} = \sqrt{\frac{27 G_c E}{256 \ell}}$$



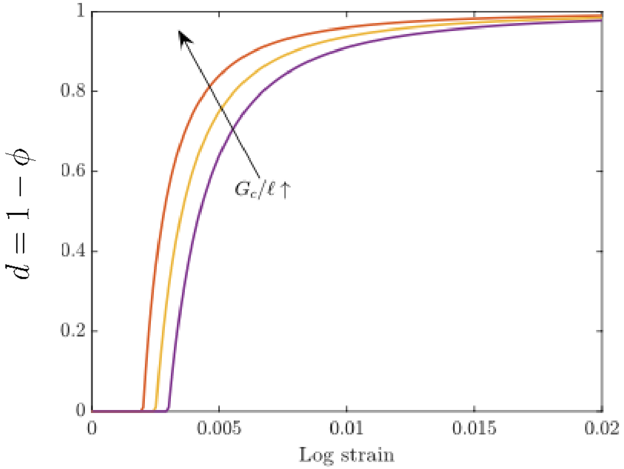
Damage begins at any level of deformation

Threshold model

Stershic *et al.* (2018)



$$\sigma_{max} = \sqrt{\frac{3 G_c E}{8 \ell}} = \sqrt{2 E \psi_{crit}}$$



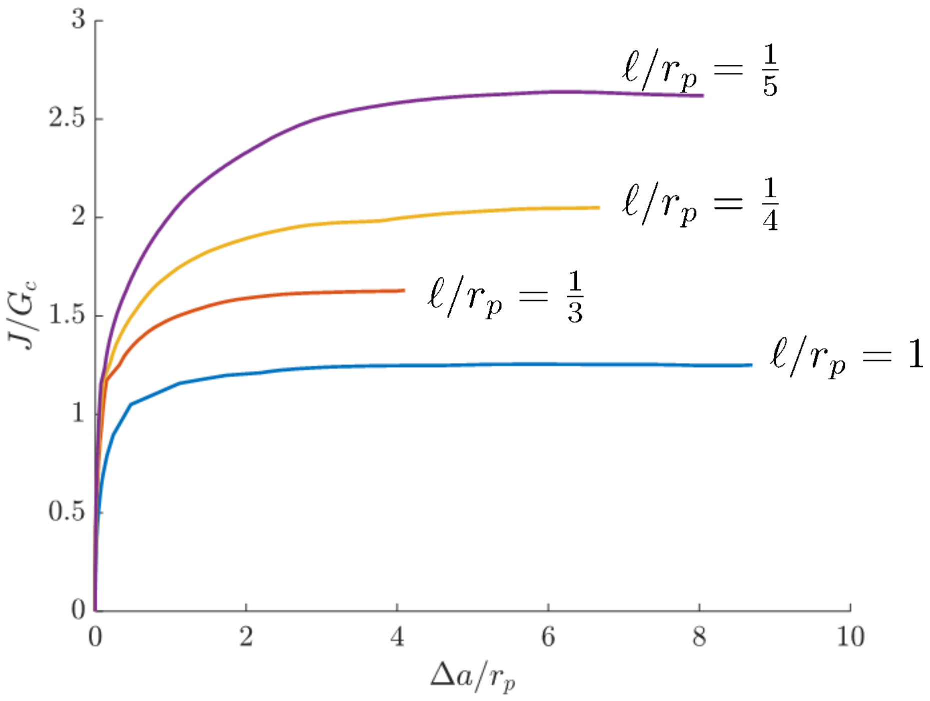
Damage begins after energy threshold is reached

$$\psi_{crit} = \frac{3 G_c}{16 \ell}$$

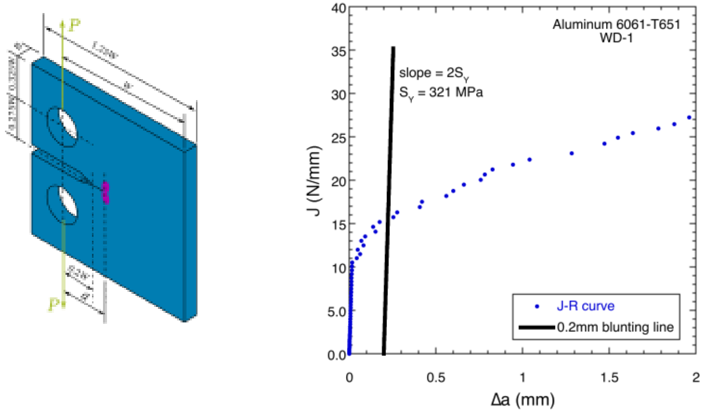
- Critical stress depends on length scale ℓ. This has been proven to work well on brittle materials.
- It is inappropriate for plastic materials, where a finite yield stress determines non-trivial material behavior.

Crack growth resistance predictions

Stershic *et al.* (2018)



- ℓ is indeed a material parameter!
- Serves a similar role as cohesive strength in cohesive zone models
- Can calibrate ℓ to standard fracture tests



Data courtesy of Chris San Marchi (SNL)

New Phase Field Model

Cohesive / Lorentz Model – new parameter ψ_{crit}

Talamini *et al.* (2021)

Total Energy Functional:

$$\hat{\psi}^* = \min_{u,z,\phi} \left(\int_\Omega \hat{\psi}_{\text{mech}}(u, z, \phi) + \hat{\psi}_{\text{frac}}(G_c, \phi, \nabla\phi)\, d\,\Omega \right)$$

Euler-Lagrange Equations:

$$\nabla \cdot \frac{\partial \psi}{\partial \nabla u} - \frac{\partial \psi}{\partial u} = 0 \qquad \nabla \cdot \frac{\partial \psi}{\partial z} - \frac{\partial \psi}{\partial z} = 0$$

$$\nabla \cdot \frac{\partial \psi}{\partial \nabla \phi} - \frac{\partial \psi}{\partial \phi} = 0$$

Phase-Field Evolution

$$\frac{3G_c\ell}{8}\Delta\phi - \left(g'(\phi)\psi^e + h'(\phi)\psi^p\right) + \frac{3G_c\ell}{8} = 0$$

(nonlinear PDE! , generally)

Driving Energies & Degradation Functions:

$$\hat{\psi}_{\text{mech}}(u, z, \phi) = g(\phi)\psi^e(u, z) + h(\phi)\psi^p(z)$$

$$g(\phi) = h(\phi) = \frac{\phi^2}{\left(1 - \left(\frac{3G_c}{16\ell\psi_{crit}} - 1\right)(1 - \phi)\right)^2}$$

If $\psi_{crit} = \frac{3G_c}{16\ell}$, threshold model recovered:

$$g(\phi) = h(\phi) = \phi^2$$

Fracture Energy Approximation Functional:

$$\hat{\psi}_{\text{frac}}(G_c, \phi, \nabla\phi) = G_c \frac{3}{8\ell}\left((1 - \phi) + \ell^2 \nabla\phi \cdot \nabla\phi\right)$$

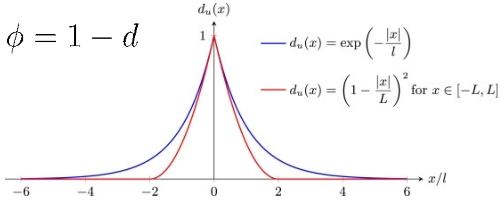
$$\updownarrow$$

$$1 + 2\ell^2 \Delta\phi = 0$$

$$\updownarrow$$

$$\phi(x) = 1 - \left(1 - \frac{|x|}{\sqrt{2}\ell}\right)^2$$

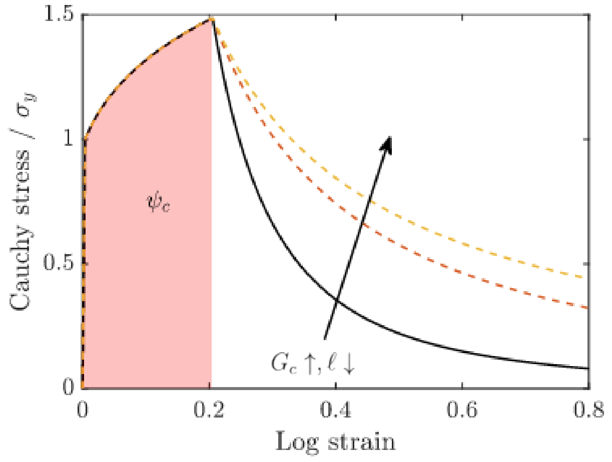
$\phi = 1 - d$



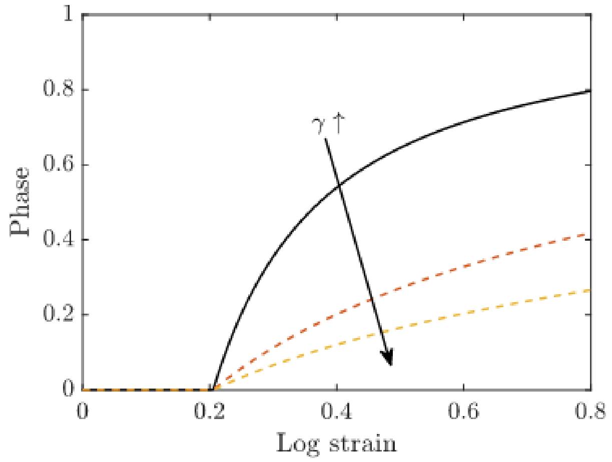
New Phase Field Model

Cohesive / Lorentz Model

Talamini *et al.* (2021)



