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SAND2021-8929C

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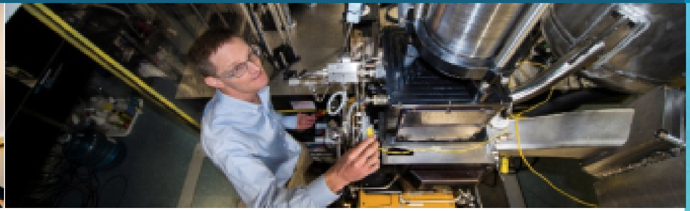
A variational phase-field model of ductile fracture



PRESENTED BY

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USNCCM 16

July 25-29, 2021

SAND NUMBER

U.S. DEPARTMENT OF ENERGY NNSA National Nuclear Security Administration

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Background and Objective

- Extension of phase field modeling of fracture to ductile materials is an active area of research
- We are aiming to improve the phase field predictivity in large scale yielding problems
  - More focus on fracture initiation
- Want to maintain predictivity in small-scale yielding exhibited by phase field approach
  - Toughness controlled fracture propagation
- Want correspondence with known ductile void growth mechanics

Basic kinematics

Primary fields

$\boldsymbol{\chi}(\boldsymbol{X},t)$	Deformation map
$\phi(\boldsymbol{X},t)$	Phase field (damage) $\dot{\phi} \geq 0, \quad 0 \leq \phi \leq 1$ $\phi = 0$ Intact material point $\phi = 1$ Broken material point
$\bar{\varepsilon}^p$	Equivalent uniaxial plastic strain
$\boldsymbol{F}^p$	Plastic distortion tensor

Multiplicative decomposition

$$\boldsymbol{F} = \nabla \boldsymbol{\chi} \qquad \boldsymbol{F}^e = \boldsymbol{F}\boldsymbol{F}^{p-1}$$

Flow rule

$$\dot{\boldsymbol{F}}^p \boldsymbol{F}^{p-1} = \dot{\bar{\varepsilon}}^p \boldsymbol{N}^p \qquad \dot{\bar{\varepsilon}}^p \geq 0$$

$$\mathrm{tr}\, \boldsymbol{N}^p = 0 \quad \boldsymbol{N}^p : \boldsymbol{N}^p = \frac{3}{2}$$

Model form

Free energy

$$\psi = \psi_{\text{mech}}(\boldsymbol{F}, \boldsymbol{F}^p, \bar{\varepsilon}^p, \phi) + \psi_{\text{frac}}(\phi, \boldsymbol{\nabla}\phi)$$

Mechanical free energy

$$\psi_{\text{mech}}(\boldsymbol{F}, \boldsymbol{F}^p, \bar{\varepsilon}^p, \phi) = g(\phi)\tilde{\psi}^e(\boldsymbol{F}^e) + \psi^p(\bar{\varepsilon}^p)$$

$$g(\phi) = \frac{(1-\phi)^2}{(1+\gamma\phi)^2} \qquad \gamma = \frac{3G_0}{16\ell\psi_c} - 1$$

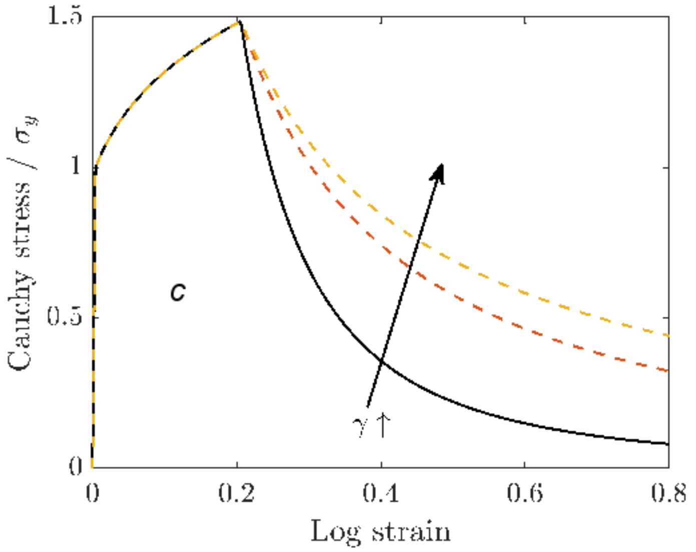
Degradation function of Lorentz et al., *C.R. Mechanique* **339** (2011)

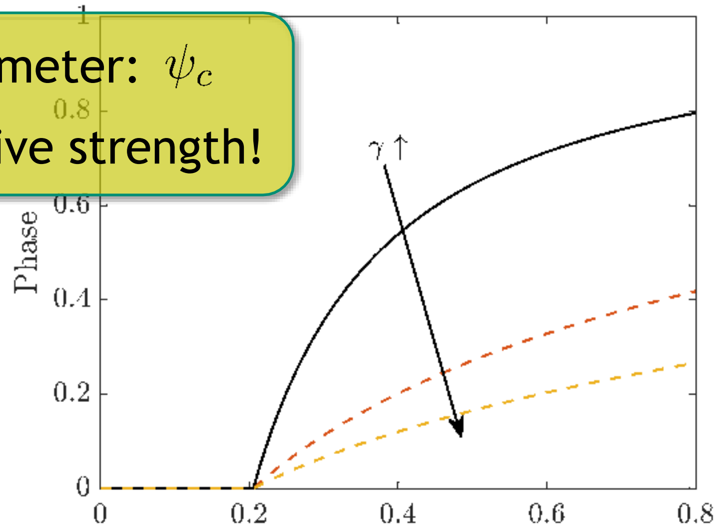
Additional parameter: ψ_c

Serves as cohesive strength!

Fracture free energy

$$\psi_{\text{frac}}(\phi, \boldsymbol{\nabla}\phi) = \frac{3G_0}{8\ell}\left(\phi + \ell^2 \|\boldsymbol{\nabla}\phi\|^2\right)$$





Elastic/plastic constitutive relations

$$\psi_{\text{mech}}(\boldsymbol{F}, \boldsymbol{F}^p, \bar{\varepsilon}^p, \phi) = g(\phi)\widetilde{\psi}^e(\boldsymbol{F}^e) + \psi^p(\bar{\varepsilon}^p)$$

Intact strain energy

$$\widetilde{\psi}^e(\boldsymbol{\varepsilon}^e) = \mu \operatorname{dev} \boldsymbol{\varepsilon}^e : \operatorname{dev} \boldsymbol{\varepsilon}^e + \frac{\kappa}{2} \operatorname{tr}(\boldsymbol{\varepsilon}^e)^2, \qquad \boldsymbol{\varepsilon}^e = \frac{1}{2} \log\left(\boldsymbol{F}^{eT} \boldsymbol{F}^e\right)$$

Hencky elastic strain

Defect energy

Power law hardening

$$\psi^p(\bar{\varepsilon}^p) = \frac{n\sigma_y\varepsilon_0}{n+1}\left(1 + \frac{\bar{\varepsilon}^p}{\varepsilon_0}\right)^{\frac{n+1}{n}} \longrightarrow \quad S(\bar{\varepsilon}^p) := \frac{\partial \psi^p(\bar{\varepsilon}^p)}{\partial \bar{\varepsilon}^p} = \sigma_y \left(1 + \frac{\bar{\varepsilon}^p}{\varepsilon_0}\right)^{1/n}$$

