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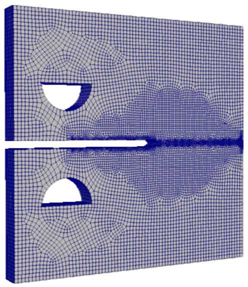

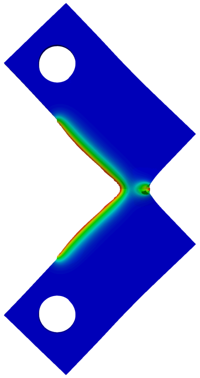

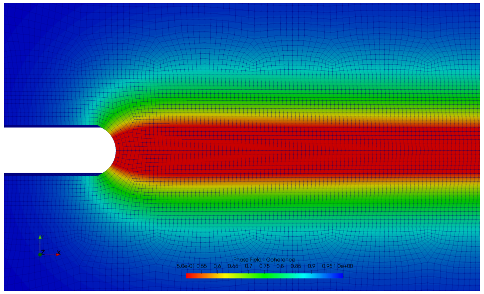

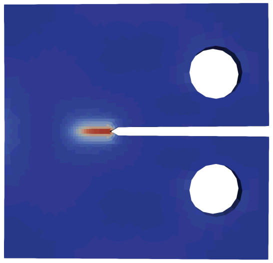

Ductile Fracture Representation Using the Phase-Field Model in SIERRA

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Sandia National Laboratories / California

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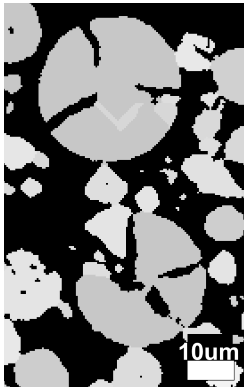
Overview

- Motivation & Objectives
- Common Models
  - Classical, “AT-2”
  - Threshold, “AT-1”
- Capabilities
  - Implicit & explicit & mixed integration
- Challenges, overcoming them
- Addressing Plasticity
  - Moving to cohesive model
- Future directions

Overview

- Motivation:
  - Need to model fracture in many industries:
    - Aerospace/naval/defense
    - Manufacturing
    - Automobile
    - Wind energy systems
    - Batteries / energy storage
    - Biological materials
  - Most emphasis has been in brittle fracture, many relevant materials are ductile
  - SIERRA users overwhelmingly use explicit time integration for dynamic simulations



Cathode Particle Fracture

- Objectives:
  - Implement phase field model in SIERRA (fully 3-D, parallel, HPC-ready, multi-physics)
  - High model credibility from verification & validation
  - Computationally efficient
  - Capable with implicit and explicit time integration

Common Models

- Phase Field Fracture Concept:

$$\Psi = \int_\Omega \psi \, d\Omega = \int_\Omega \tilde{\psi}^{\mathrm{e}}(\varepsilon^e) + \tilde{\psi}^p(\varepsilon^p) d\Omega + \int_\Gamma G_c d\Gamma$$
$$\rightarrow \int_\Omega g(c)\tilde{\psi}^{\mathrm{e}}(\varepsilon^e) + h(c)\tilde{\psi}^p(\varepsilon^p) + f(c, \nabla c, l) G_c \, d\Omega$$

  - Fracture energy: volumetric expression replaces surface energy functional
  - Γ-convergent: expressions equivalent in limit $l \to 0^+$
- Classical, AT-2

$$\psi = \mathrm{c}^2 * \left(\tilde{\psi}^{\mathrm{e}}(\varepsilon^e) + \tilde{\psi}^p(\varepsilon^p)\right) + \frac{G_c}{4l}\left((1-c)^2 + 4l^2|\nabla c|^2\right)$$

  - Drawbacks:
    - Damage everywhere
    - Damage irreversibility not intrinsic to mathematical formulation
- Threshold, AT-1

$$\psi = \mathrm{c}^2 * \left(\tilde{\psi}^{\mathrm{e}}(\varepsilon^e) + \tilde{\psi}^p(\varepsilon^p)\right) + 2\psi_{crit}\left((1-c) + l^2|\nabla c|^2\right)$$

  - Damage only grows after critical energy condition reached, only in neighborhood of cracks
  - Drawbacks:
    - Damage irreversibility not intrinsic to mathematical formulation

Capabilities

- Classical (AT-2) & Threshold (AT-1) models implemented in common framework:
  - Euler-Lagrange equations derived by variational derivative of energy functional