$$\sigma_{max} = \sqrt{2E\psi_{crit}}$$

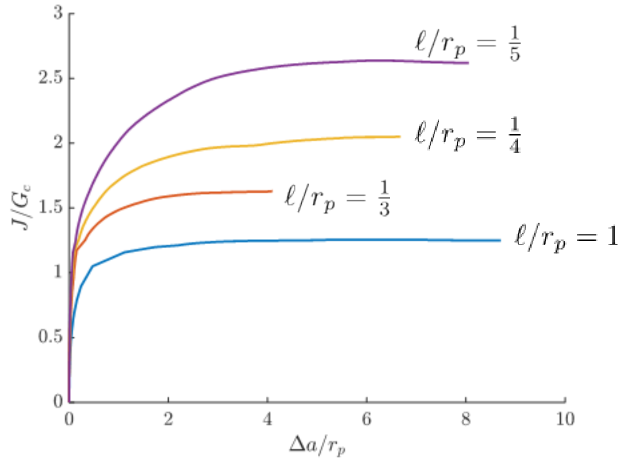


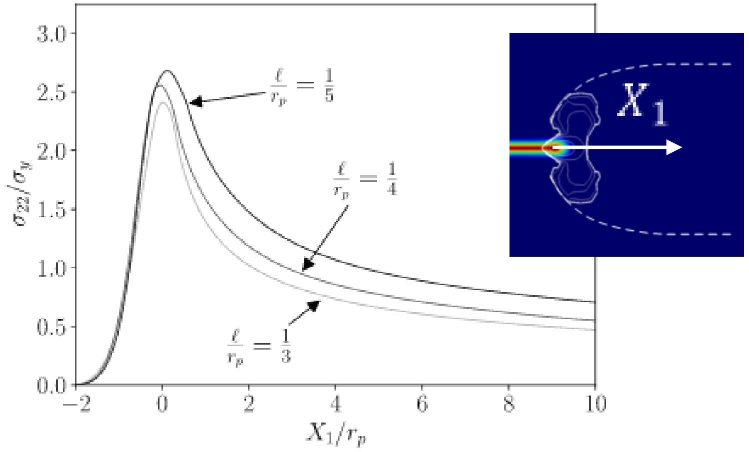
Damage begins after energy threshold is reached

- Critical strength now independent of length scale
- ψ_{crit} is a material parameter with physical interpretation – energy threshold
- ℓ is a numerical parameter

New Phase Field Model

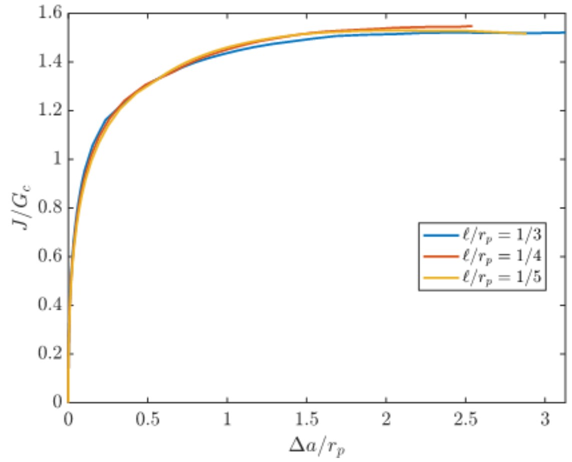
Threshold model

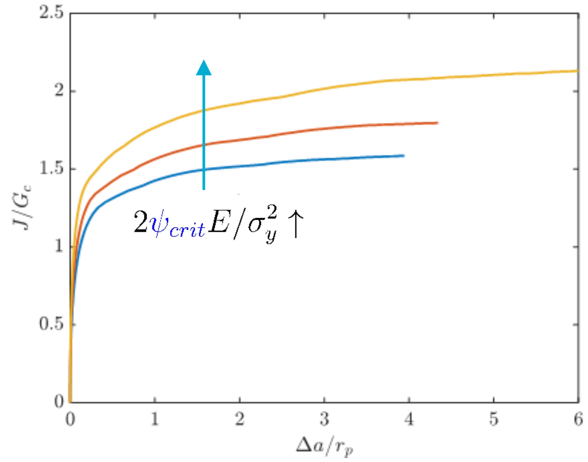


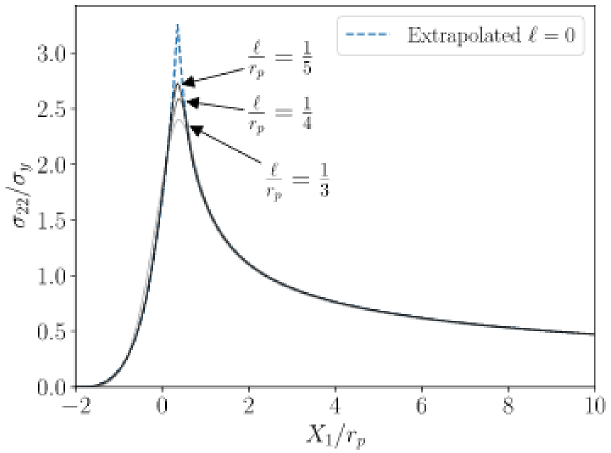


Cohesive / Lorentz Model

Talamini *et al.* (2021)







- Yields convergent R-curve behavior (wrt length scale)
- Can now adjust length scale to problem size
- Can increase process zone size (engineering approximation) to ease mesh requirements

Plastic-Damage Coupling

Hu *et al.* (2021)

Consider Plastic-Damage Coupling:

- Plastic Yield Surface (from $\nabla \cdot \frac{\partial \psi}{\partial z} - \frac{\partial \psi}{\partial z} = 0$):

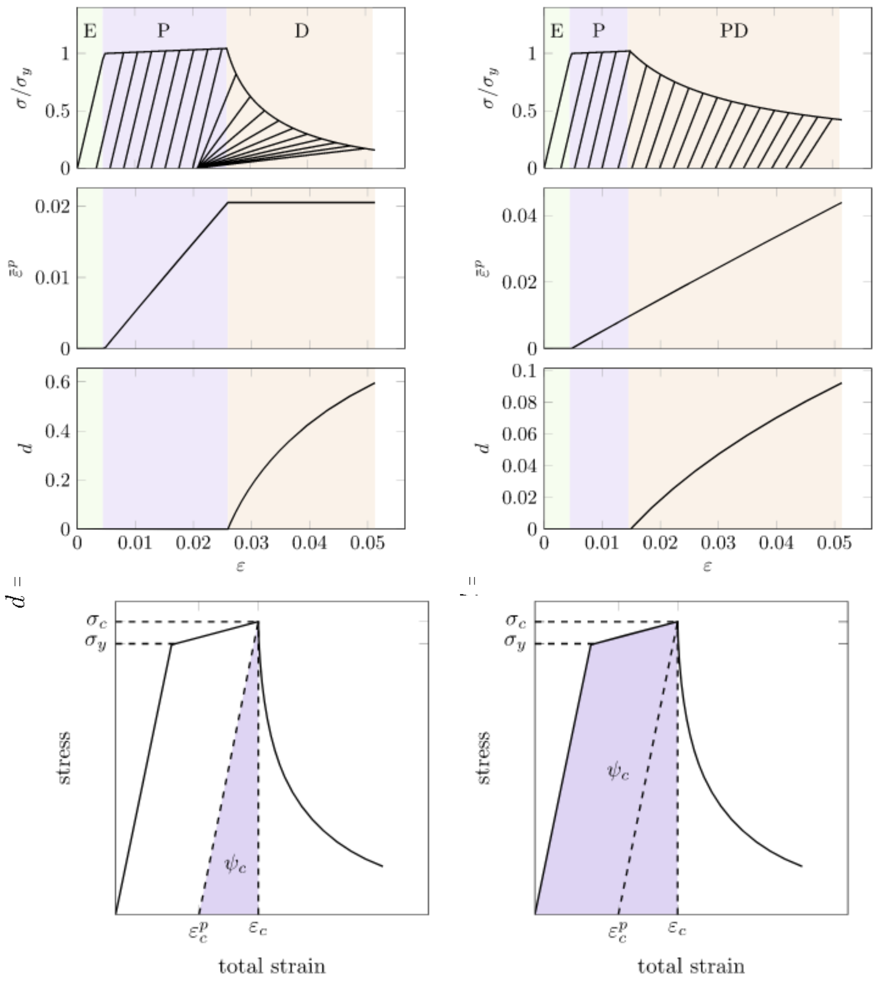
  $\rightarrow g(\phi)\sigma_{eff}(u, z) = h(\phi)\sigma_y(z)$

- Full plastic contribution (E-P-PD), $h(\phi) = g(\phi)$
  - fracture driving energy = $\psi^e + \psi^p$
  - yield surface: $\sigma_{eff}(u, z) = \sigma_y(z)$ (usual)

- No plastic contribution (E-P-D), $h(\phi) = 1$
  - fracture driving energy = ψ^e
  - yield surface: $g(\phi)\,\sigma_{eff}(u, z) = \sigma_y(z)$