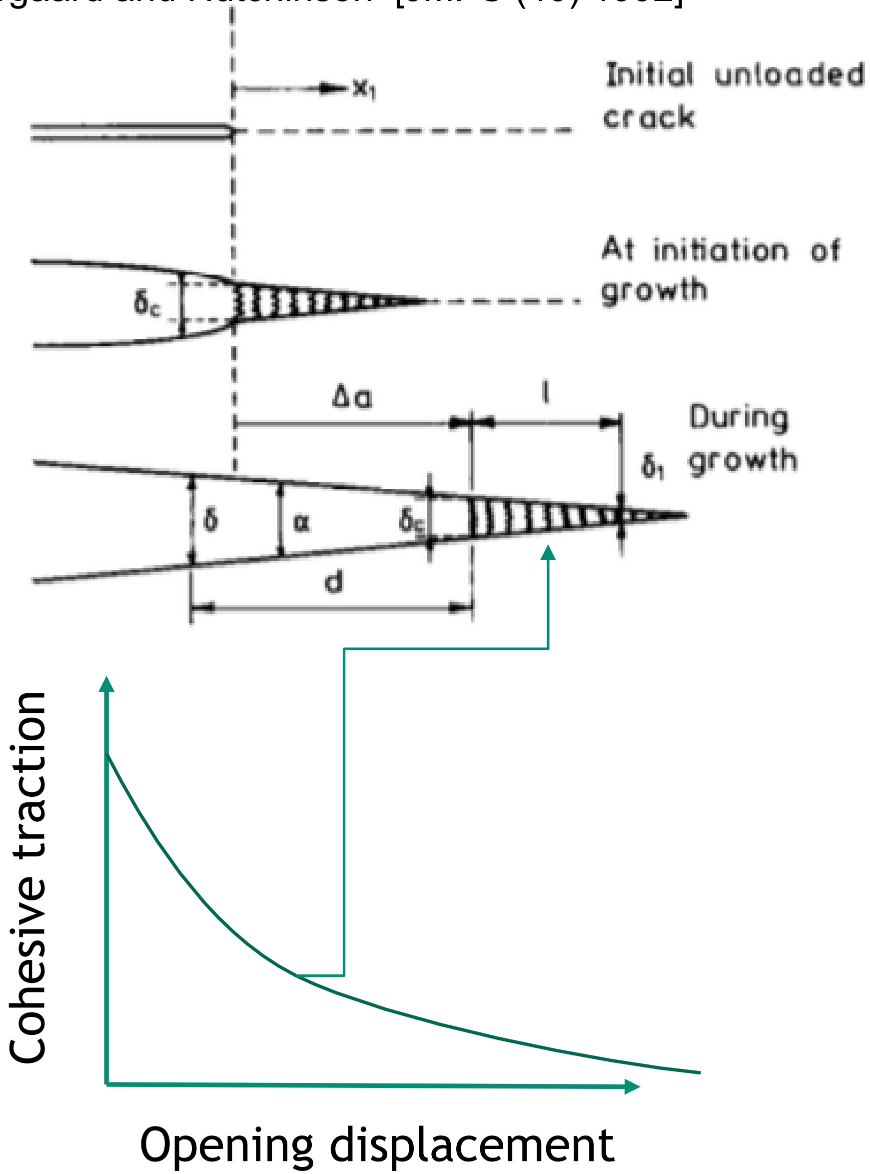
Dual kinetic potential

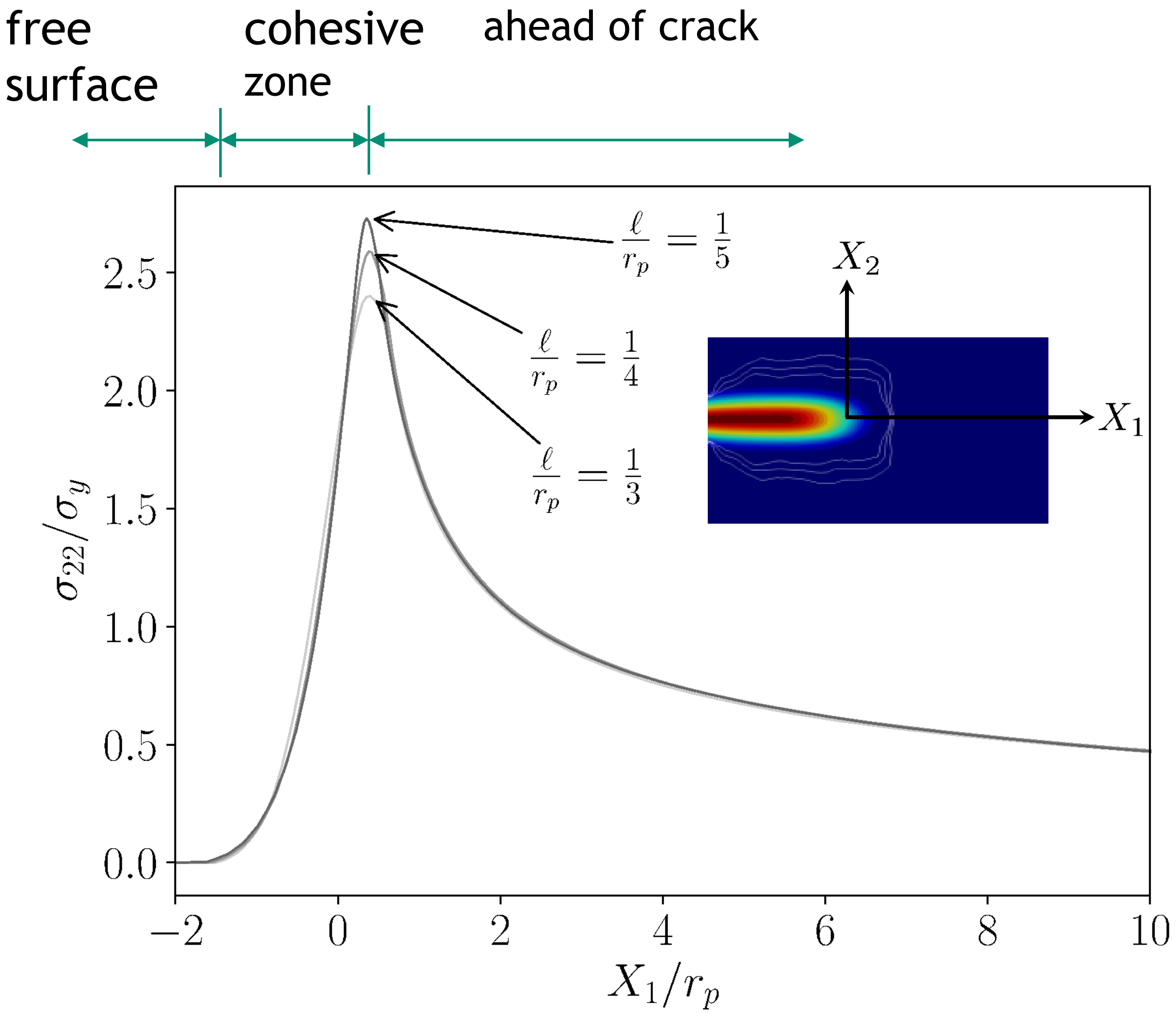
Power law rate sensitivity

$$\Pi^*(\dot{\bar{\varepsilon}}^p) = \frac{m\sigma_y\dot{\varepsilon}_0}{m+1}\left(\frac{\dot{\bar{\varepsilon}}^p}{\dot{\varepsilon}_0}\right)^{\frac{m+1}{m}} \longrightarrow \quad S_{\text{vis}}(\dot{\bar{\varepsilon}}^p) = \frac{\partial \Pi^*(\dot{\bar{\varepsilon}}^p)}{\partial \dot{\bar{\varepsilon}}^p} = \sigma_y \left(\frac{\dot{\bar{\varepsilon}}^p}{\dot{\varepsilon}_0}\right)^{\frac{1}{m}}$$