Stationary Functional

$$\delta\Psi = 0$$

Damaged Mechanical Solve

Phase Field Solve

E-L:

$$\nabla \cdot \left(\frac{\partial \psi}{\partial \varepsilon}\right) = 0$$

$$\nabla \cdot \left(\frac{\partial \psi}{\partial \nabla c}\right) - \frac{\partial \psi}{\partial c} = 0$$

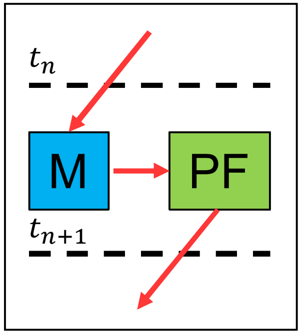
$$\left(\frac{2\tilde{\psi} l}{G_c} + 1\right) c - l^2 \Delta c = 1$$

$$\frac{\tilde{\psi}}{\psi_{crit}} c - 2 l^2 \Delta c = 1$$

- Phase-field solve accomplished using a linear reaction-diffusion solver
  - General form: $Rc - D\Delta c = S$

Capabilities

- Implicit Mechanics / Implicit Phase-Field
- Explicit Mechanics / Implicit Phase-Field
- Explicit Mechanics / Explicit Phase-Field



Staggering Scheme

- All are fully-3D & fully-parallelized / HPC ready
- All are staggered solve:
  - Mechanical update then phase-field update each step
  - Option to update phase field less often:
    - every “X” timesteps (especially for Explicit/Implicit)

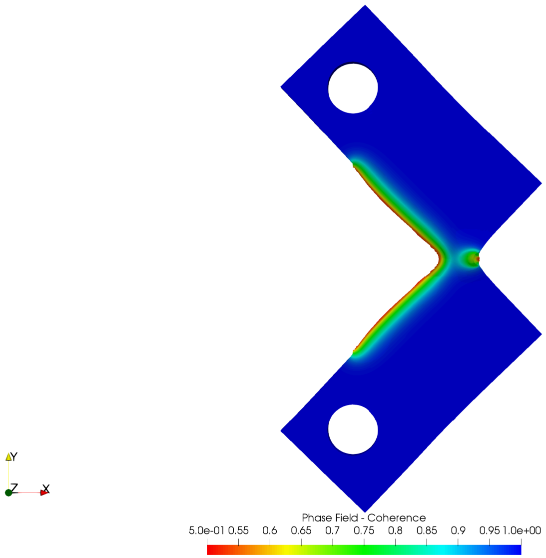
- Explicit/Implicit Timing:

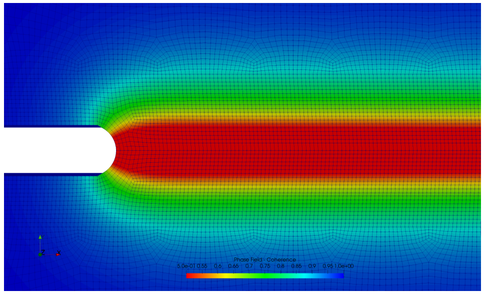
Mesh	Δt (s)	FeFp cpu*time (No Phase-Field Solve: Mechanical only)	PFFeFp-L cpu*time (“Local” Phase-Field Solve: $D = 0 \rightarrow c = S/R$)	PFFeFp-NL cpu*time (Full Phase-Field Implicit Solve $Rc - D\Delta c = S$)
$\tilde{h} = 1$	1.75e-5	9m2s	13m5s	27m23s
$\tilde{h} = 1/2$	9.06e-6	5h9m	7h16m	11h39m
$\tilde{h} = 1/4$	4.57e-6	53h41m	79h20m	155h18m