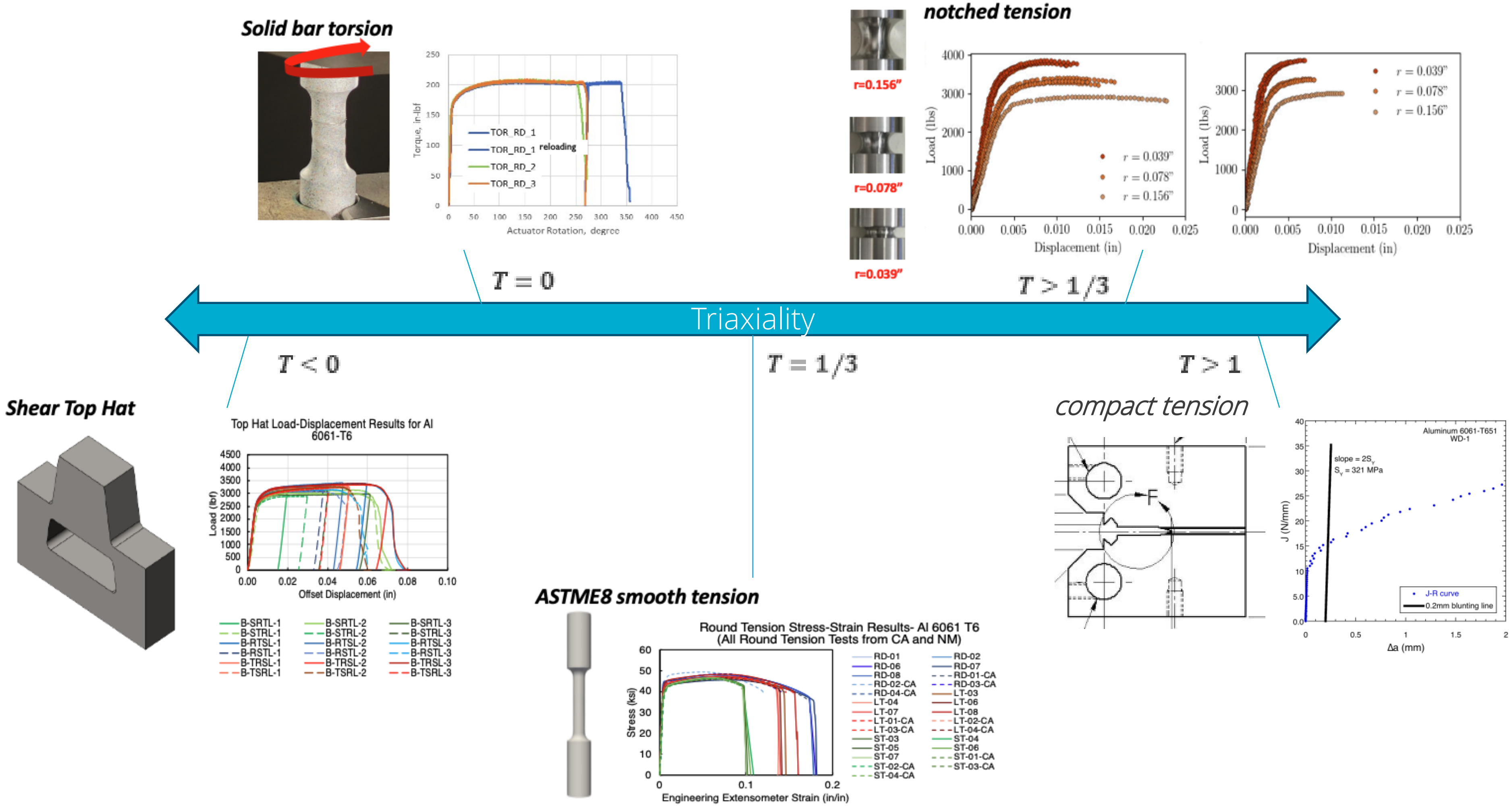
    $\rightarrow$ no yielding after damage