Approach to a cohesive zone model

Tvergaard and Hutchinson [JMPS (40) 1992]





Variational formulation

Minimize $I(\dot{\boldsymbol{\chi}}, \dot{\phi}, \dot{\bar{\varepsilon}}^p, \boldsymbol{N}^p) = \int_{B_0} \left(\dot{\psi} + \Pi^*\right) \mathrm{d}V - G_{\text{ext}}(\dot{\boldsymbol{\chi}})$

$$\dot{\phi} \geq 0$$
$$\dot{\bar{\varepsilon}}^p \geq 0$$
$$0 \leq \phi \leq 1$$

Splits naturally into 2 subproblems:

1. Variational constitutive update (local)

$$\mathcal{W}^{\text{eff}}(\boldsymbol{\nabla}\dot{\boldsymbol{\chi}}, \dot{\phi}, \boldsymbol{\nabla}\dot{\phi}) = \inf_{\substack{\dot{\bar{\varepsilon}}^p, \boldsymbol{N}^p \\ \dot{\bar{\varepsilon}}^p \geq 0}} \dot{\psi} + \Pi^*$$

cf. M Ortiz and L Stainier, *Comp Meth Appl Mech Engrg* 171 (1999) 419-444

2. Equilibrium search (nonlocal)

minimize $I^{\text{eff}}(\dot{\boldsymbol{\chi}}, \dot{\phi}) = \int_{B_0} \mathcal{W}^{\text{eff}}(\boldsymbol{\nabla}\dot{\boldsymbol{\chi}}, \dot{\phi}, \boldsymbol{\nabla}\dot{\phi}) \, \mathrm{d}V - G_{\text{ext}}(\dot{\boldsymbol{\chi}})$

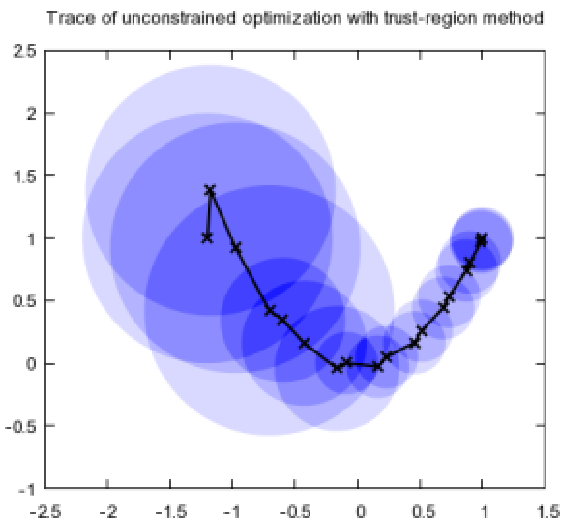
subject to $\dot{\phi} \geq 0 \qquad 0 \leq \phi \leq 1$

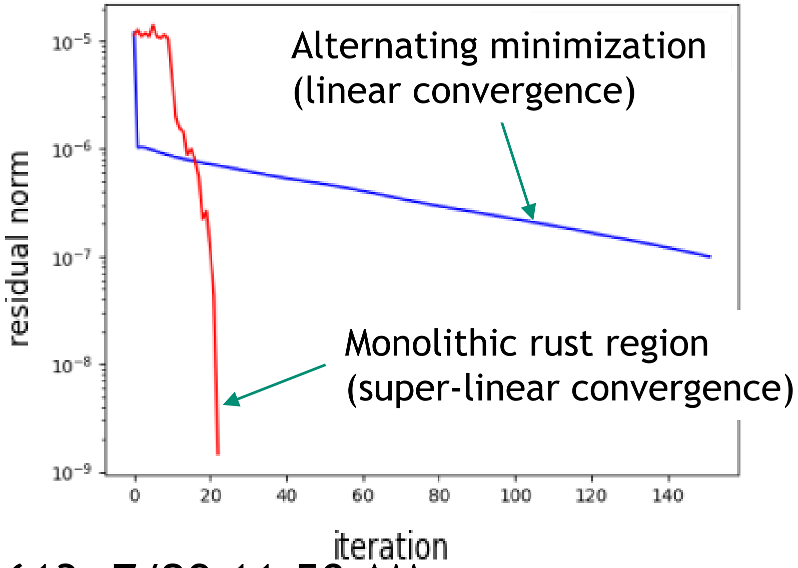
Talamini et al. “Attaining regularization length insensitivity in phase-field models of ductile failure”, *CMAME* 2021

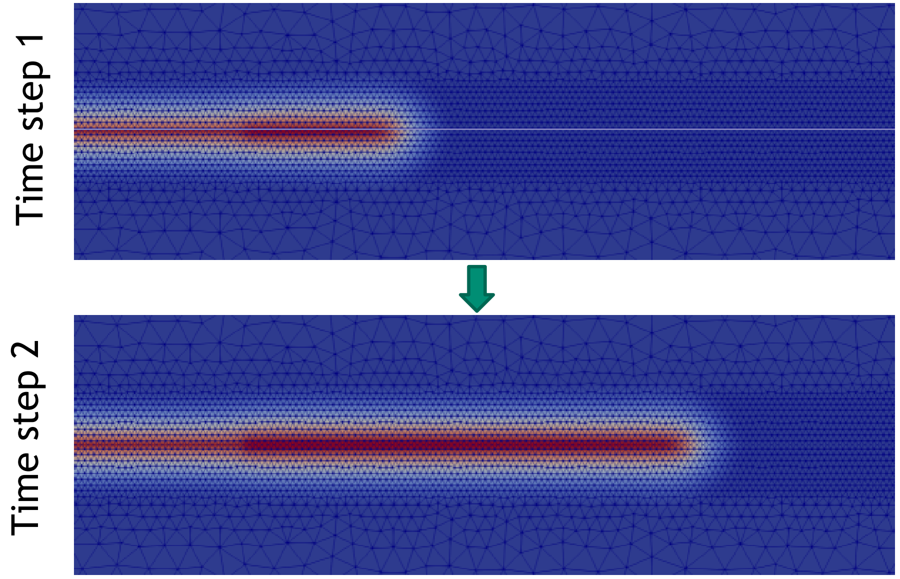
Solver implementation

- Machine learning has led to a recent growth in non-convex optimization research
- **We use our variational formulation to leverage this**

Monolithic trust region solver
1. Local quadratic model
2. Inner iterations use preconditioned linear CG
3. Aggressively move in directions of negative curvature – **avoids unstable & unphysical saddle points**