Explicit/Implicit expensive! motivation for explicit/explicit model

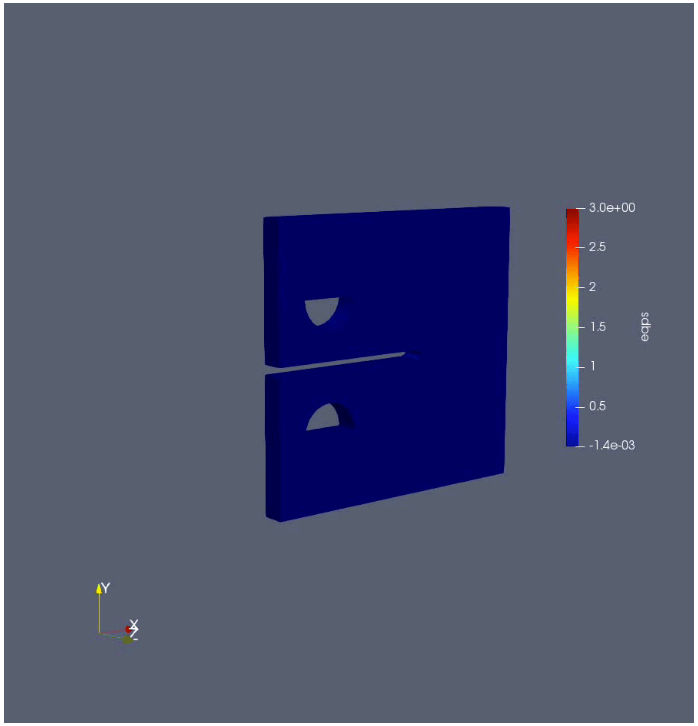
Capabilities

- Minimum qualification…. we can solve the mode-I fracture problem!





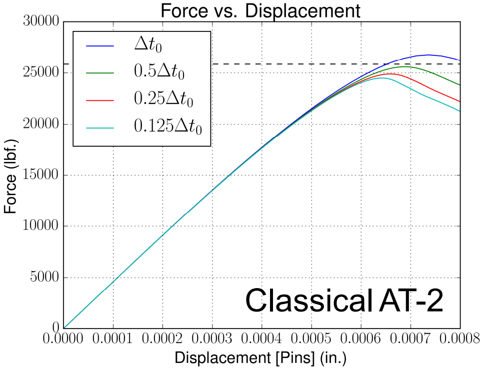
Undeformed View (No visual threshold, zoomed):



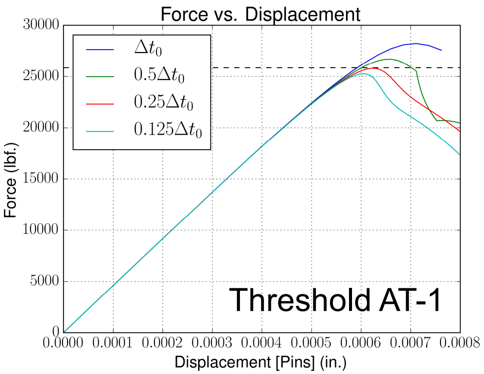
Visual threshold at $c = 0.5$

Capabilities – Implicit/Implicit

- Verification test: toughness
  - Geometry: compact tension specimen (ASTM E1820)
  - Prescribe fracture toughness G_c in material model
  - Observe peak force at crack initiation
  - Calculate ideal peak force from toughness & geometry using ASTM relation A2.2
  - Compare results



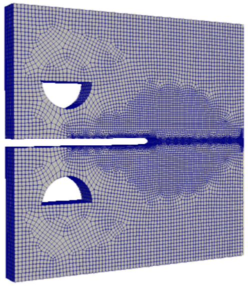
- Model results approximate the expected value
  - Possible explanations for discrepancy:
    - Finite/coarse mesh density
    - Finite length scale (convergent as $l \rightarrow 0^+$)

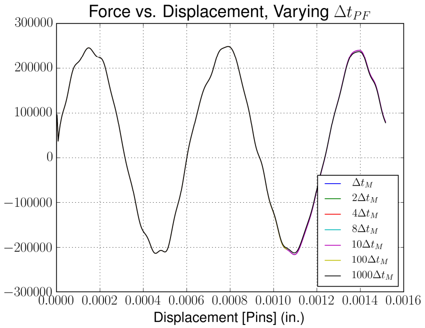


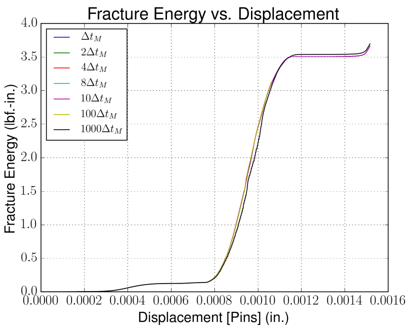
- Temporal sensitivity… wait 4 minutes!