E-P-D $h(\phi) = 1$ E-P-PD $g(\phi) = h(\phi)$



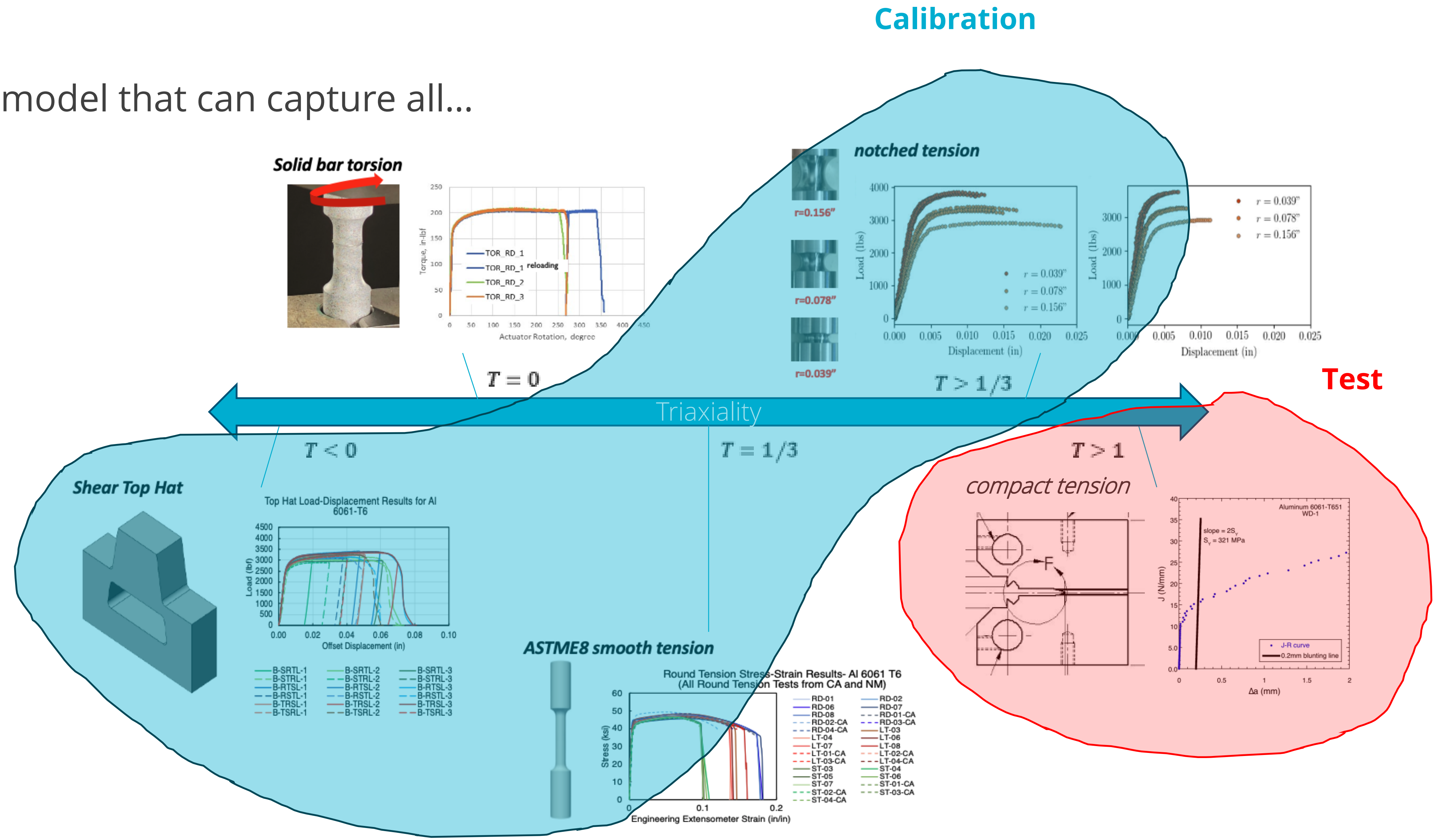
Model Objective

One model that can capture all…



Model Objective

One model that can capture all…

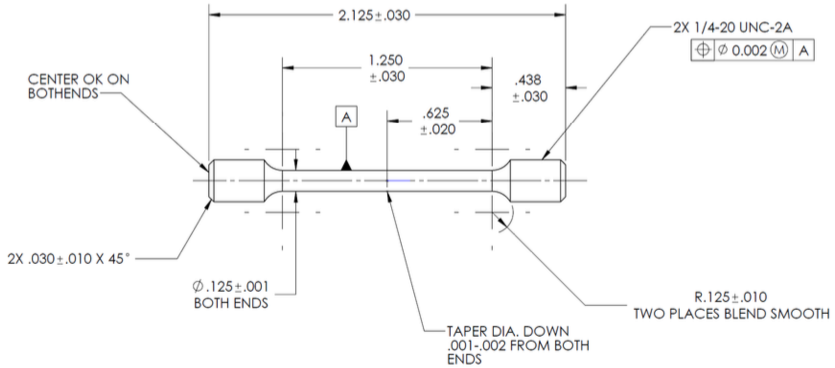


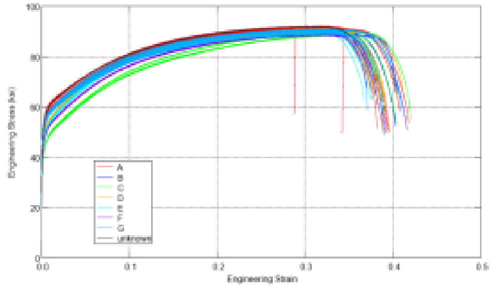
Characterization Data

Material:
304L Stainless Steel

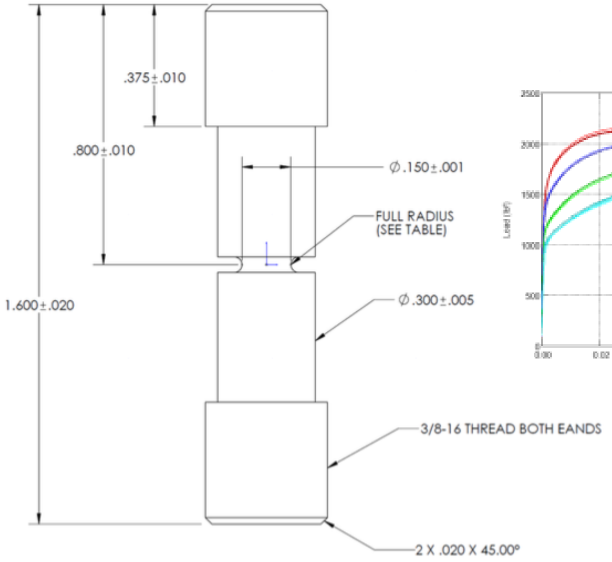
Uniaxial Tension

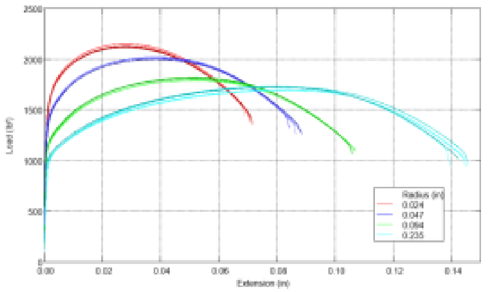
K. Mac Donald & B. Antoun



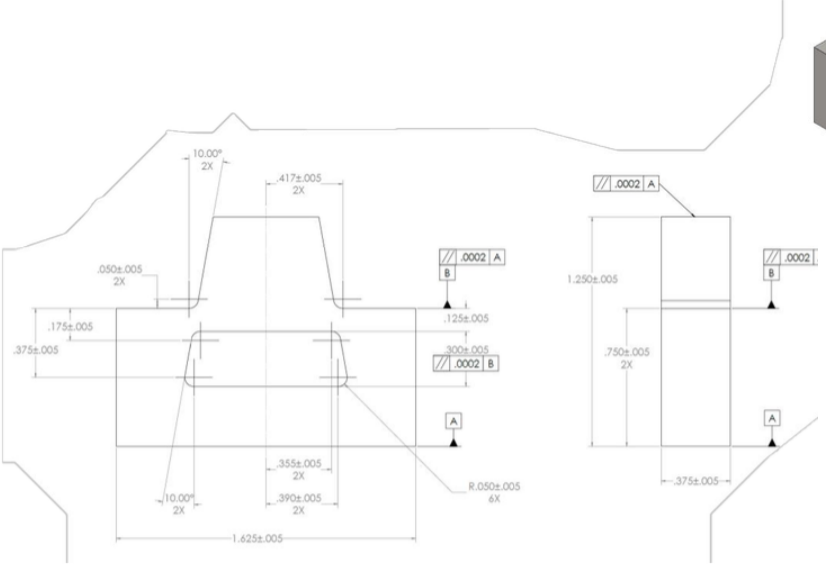


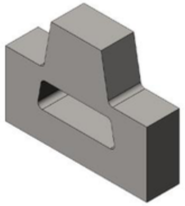
Notched Tension

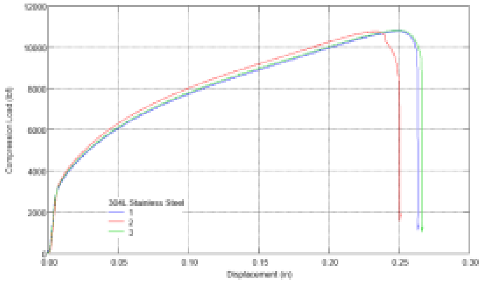




Shear Top Hat







Calibration Process

Multistage calibration process (MatCal):

1. Plasticity Calibration
   - Uniaxial Tension
     - Stress/strain curve (plastic hardening portion)
   - Notched Tension, R0.094”
     - Load/displacement curve (plastic hardening portion)

2. Phase-Field Damage Calibration
   - Uniaxial Tension
     - Max. displacement
   - Notched Tension, R0.094”
     - Max. displacement
   - Shear Top Hat
     - Load/displacement curve
     - Max. displacement

Calibration Process

Voce Hardening:

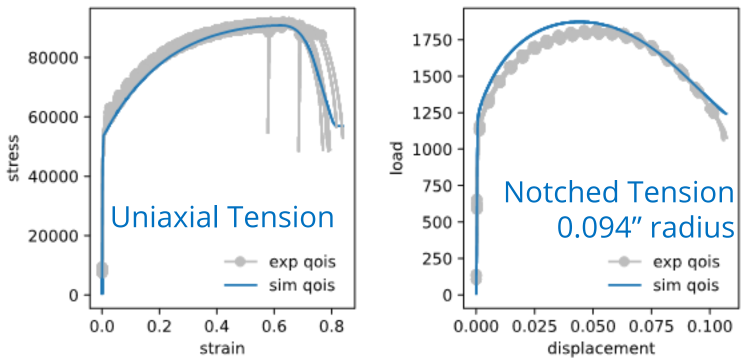
$$\sigma_y = {\color{red}Y} + {\color{red}A}\left(1 - \exp(-{\color{red}n}\bar{\varepsilon}^p)\right)$$

Multistage calibration process (MatCal):

1. Plasticity Calibration: Y, A, n
   - Uniaxial Tension (series A, upper bound)
     - Stress/strain curve (plastic portion)
   - Notched Tension, R0.094"
     - Load/displacement curve (plastic portion)

2. Phase-Field Damage Calibration
   - Uniaxial Tension
     - Max. displacement
   - Notched Tension, R0.094"
     - Max. displacement
   - Shear Top Hat
     - Load/displacement curve
     - Max. displacement

MatCal Calibration – 304L, PhaseFieldFeFp plasticity
3483 evaluations x 2 models x 3 parameters
(~ 3 days runtime)



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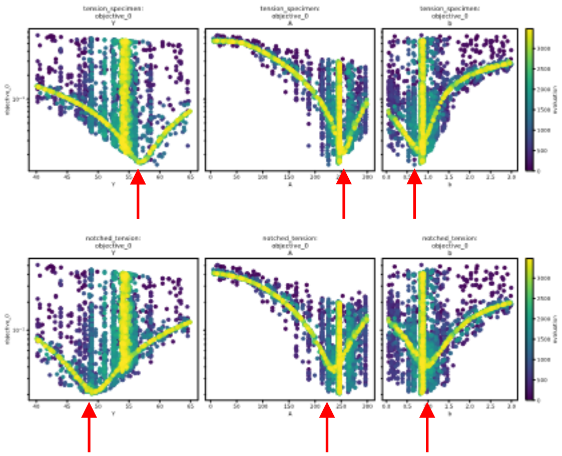
Uniaxial Tension

Notched Tension
0.094" radius



The different model problems have distinct preferences…
MatCal tries to balance uniaxial & notched tension data

Calibration Process

Multistage calibration process:

1. Plasticity Calibration
   - Uniaxial Tension
     - Stress/strain curve (plastic hardening portion)
   - Notched Tension, R0.094”
     - Load/displacement curve (plastic hardening portion)

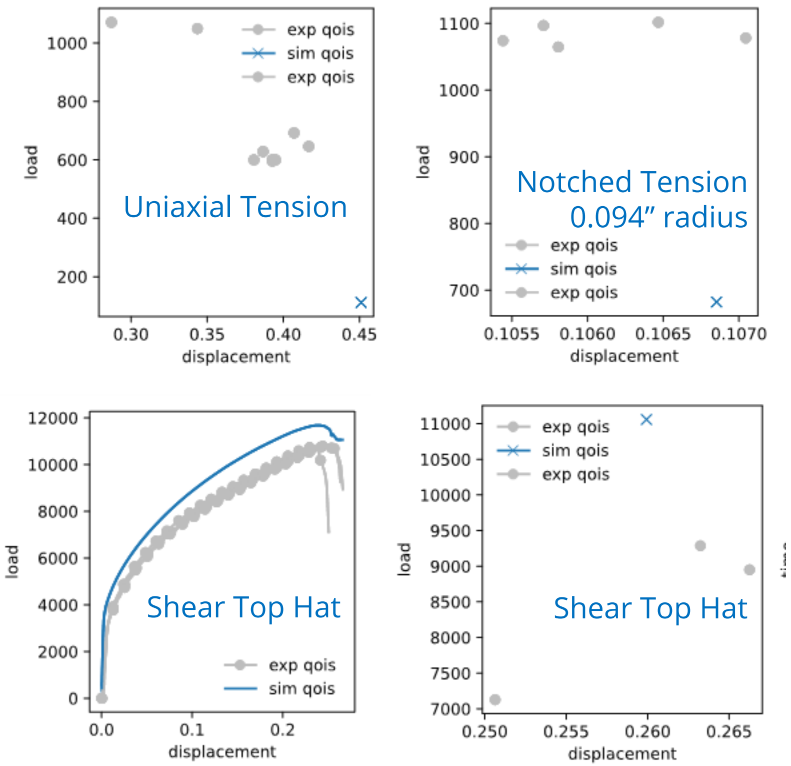
2. Phase-Field Damage Calibration: G_c, ψ_c
   - Uniaxial Tension
     - Max. displacement
   - Notched Tension, R0.094”
     - Max. displacement
   - Shear Top Hat
     - Load/displacement curve

Cohesive Phase Field (Lorentz model):

$$g(\phi) = h(\phi) = \frac{\phi^2}{\left(1 - \left(\frac{3G_c}{16\ell\psi_{crit}} - 1\right)(1-\phi)\right)^2}$$

$$\hat{\psi}_{\text{frac}}(G_c, \phi, \nabla\phi) = G_c \frac{3}{8\ell}\left((1-\phi) + \ell^2 \nabla\phi \cdot \nabla\phi\right)$$

MatCal Calibration – 304L, PhaseFieldFeFp plasticity
1320 evaluations x 3 models x 2 parameters
(~ 6 days runtime)



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Calibration Process

Multistage calibration process:

1. Plasticity Calibration
   - Uniaxial Tension
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2. Phase-Field Damage Calibration: G_c, ψ_c
   - Uniaxial Tension
     - Max. displacement
   - Notched Tension, R0.094”
     - Max. displacement
   - Shear Top Hat
     - Load/displacement curve
     - Max. displacement