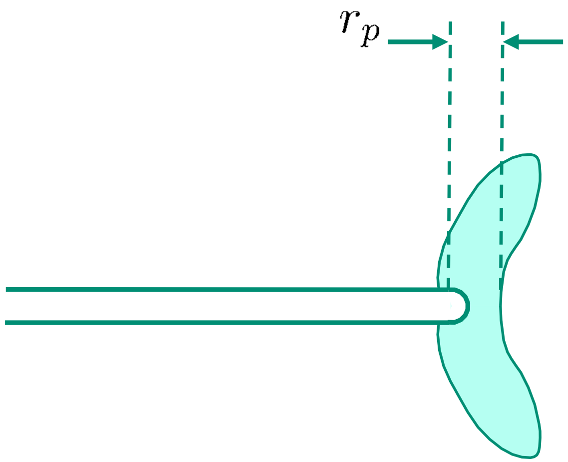
Robustly propagates damage across multiple elements in a single load-step

*See talk by M Tupek, MS 613, 7/29 11:50 AM

INTERNAL LENGTH SCALE AND CRACK GROWTH RESISTANCE

Role of phase field length scale

- Plasticity introduces an additional length scale to fracture problem:



Plane strain estimate: $r_p = \dfrac{EG_0}{3\pi(1-\nu^2)\sigma_y^2}$

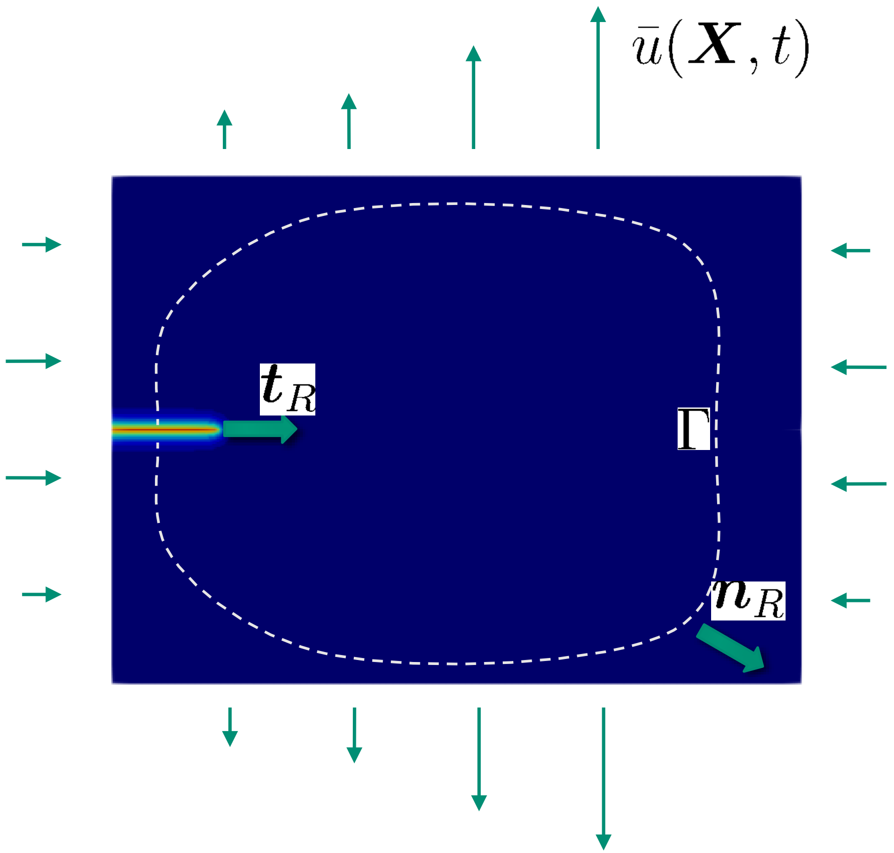
- Ratio ℓ / r_p could become meaningful in terms of predicted response
- Propose to characterize this effect through **crack growth resistance**
- Functional dependence of crack growth resistance must have the form

$$\frac{G_R}{G_0} = f\left(\frac{\Delta a}{r_p}, \frac{\ell}{r_p}, \frac{\sigma_y}{E}, n, \epsilon_0, \nu\right)$$

- Cf. classic paper of Tvergaard and Hutchinson [JMPS (40) 1992]

Procedure

Simulate plane strain mode I crack growth in nearly infinite domain



Note: not to scale, domain is much larger

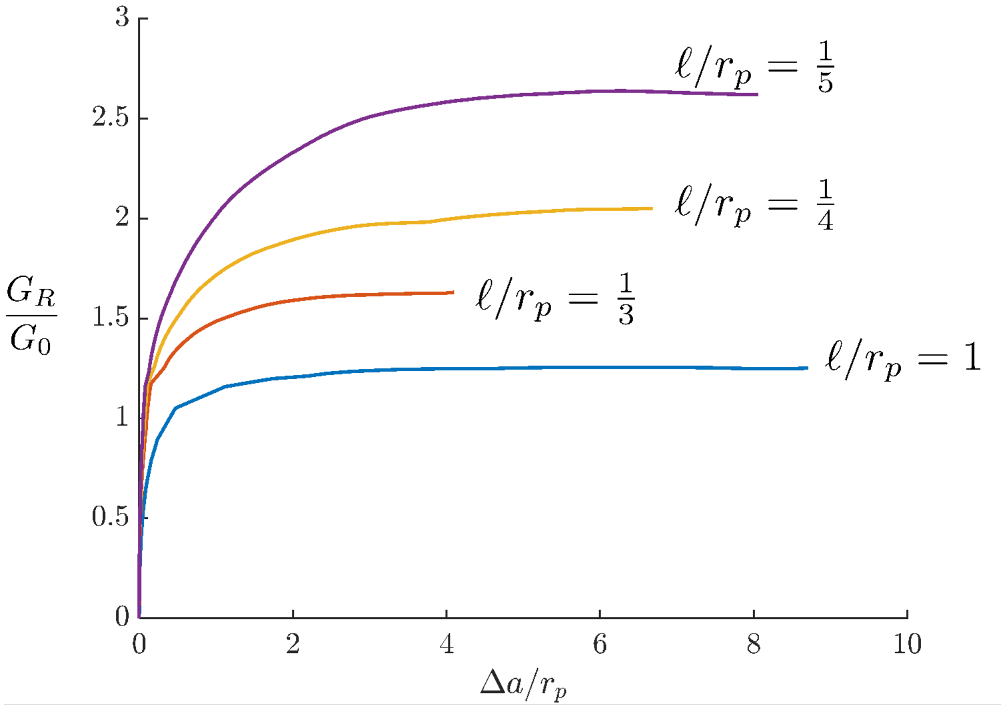
1. Choose ℓ / r_p
2. Drive stable crack growth through "surfing" boundary conditions[†]
3. Compute crack length vs time $a = \frac{3}{8\ell} \int_{B_0} \left(\phi + \ell^2 \|\nabla \phi\|^2 \right) \mathrm{d}A$
4. Compute energy release rate vs time via J-integral

$$G_R = J := \int_\Gamma \boldsymbol{t}_R \cdot \left[\tilde{\psi}^e \mathbf{1} - \nabla u^T \boldsymbol{P} \right] \boldsymbol{n}_R \, \mathrm{d}s$$