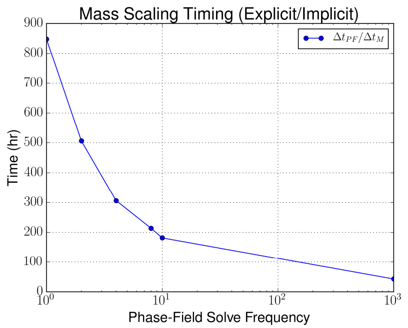
Capabilities – Explicit/Implicit

- Explicit Mechanics / Implicit Phase-Field solve is costly
  - Option to update phase field less often
    - Every "X" timesteps
- A quick test on a dynamic problem
  - ASTM E1820 compact tension specimen
  - 6061-T6 Aluminum
  - Quick loading: 1 in/s for 60ms









- Very similar force/displacement & fracture energy responses
- Great simulation time savings realized
- Still to do.... testing on a less-dynamic problem

Capabilities – Explicit/Explicit

- Addition of non-conservative viscosity term in Euler-Lagrange equation:
  - Viscous Dissipation: $V = \frac{1}{2}\eta\dot{c}^2$
  - Euler-Lagrange: $\nabla \cdot \left(\frac{\partial\psi}{\partial\nabla c}\right) - \frac{\partial\psi}{\partial c} = -\frac{\partial V}{\partial\dot{c}}$
  - Phase-Field update: $\eta\dot{c} = \begin{cases} 2\tilde{\psi}c - \frac{G_c}{2l}(1-c) - 2G_c l\Delta c \\ 2\tilde{\psi}c - 2\psi_{crit} - 4\psi_{crit}l^2\Delta c \end{cases}$ & $\dot{c} \geq 0$
  - Damage irreversibility not intrinsic to mathematical formulation, artificial dissipation
- Stability:
  - Parabolic systems inherently transmit information instantaneously
  - Limit timestep to keep crack/damage propagation speed at/under elastic wave speed, v_c
  - Strategy: choose smallest phase viscosity η such that $(\Delta t)_{\mathrm{M}} \leq (\Delta t)_{PF}$

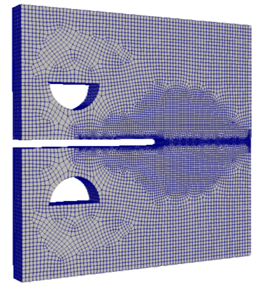
$$\frac{\eta}{(\Delta t)_{PF}} \geq \left\{\frac{2G_c l}{(\Delta x)^2}, \frac{4\psi_{crit}l^2}{(\Delta x)^2}\right\} \rightarrow (\Delta t)_{PF} \leq \left\{\frac{\eta(\Delta x)^2}{2G_c l}, \frac{\eta(\Delta x)^2}{4\psi_{crit}l^2}\right\}, (\Delta t)_M \leq \frac{\Delta x}{v_c}$$

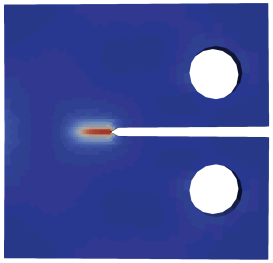
$$\eta \geq \tilde{\eta} = \left\{\frac{2G_c l}{\Delta x\, v_c}, \frac{4\psi_{crit}l^2}{\Delta x\, v_c}\right\}$$

Reference: Tupek, MR. "Cohesive phase-field fracture and a PDE constrained optimization approach to fracture inverse problems". SAND2016-9510. 2016.

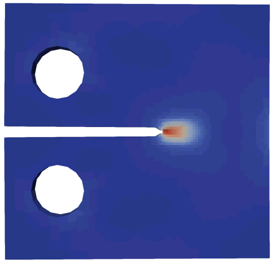
Capabilities – Explicit/Explicit

- New capability….
- A quick test on a dynamic problem
  - ASTM E1820 compact tension specimen
  - 6061-T6 Aluminum
  - Quick loading: 1 in/s for 60ms



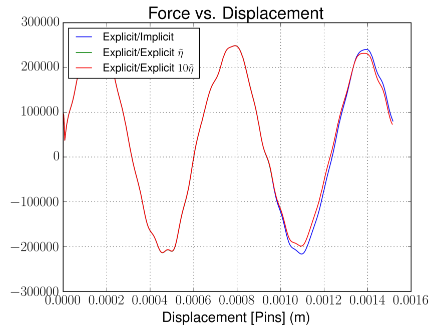


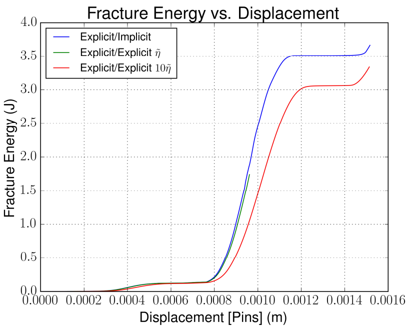
Interior Midplane



Exterior

- Similar force/displacement response
- Drawback of viscosity model: sensitivity (excess dissipation)