Cohesive Phase Field (Lorentz model):

$$g(\phi) = h(\phi) = \frac{\phi^2}{\left(1 - \left(\frac{3G_c}{16\ell\psi_{crit}} - 1\right)(1-\phi)\right)^2}$$

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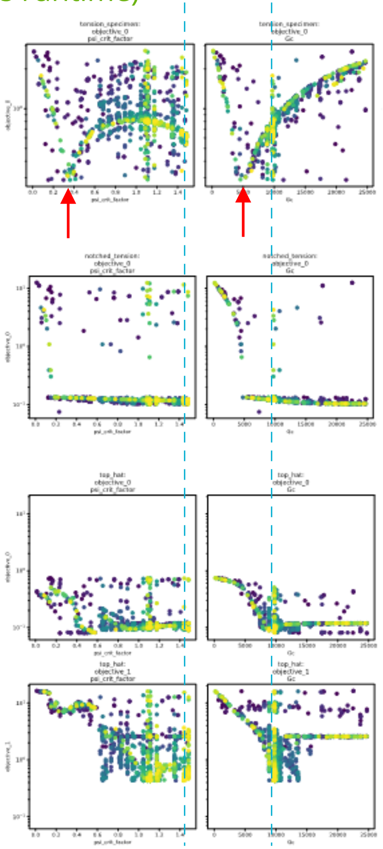

Uniaxial Tension

Notched Tension
0.094” radius

Shear Top Hat

Calibration Process

Multistage calibration process:

1. Plasticity Calibration
   - Uniaxial Tension
     - Stress/strain curve (plastic hardening portion)
   - Notched Tension, R0.094"
     - Load/displacement curve (plastic hardening portion)

2. Phase-Field Damage Calibration: G_c, ψ_c
   - Uniaxial Tension
     - Max. displacement
   - Notched Tension, R0.094"
     - Max. displacement
   - Shear Top Hat
     - Load/displacement curve

Cohesive Phase Field (Talamini model):

$$g(\phi) = h(\phi) = \frac{\phi^2}{\left(1 - \left(\frac{3G_c}{16\ell\psi_{crit}} - 1\right)(1-\phi)\right)^2}$$

$$\hat{\psi}_{\text{frac}}(G_c, \phi, \nabla\phi) = G_c \frac{3}{8\ell}\left((1-\phi) + \ell^2 \nabla\phi \cdot \nabla\phi\right)$$

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1320 evaluations x 3 models x 2 parameters
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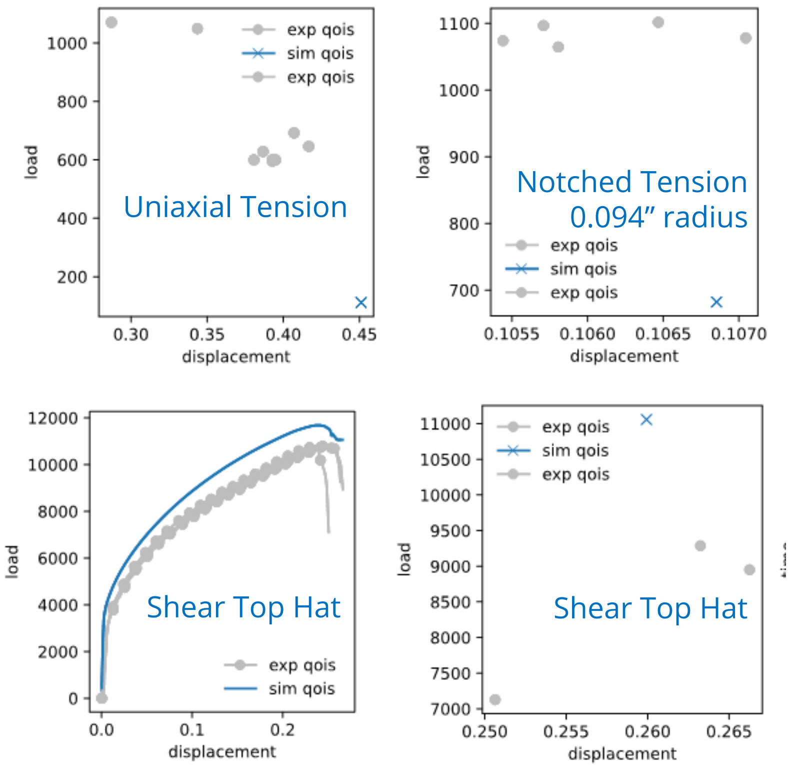

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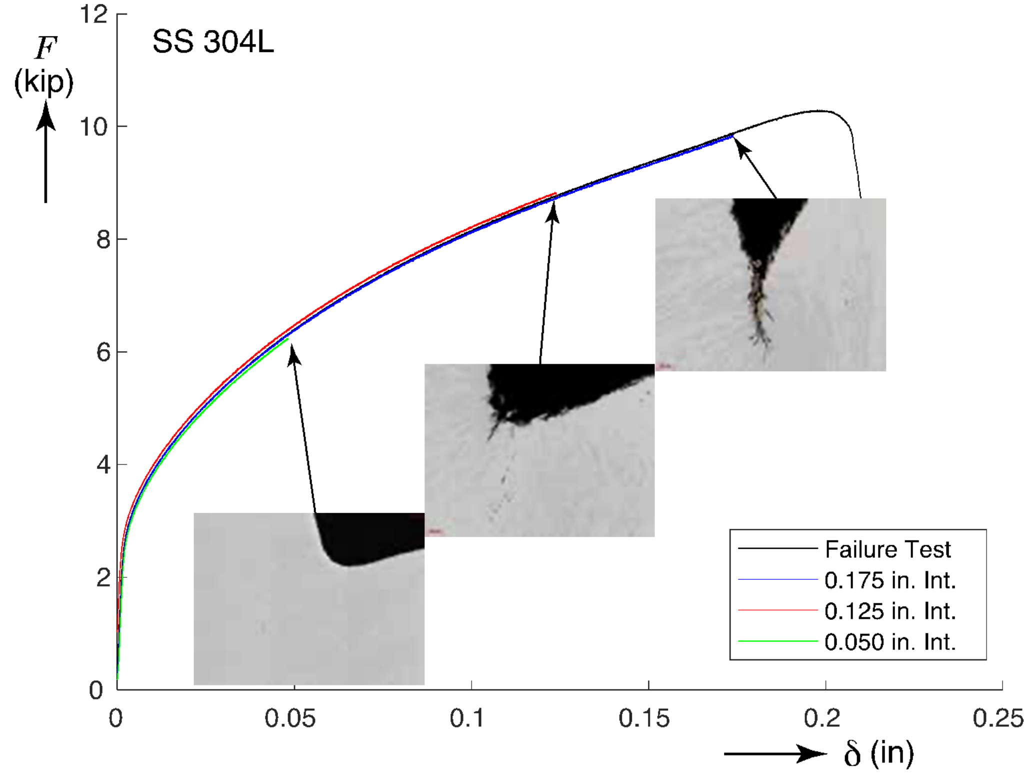
Calibration – Validation Comparison

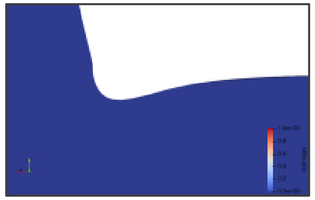
Top hat calibration – comparison to experimental imagery

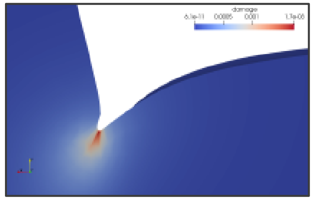
- Imagery shows damage growth before peak force
- Model similarly predicts similar damage patterns / timings

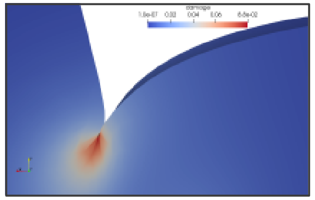
E. Corona, *et al.* (2021): SAND2021-1752



$$d = 1 - g(\phi) = 1 - \frac{\phi^2}{\left(1 - \left(\frac{3G_c}{16\ell\psi_{crit}} - 1\right)(1-\phi)\right)^2}$$