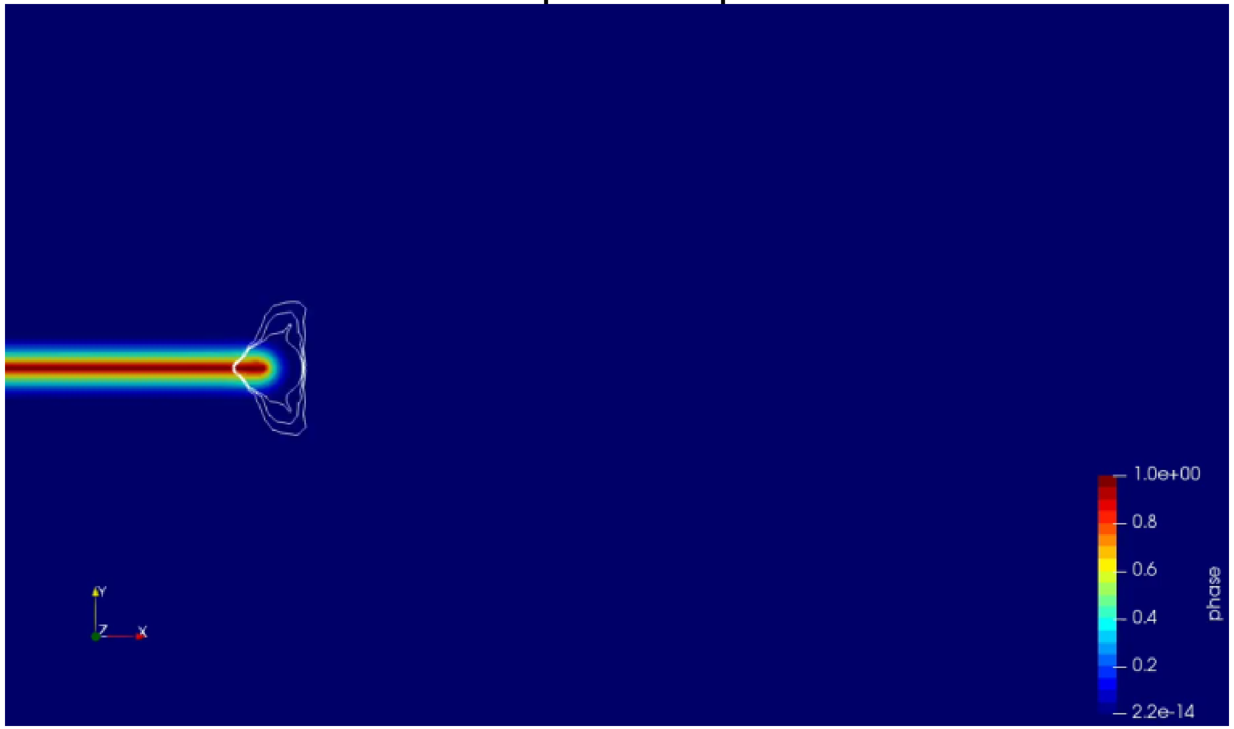
[†] MZ Hossain et al. *J. Mech. Phys Solids* (71) 2014

Crack growth resistance predictions, Part I

Classic Ambrosio-Tortorelli model form



Isolines of equivalent plastic strain

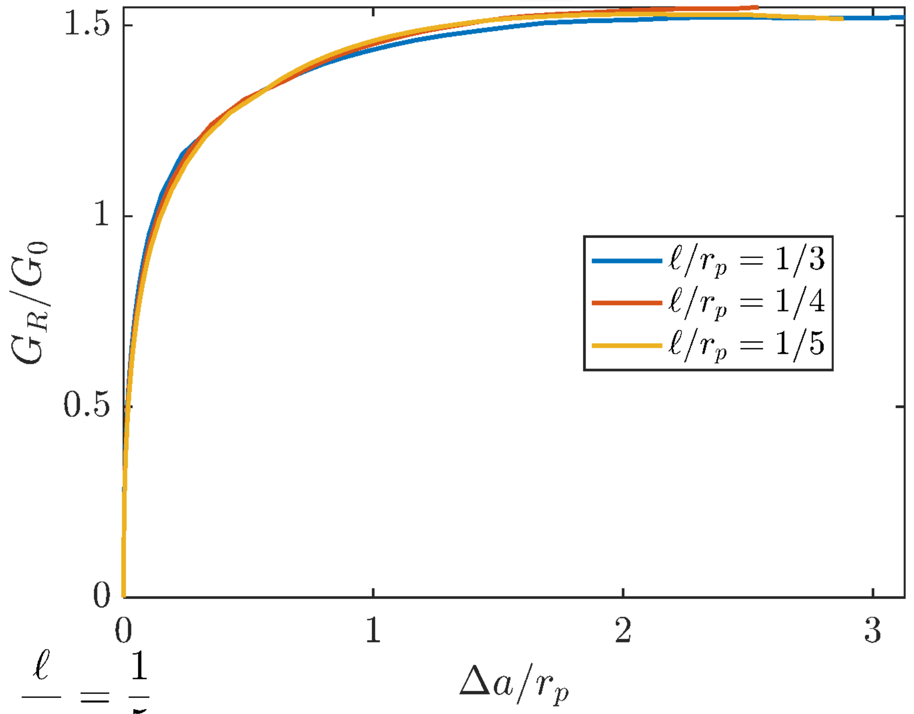


- Zone of active plastic straining grows with crack extension
- Eventually becomes fully developed
- Far-field resistance starts at G_0 and grows to steady-state value due to this additional dissipation
- ℓ must be considered a material parameter

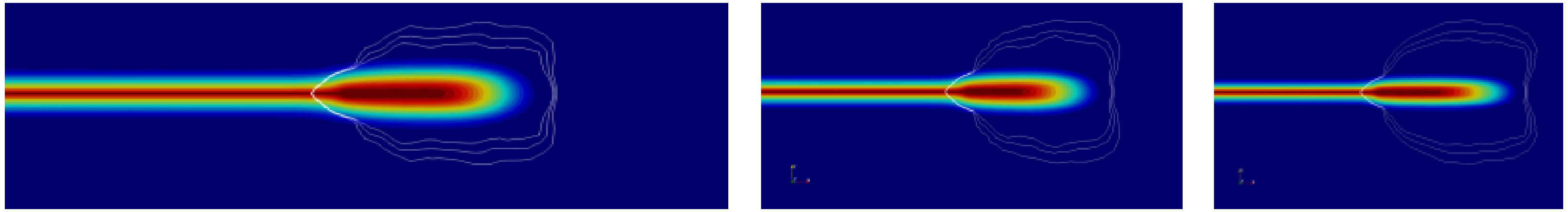
Crack growth resistance predictions, Part II

$$\frac{G_R}{G_0} = f\left(\frac{\Delta a}{r_p}, \frac{\ell}{r_p}, \frac{\psi_c}{\sigma_y \epsilon_0}, n, \epsilon_0, \nu\right)$$

- Crack growth resistance prediction is now insensitive to ℓ/r_p
- We can consider ℓ as a mathematical regularization parameter again



$\frac{\ell}{r_p} = \frac{1}{3}$ $\frac{\ell}{r_p} = \frac{1}{4}$ $\frac{\ell}{r_p} = \frac{1}{5}$

