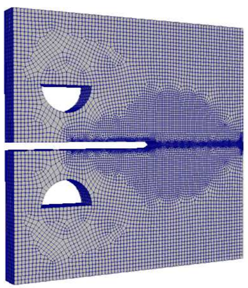
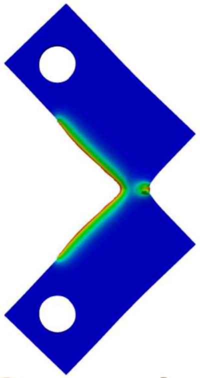
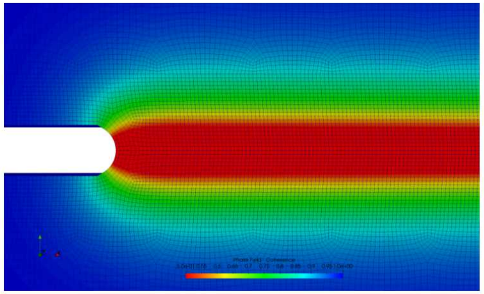
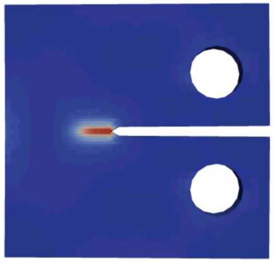
SAND2019-8673C









Advances in Quasistatic and Dynamic Phase-Field Implementation for Ductile Failure in SIERRA

A. Stershic, B. Talamini, J. Ostien, M. Tupek

Sandia National Laboratories / California

USNCCM 15; Austin, TX; July 29, 2019

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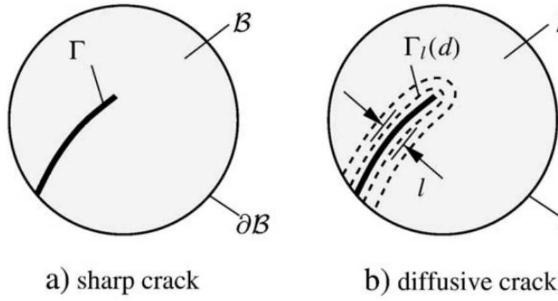
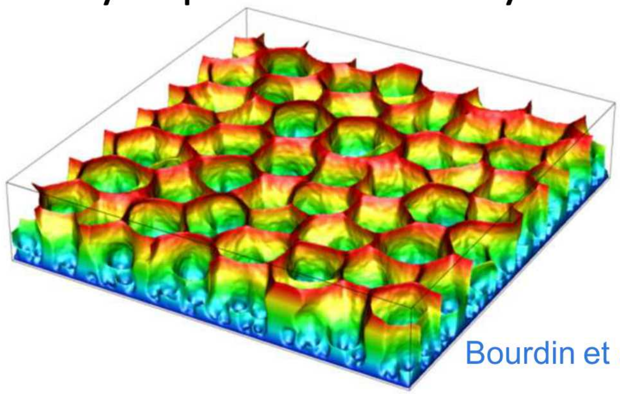
Phase field approach to fracture

- Cracks represented as smeared field



Miehe et al (2011)

- Advantages: no sharp discontinuities, naturally captures arbitrary crack paths, branching, merging



Bourdin et al (2014)

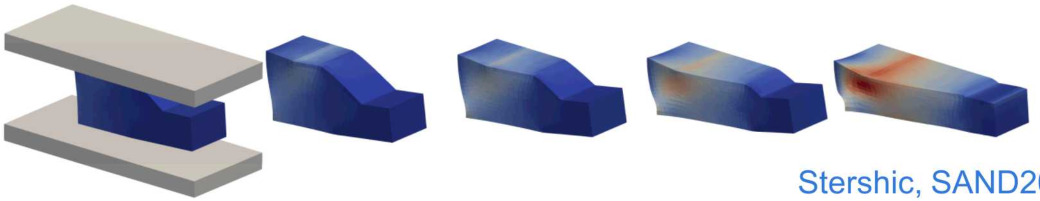
- Genesis in linear elastic brittle fracture
- Approaches for ductile failure have started appearing and are under development