u = 0.05 in


u = 0.13 in

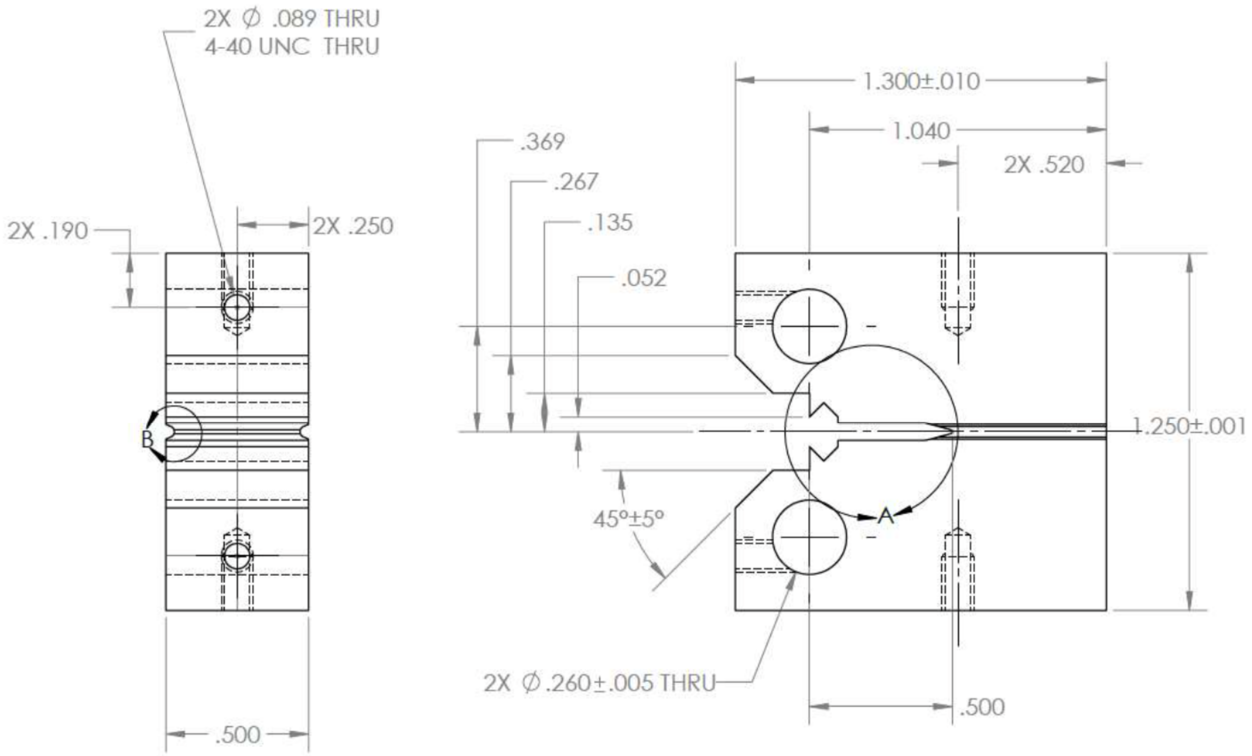

u = 0.13 in

Damage magnitude is lower than expected though material too tough?

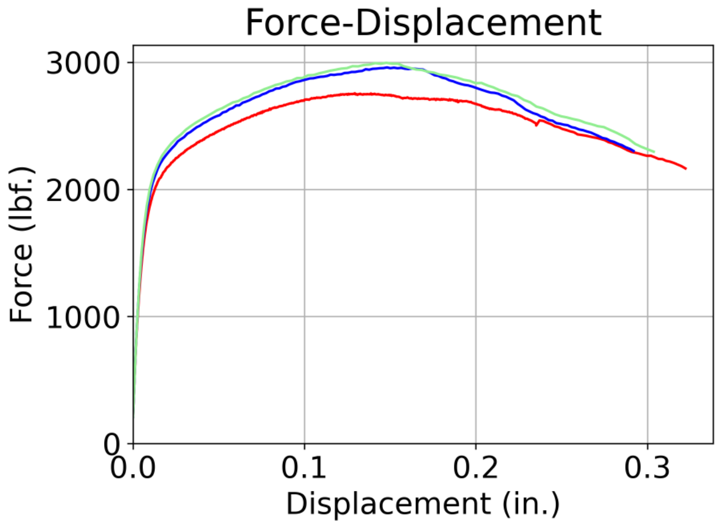
Also, note initiation of uncaptured self-contact

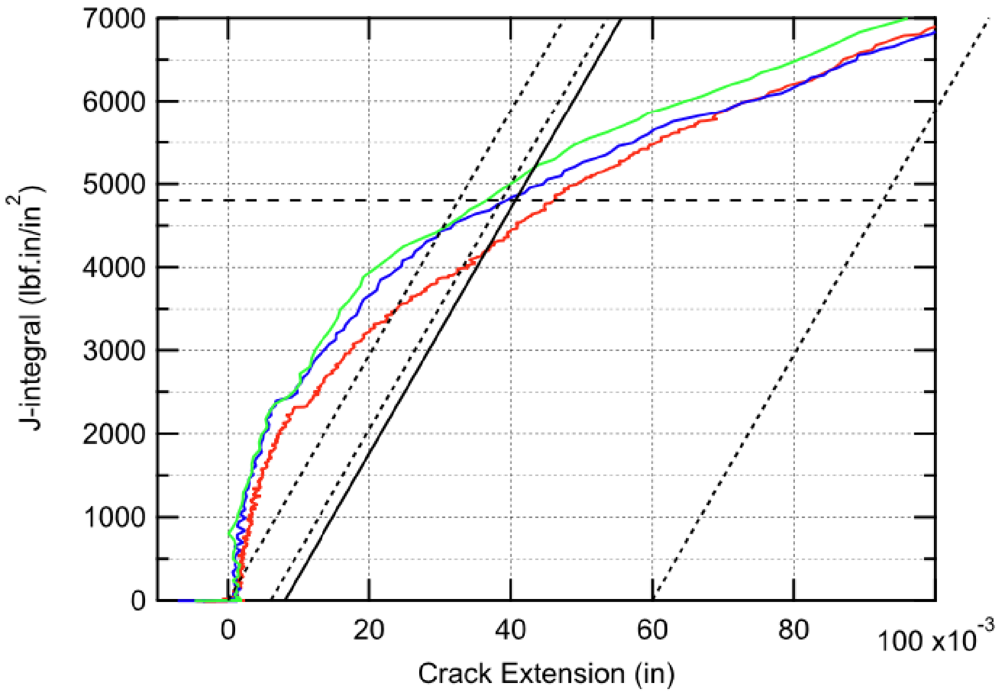
Validation Problem

Compact tension specimen, with side groove



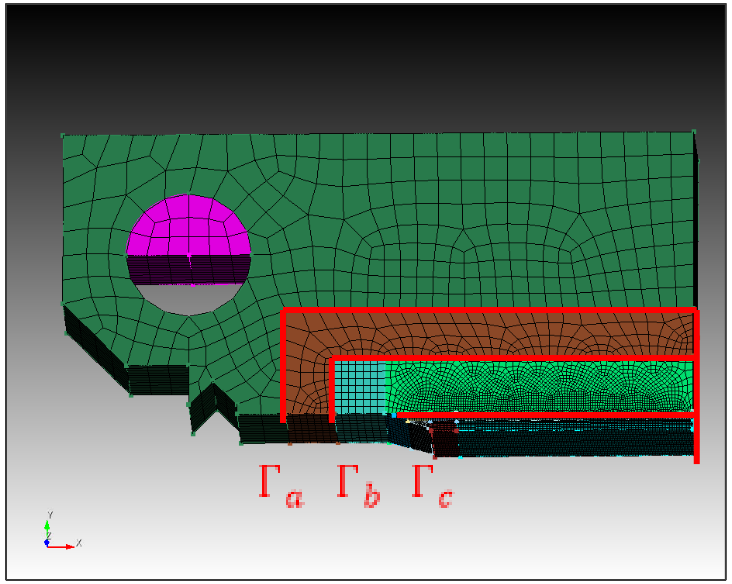
K. Mac Donald & B. Antoun





Validation Problem

How to measure J-integral:



Surface integrals:

$$\int_\Gamma L_i \left(\psi \delta_{ij} - (F - \delta)_{ki} P_{kj}\right) n_j \, dA$$

2. ASTM E1820 (A2.4 – Basic Test Method)

$$J = J_{el} + J_{pl}$$

$$J = J_{e/0} + \frac{J_{p/0}}{1 + \left(\frac{\alpha - 0.5}{\alpha + 0.5}\right) \frac{\Delta a}{b_o}}$$

$$J = \frac{K^2(1 - \nu^2)}{E} + J_{pl}$$

$$J_{pl} = \frac{\eta_{pl} A_{pl}}{B_N b_o}$$

$$K_{(i)} = \frac{P_{(i)}}{(BB_N W)^{1/2}} f\left(\frac{a_i}{W}\right)$$

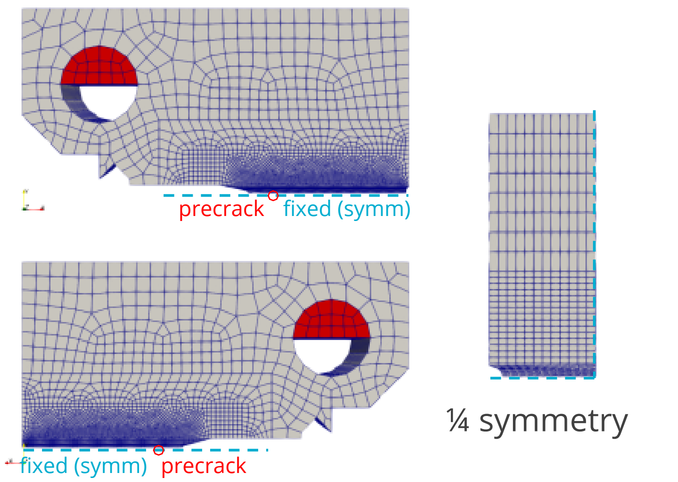
$$f\left(\frac{a_i}{W}\right) = \qquad (A2.3)$$

$$\frac{\left\{\left(2 + \frac{a_i}{W}\right)\left[0.886 + 4.64\left(\frac{a_i}{W}\right) - 13.32\left(\frac{a_i}{W}\right)^2 + 14.72\left(\frac{a_i}{W}\right)^3 - 5.6\left(\frac{a_i}{W}\right)^4\right]\right\}}{\left(1 - \frac{a_i}{W}\right)^{3/2}}$$