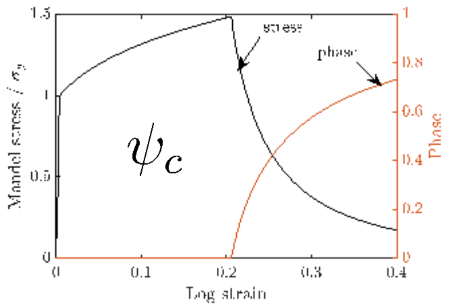


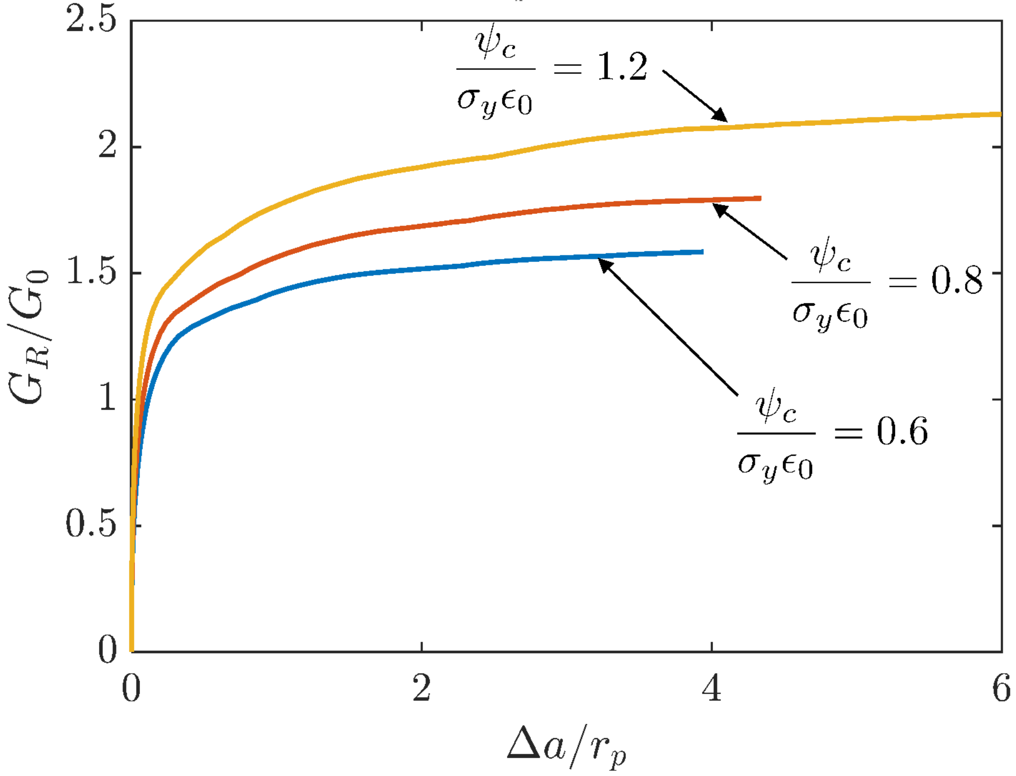
Isolines of equivalent plastic strain

Effect of threshold energy in cohesive model

$$\frac{G_R}{G_0} = f\left(\frac{\Delta a}{r_p}, \frac{\ell}{r_p}, \boxed{\frac{\psi_c}{\sigma_y \epsilon_0}}, n, \epsilon_0, \nu\right)$$

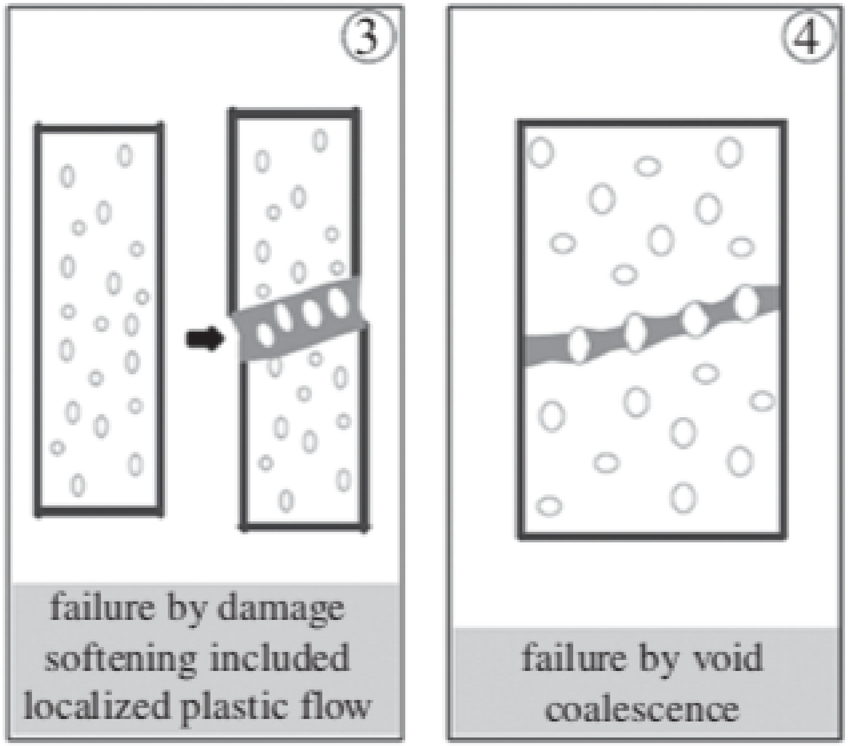
- R-curve can be tuned by threshold energy parameter ψ_c
- Model distinguishes fracture strength from regularization
- Opens pathway to enriching fracture physics: modulate strength locally without unphysical widening/narrowing of crack representation





Improving LSY ductile failure predictivity

- Many alloys fail by void growth & coalescence
- Initial stable growth well approximated by RVE void growth mechanics (Rice-Tracey, Gurson, many more)
- Usually based on RVE calculations – valid when zone surrounding void can be considered in isolation
- In contrast, coalescence is inherently nonlocal



Tekoglu et al. *Phil Trans R Soc A* **373** 20140121

Idea:
- Use classic void growth mechanics to characterize the initial stable void growth,
- Use phase field to capture coalescence and macroscopic localization

Improving LSY ductile failure predictivity

1. Capture void fraction evolution with void growth mechanics relation:

$$\dot{f} = \hat{\mathcal{F}}(f, \frac{\sigma_m}{\bar{\sigma}}, \dot{\bar{\varepsilon}}^p)$$

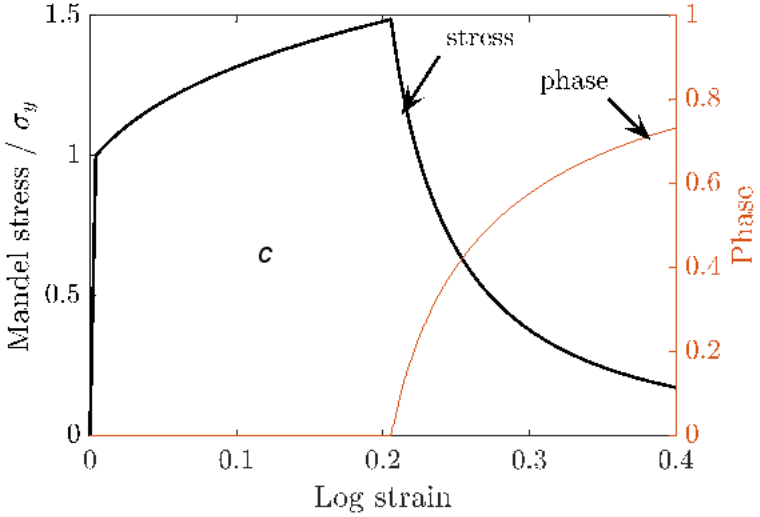
For example, Rice-Tracey: $\dot{f} = C_0 \exp\left(C_1 \frac{3\sigma_m}{2\bar{\sigma}}\right)\dot{\bar{\varepsilon}}^p$