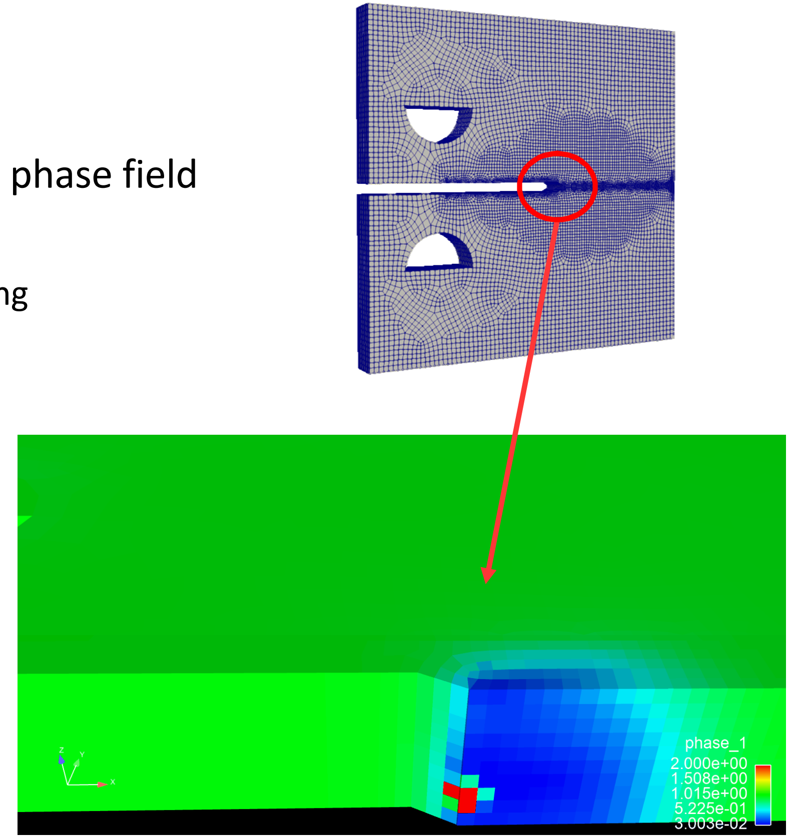




- Still need to do…
  - Timing study to quantify efficiency gains
  - A less-dynamic problem to verify toughness returned

Overcoming Challenges

- Stability (Explicit/Explicit):
  - For stability, need to maintain $(\Delta t)_{\mathrm{M}} \leq (\Delta t)_{PF}$
  - When mechanical timestep grows… trouble for phase field
  - Solutions:
    - Increase viscosity parameter η from the beginning
      - Increases artificial dissipation…
    - Adaptively set η based on mechanical timestep



- Sub-zero coherence (Explicit/Explicit):
  - Possible for $c < 0$ due to explicit integration
  - Solutions:
    - Bound c at quadrature points or nodes
    - Lagrange multiplier constraint

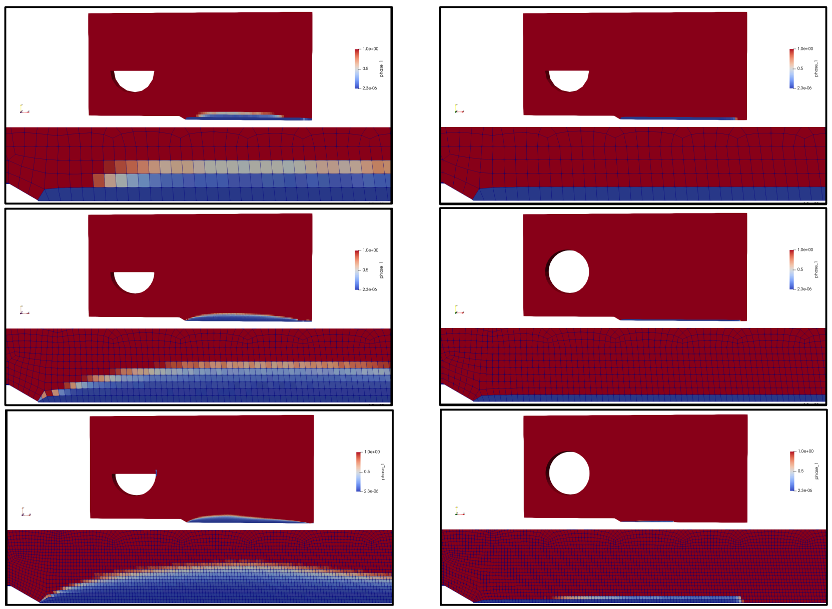
Overcoming Challenges

- Temporal sensitivity (Implicit/Implicit):
  - Artifact of staggered solve
  - Example from "local" (no gradient term) phase field solve