Preliminary Results

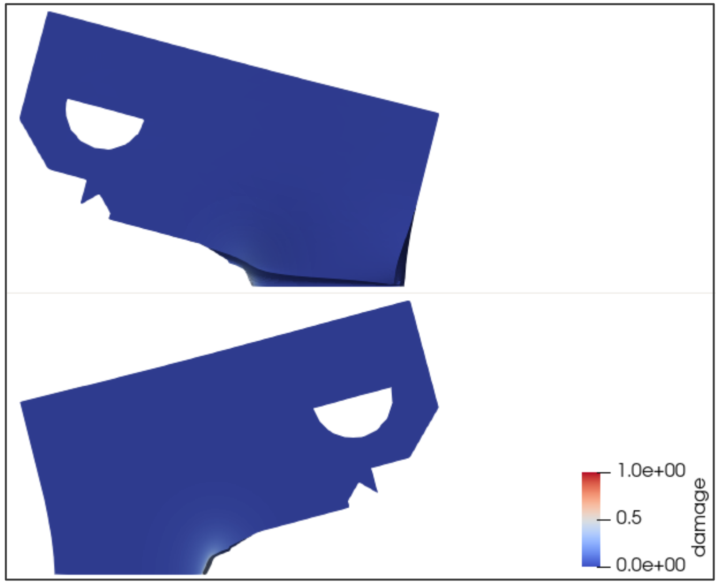
2-parameter calibration: : G_c, ψ_c

Model

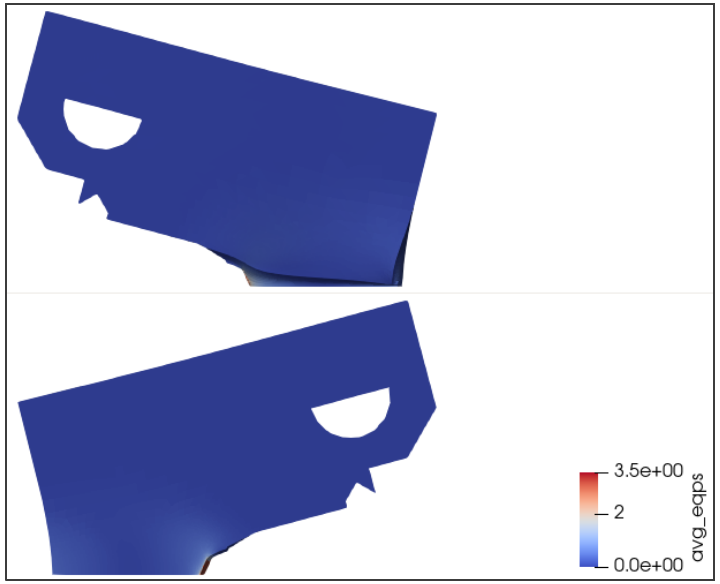


CTS Mesh, fine element = 0.0025”

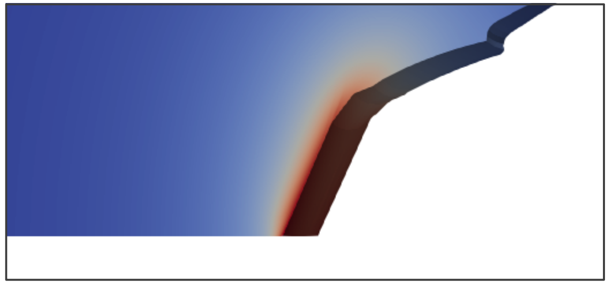
Phase @ Max. Displacement



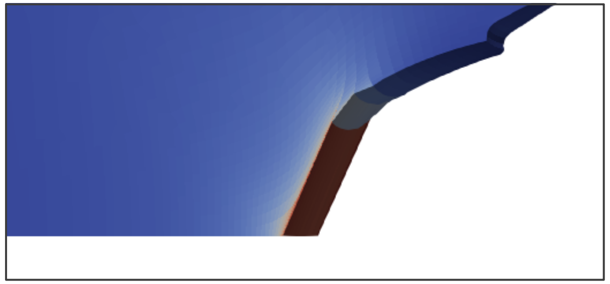
EQPS @ Max. Displacement



Zoomed view



Zoomed view

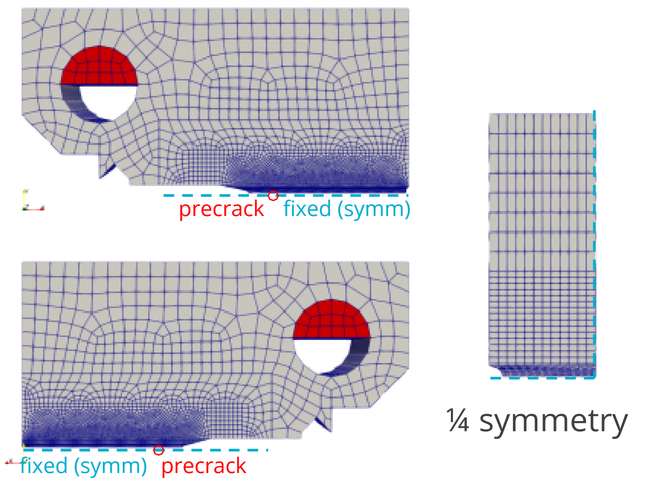


- High ductility, but concentrated in one element at sharp crack tip
- Crack isn’t propagating; damage slow to develop

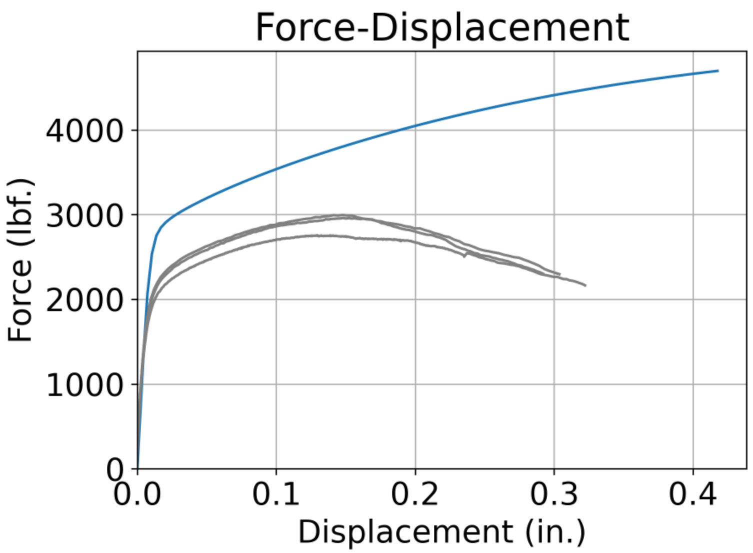
Preliminary Results

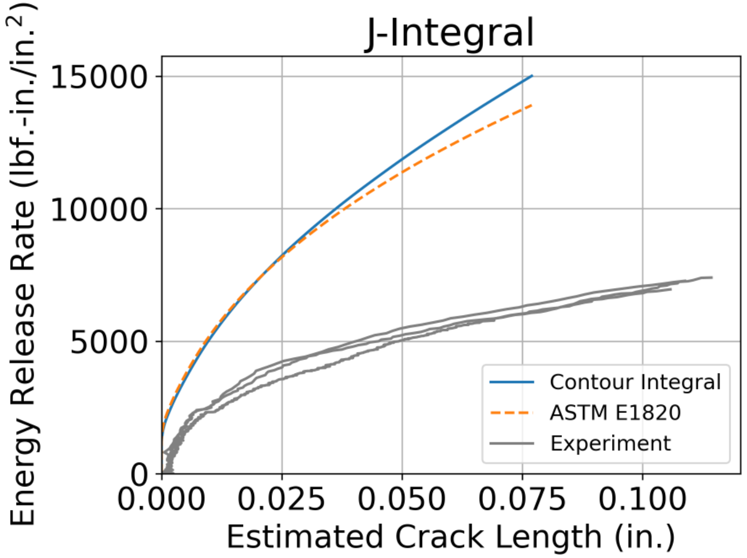
2-parameter calibration: G_c, ψ_c

Model



CTS Mesh, fine element = 0.0025”



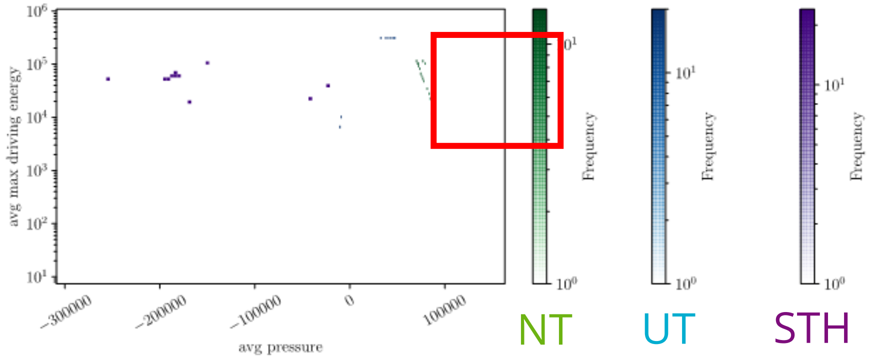


- (F/D) Small error in plasticity, now magnified
- Phase Field model too tough, over-estimating J-R curve

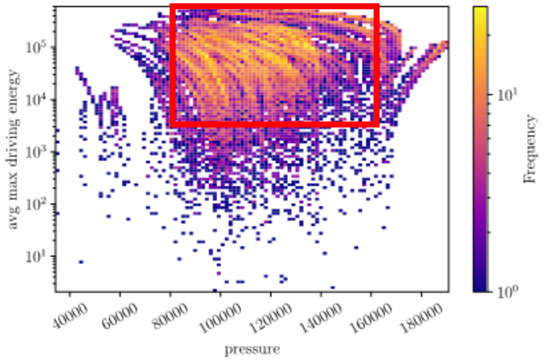
Interpretation

- Using upper-bound uniaxial tension series seems to have biased plasticity model
  - Tangible difference in plasticity model in shear top-hat
  - Even worse for compact tension
- Difficulty of modeling plasticity at infinitely sharp crack tip
  - Majority of plasticity & damage occurs on the one-element tip
- Phase Field model too stiff!
  - Characterization data (UT, NT, STH) don't contain strong singularities like CT does → too much extrapolation in using calibration for CT?