2. Evolve critical fracture energy density with changing void fraction:

$$\psi_c = \hat{\psi}_c(f, \frac{\sigma_m}{\bar{\sigma}}, \ldots)$$

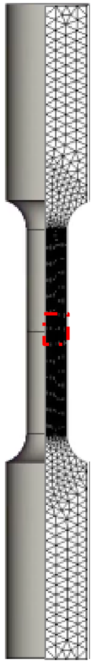
E.g., simple mixture rule: $\hat{\psi}_c(f) = (1 - f)\psi_{c,0}$

Could use more rigorous localization study based on average void size, spacing, loading conditions

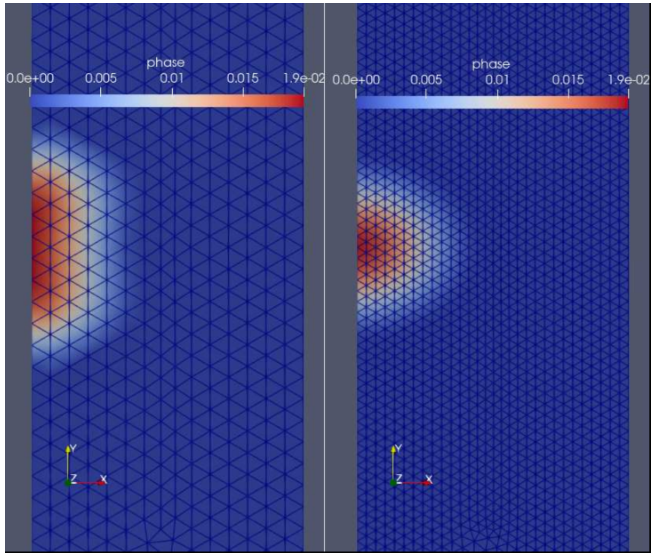


3. Phase field tends to nucleate where strain energy density exceeds critical fracture energy density

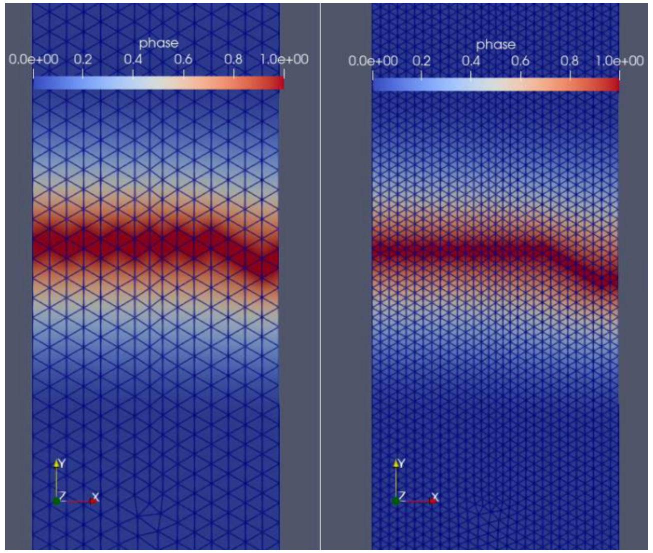
However, model mantains well-defined surface energy G_0

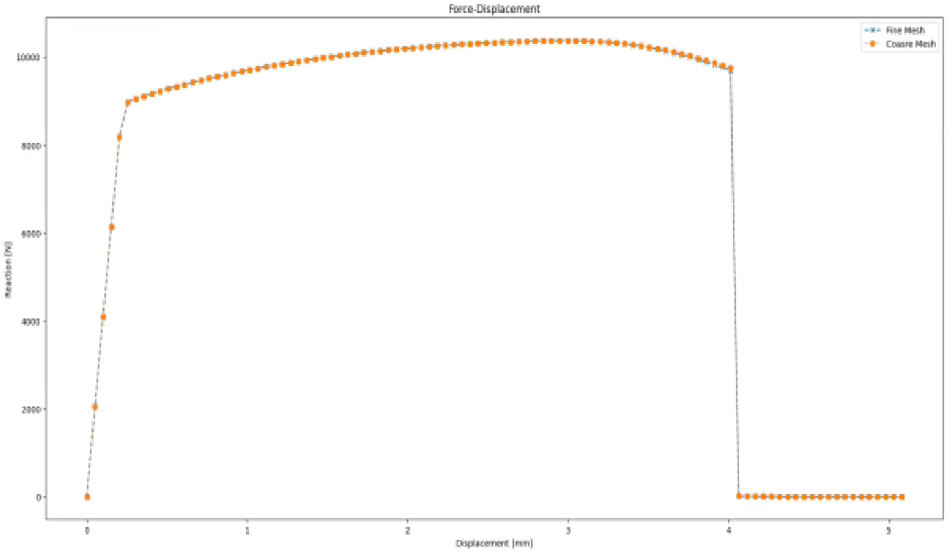


Load step before failure



Load step at failure





- Calibration of the model is in progress
- Multiple test data sources: round bar tension, notched bar, compact tension

Conclusions

- Cohesive phase field model restores role of internal length as regularization parameter for EPFM
- New model with a useful set of properties:
  - Crack nucleation dependence on stress triaxiality history
  - Consistent with classic void growth mechanics
  - Correspondence with small scale yielding: critical energy release rate still a parameter
  - Minimum principle formulation preserved
- Minimization structure can be exploited for solution, more accurate, more robust

Acknowledgements

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Thanks for your attention!

Questions?

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SUPPLEMENTAL INFORMATION

First attempt: Ambrosio-Tortorelli regularization model[1]

Free energy

$$\psi = \psi_{\text{mech}}(\boldsymbol{F}, \boldsymbol{F}^p, \bar{\varepsilon}^p, \phi) + \psi_{\text{frac}}(\phi, \boldsymbol{\nabla}\phi)$$