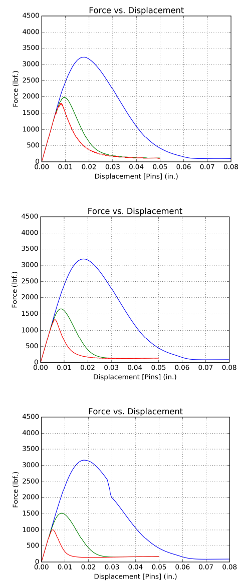
$\tilde{h} = 1$

$\tilde{h} = 1/2$

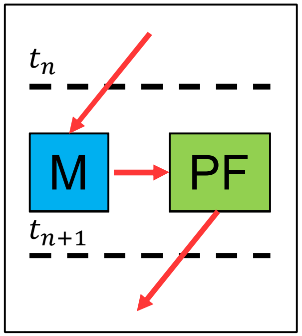
$\tilde{h} = 1/4$



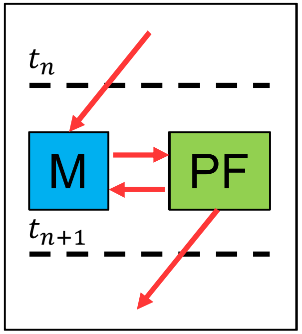
$\Delta t \leq 0.001$ $\Delta t \leq 0.0001$



  - Solutions:
    - Monolithic solve
    - Iteration within staggered solve



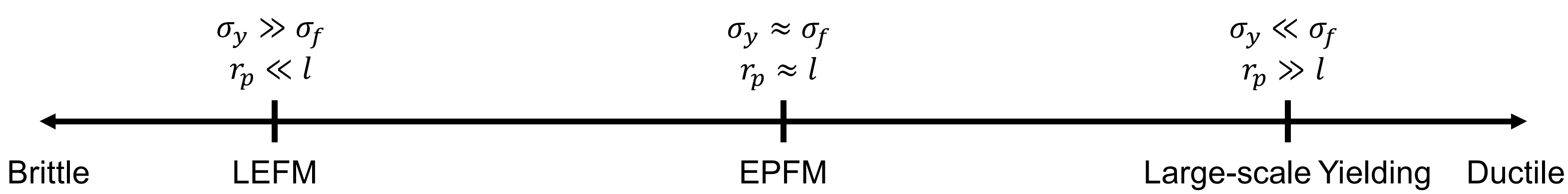
Current



Proposed

Addressing Plasticity

- Material scale continuum…
  two perspectives of plasticity in traditional approaches:
  - Length scale interpretation:
    - Phase-field models Γ-convergent to Griffith fracture as $l \to 0^+$
    - If length scale too small, plasticity dominates fracture process
    - If length scale too large, plasticity enveloped by fracture regularization
    - Numerical regularization length scale l_f incompatible with physical length scale r_p



  - Stress interpretation:
    - Regularization length scale l associated with a critical stress $\sigma_f(l)$
    - Phase-field models Γ-convergent to Griffith fracture as $l \to 0^+$
    - Associated critical stress grows correspondingly: $\sigma_f \to \infty$
    - Numerical critical stress σ_f incompatible with physical yield stress σ_y
- Motivation to move toward cohesive/Lorentz-type model

Future Directions

- Explicit/Explicit:
  - Timing study to demonstrate efficiency improvement
  - Toughness verification with “Pacman” geometry & K-field solution to eliminate dynamic effects
- Capability:
  - Integrate with rate-dependent material models
  - Integrate with XFEM
- Quality:
  - Iteration within staggered implicit solve
  - Implement cohesive/Lorentz-type model and non-linear update PDE solve
  - More intelligently address damage irreversibility & sub-zero coherence
    - Perhaps with Lagrange multipliers
- Efficiency:
  - Integrate with adaptive mesh refinement/coarsening for greater efficiency

- Acknowledgement: John Dolbow & Rudy Geelen (Duke University)

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