Calibration Space:



Compact Tension Test



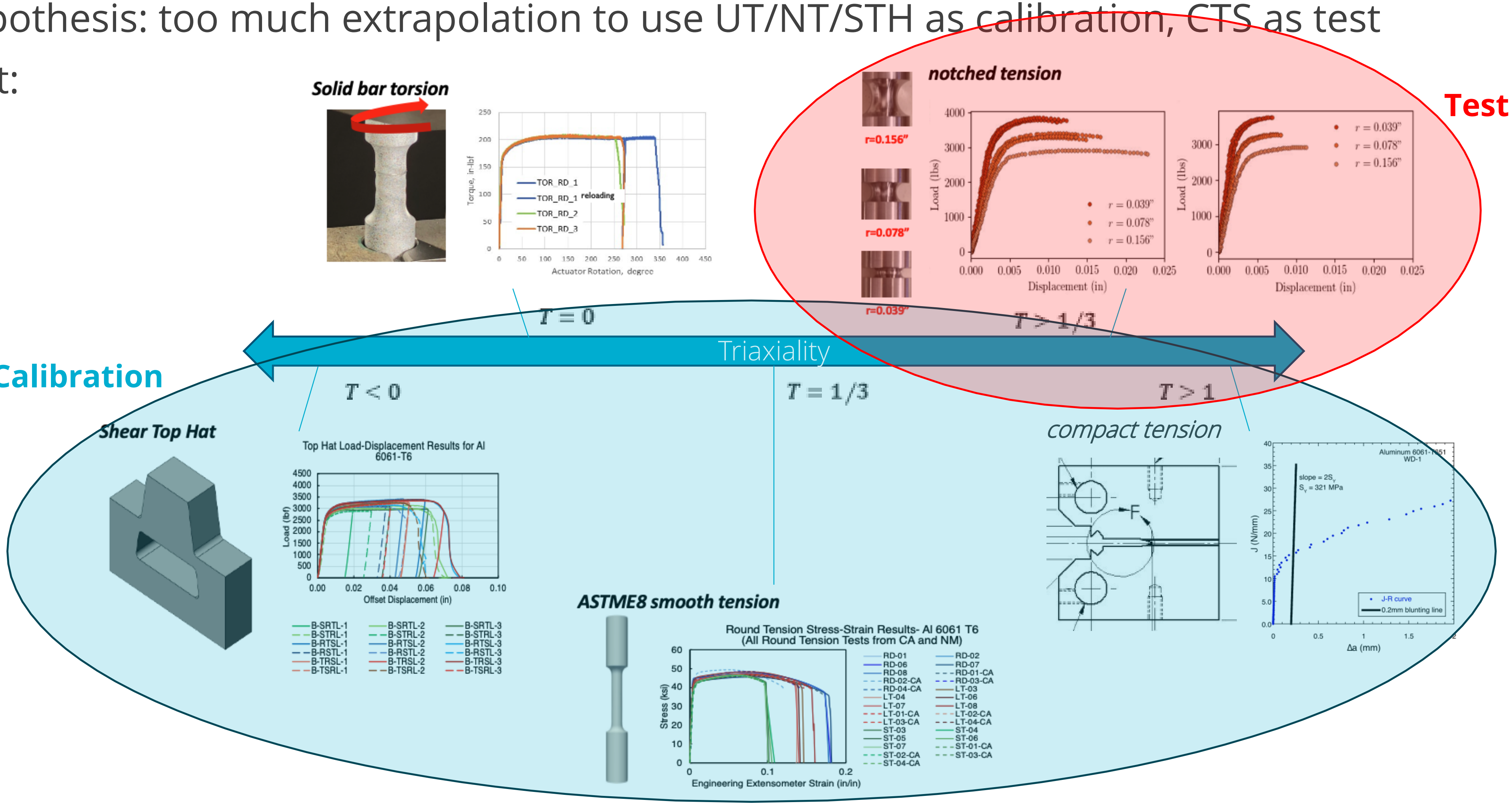
Next Steps for Continued Investigation

- Assess calibration space:
  - Compare driving energies in calibration vs CTS
- Top Hat model used in calibration is implicit, self-contact OFF
  - → consider explicit dynamics w/ mass scaling, self-contact ON
- Re-calibration:
  - Improve plasticity:
    - Incorporate all/median UT data, rather than upper bound
    - Add all NT series?
    - Add Top Hat?
  - Improve damage calibration:
    - Leave Top Hat out from damage calibration (CTS isn't shear), and include more NT series?
    - Calibrate to CTS and test on NT & Top Hat?
    - Calibrate on all models – possible?
- Capture missing physics:
  - Add new plastic-damage coupling and repeat as 2- & 3-parameter calibrations

Reverse Calibration

Hypothesis: too much extrapolation to use UT/NT/STH as calibration, CTS as test

Test:



New Proposed Model Form – Revisit Plastic-Damage Coupling

Hu *et al.* (2021)

Consider Plastic-Damage Coupling:

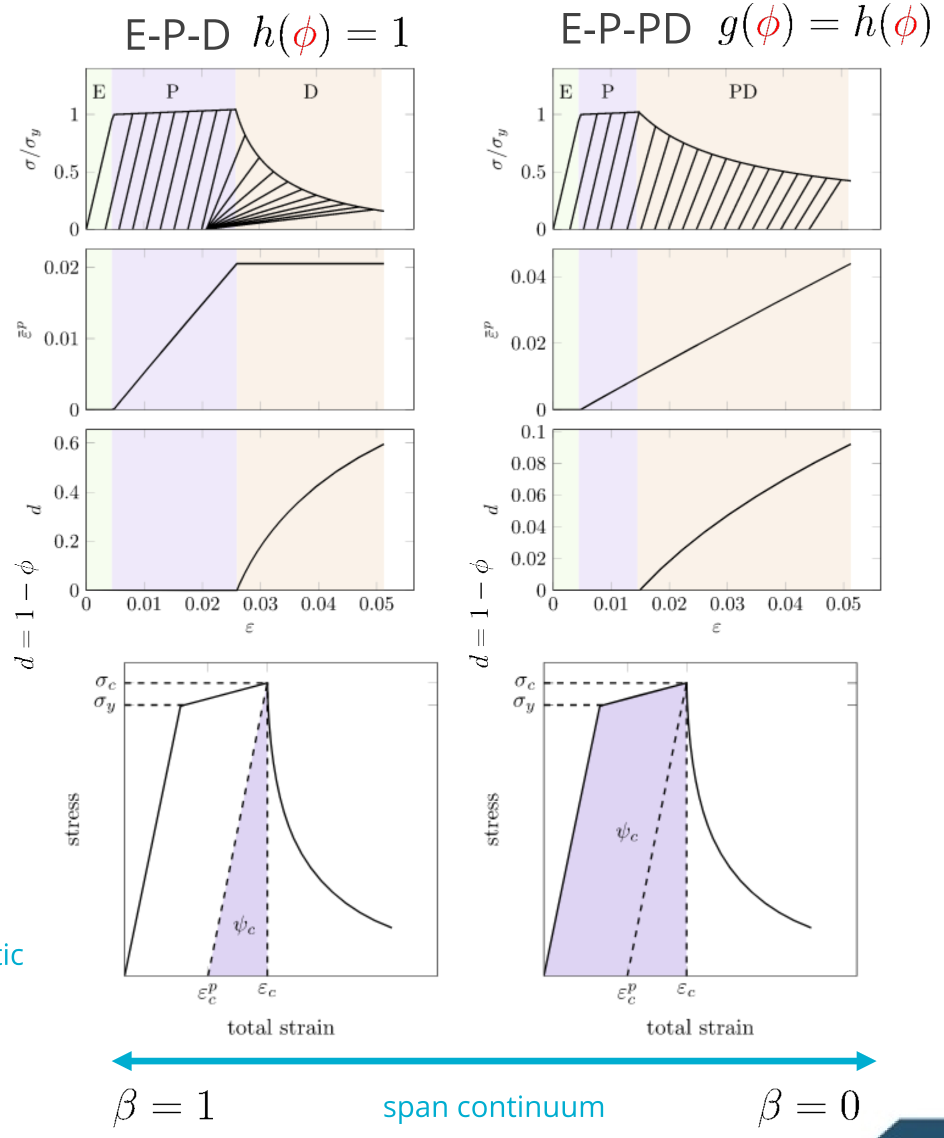
- Plastic Yield Surface (from $\nabla \cdot \frac{\partial \psi}{\partial z} - \frac{\partial \psi}{\partial z} = 0$):

  $\rightarrow g(\phi)\sigma_{eff}(u,z) = h(\phi)\sigma_y(z)$

- Full plastic contribution (E-P-PD), $h(\phi) = g(\phi)$
  - fracture driving energy = $\psi^e + \psi^p$
  - yield surface: $\sigma_{eff}(u,z) = \sigma_y(z)$ (usual)

- No plastic contribution (E-P-D), $h(\phi) = 1$
  - fracture driving energy = ψ^e
  - yield surface: $g(\phi)\,\sigma_{eff}(u,z) = \sigma_y(z)$

    → no yielding after damage



fracture adiabatic

$$h(\phi)\psi^p \rightarrow (1-\beta)g(\phi)\psi^p + \beta\psi^p$$

Thank you!

Thanks for your attention   Any questions?

Andrew Stershic, PhD PE
Sandia National Laboratories
Multi-Physics Modeling & Simulation
Livermore, CA
ajsters@sandia.gov

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