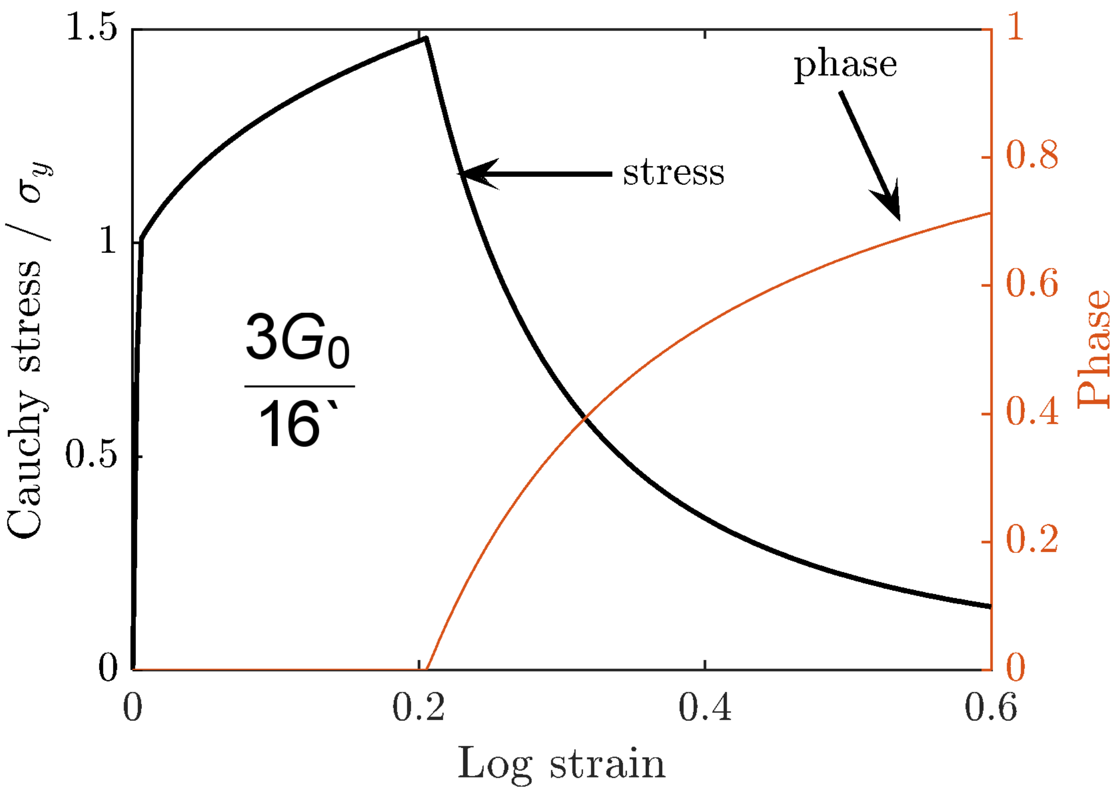
Mechanical free energy

$$\psi_{\text{mech}}(\boldsymbol{F}, \boldsymbol{F}^p, \bar{\varepsilon}^p, \phi) = g(\phi)\left(\widetilde{\psi}^e(\boldsymbol{F}^e) + \widetilde{\psi}^p(\bar{\varepsilon}^p)\right)$$

$$g(\phi) = (1-\phi)^2$$

Fracture free energy

$$\psi_{\text{frac}}(\phi, \boldsymbol{\nabla}\phi) = \frac{3G_0}{8\ell}\left(\phi + \ell^2\|\boldsymbol{\nabla}\phi\|^2\right)$$



[1]Bourdin, B., Francfort, G.A., Marigo, J.-J., 2000 J. Mech. Phys. Solids 48 (4), 797-826.

Variational formulation

cf. M Ortiz and L Stainier, *Comp Meth Appl Mech Engrg* 171 (1999) 419-444

Infimize $$I(\dot{\boldsymbol{\chi}}, \dot{\phi}, \dot{\bar{\varepsilon}}^p, \boldsymbol{N}^p) = \int_{B_0} \left(\dot{\psi} + \Pi^* + \Delta^*\right) \mathrm{d}V - G_{\mathrm{ext}}(\dot{\boldsymbol{\chi}})$$

with $$\dot{\phi} \geq 0$$ $$\dot{\bar{\varepsilon}}^p \geq 0$$ $$0 \leq \phi \leq 1$$

Euler-Lagrange equations

Linear momentum $$\nabla \cdot \boldsymbol{P} + \boldsymbol{b}_0 = \boldsymbol{0}$$

Phase evolution $$\frac{G_c \ell^2}{2 c_h} \nabla^2 \phi - g'(\phi) \hat{\psi}_{\mathrm{mech}} - \frac{G_c}{4 \ell c_h} h'(\phi) = \eta \dot{\phi}$$

Yield condition $$\boldsymbol{M} : \boldsymbol{N}^p - Y^{\text{eq}} = Y^{\text{neq}}$$

Flow direction $$\boldsymbol{N}^p = \sqrt{\frac{3}{2}} \frac{\mathrm{dev}\, \boldsymbol{M}}{\|\mathrm{dev}\, \boldsymbol{M}\|}$$

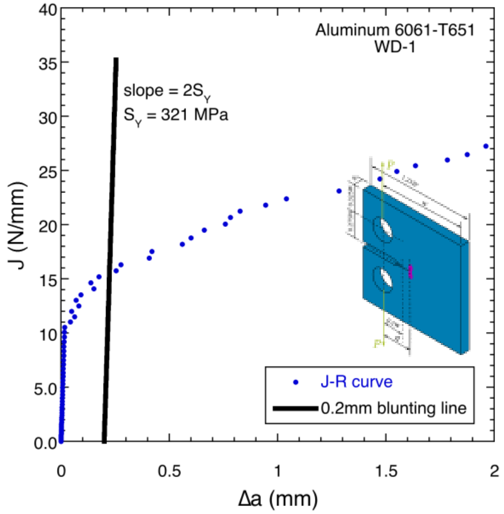
(all of the above) in B_0

$$\boldsymbol{P}\boldsymbol{n}_0 = \hat{\boldsymbol{t}}_0 \quad \text{on } \partial_t B$$

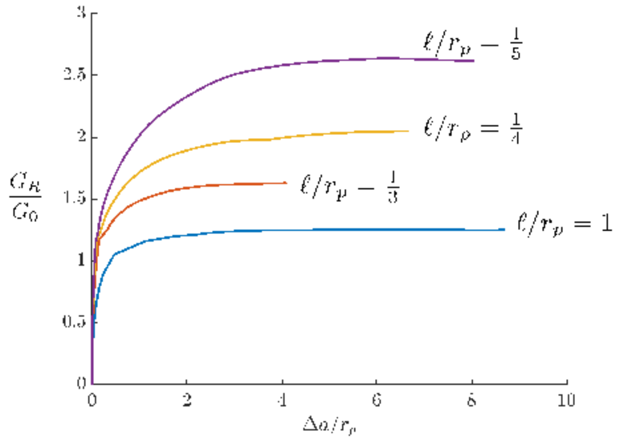
$$\nabla \phi \cdot \boldsymbol{n}_0 = 0 \quad \text{on } \partial B$$

Is the model form sufficient?

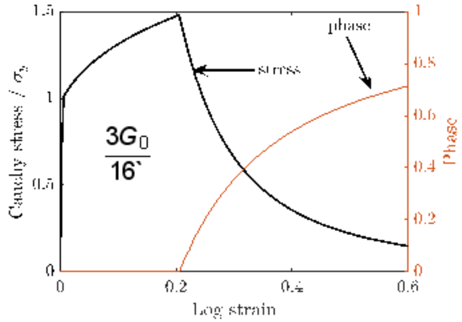
- Sometimes …
  - EPFM rules: limited plasticity, scale separation
  - Can calibrate ℓ to standard fracture tests



Chris San Marchi (SNL)



- However, convergence with respect to ℓ lost
- Nucleation and regularization have become entangled



Volumetric locking

- Hu-Washizu formulation used to avoid locking (4 fields - $\boldsymbol{u}, \phi, p, J$)
- LBB stable interpolation
  - Continuous P2 + cubic bubble for displacement
  - Element-wise P1 for pressure and Jacobian (no inter-element continuity)
- Pressure and Jacobian DOF are condensed out at element level