B Bourdin, J-J Marigo, C Maurini, P Sicsic. *Phys Rev Lett* 112, 014301 (2014)
R Alessi, J-J Marigo, S Vidoli. *Arch Ration Mech An* 214 (2014) 575-615
C Miehe, F Aldakheel, A Raina. *Int J Plasticity 84* (2016) 1-32
C Miehe, M Hofacker, L-M Schänzel, F Aldakheel. *Comp Meth Appl Mech Engrg* 294 (2015) 486-522
M Ambati, T Gerasimov, L De Lorenzis. *Comput Mech* 55 (2015) 1017-1040

Overview

- SIERRA code & objectives
- Phase Field Formulation
- Phase Field Implementation
- Implicit Time Integration
  - Recent Efforts
    - Iterated staggered solution
    - Element Study
    - Temporal / Spatial Convergence
  - Model Validation
- Explicit Time Integration
  - Explicit Phase Field solve
  - Implicit Phase Field solve
- Future directions

SIERRA Code & Objectives



Stershic, SAND2018-4988C

- SIERRA finite element code
  - Developed by Sandia National Laboratories
  - Implicit & explicit time integration, Quasistatic & Dynamic
  - Fully parallelized for clusters, HPC
  - Finite strain formulation by default
  - Robust explicit & implicit contact
  - Constant verification & validations efforts, experimental comparisons
  - Multiphysics: thermal, electrical, chemical, etc.
- Objectives:
  - Implement ductile phase field model in SIERRA
  - Modular: can be coupled with any plasticity model
  - Computationally efficient
  - Capable with implicit and explicit time integration
  - Convergent: high model credibility from verification & validation

Phase Field Formulation

- 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

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

- 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:
  - (Classical) Damage from any loading, even distant from stress concentration
  - Damage irreversibility not intrinsic to mathematical formulation
  - Interpretation of length scale – is infinitesimal l required?
    - What about critical stress?
    - What about mesh resolution?

Phase Field Implementation

Sandia National Laboratories

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

Stationary Functional

$$\delta\Psi = 0$$

Euler-Lagrange:

Damaged Mechanical Solve

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

Phase Field Solve

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

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

$$\max\left(\frac{\tilde{\psi}}{\psi_{crit}}, 1\right) c - 2 l^2 \Delta c = 1 \quad \text{Threshold}$$

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

Phase Field Implementation

- Damage irreversibility
  - Maximum driving energy history field, $\mathcal{H} = \max_t \tilde{\psi}$
    - Easy to implement
    - Deviation from Variational Consistency

Phase Field Solve

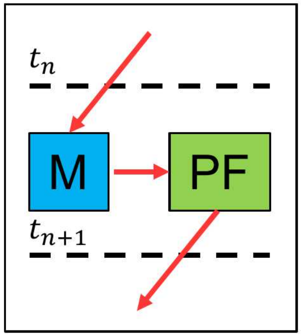
Classical	$\left(\frac{2\tilde{\psi}l}{G_c}+1\right)c - l^2\Delta c = 1$	→	$\left(\frac{2\mathcal{H}l}{G_c}+1\right)c - l^2\Delta c = 1$
Threshold	$\max\left(\frac{\tilde{\psi}}{\psi_{crit}},1\right)c - 2l^2\Delta c = 1$	→	$\max\left(\frac{\mathcal{H}}{\psi_{crit}},1\right)c - 2l^2\Delta c = 1$
			$\left(\left\langle\frac{\mathcal{H}}{\psi_{crit}}-1\right\rangle_+ + 1\right)c - 2l^2\Delta c = 1$

- Augmented Lagrangian approach using Inequality-constrained PDE solve
  - Difficult to implement in Sierra framework, but interested to explore

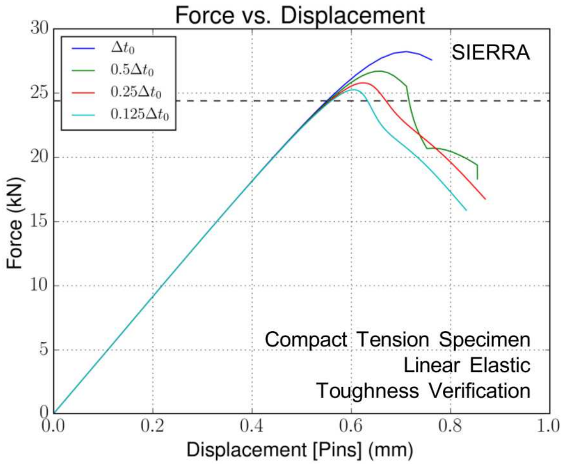
IMPLICIT TIME INTEGRATION

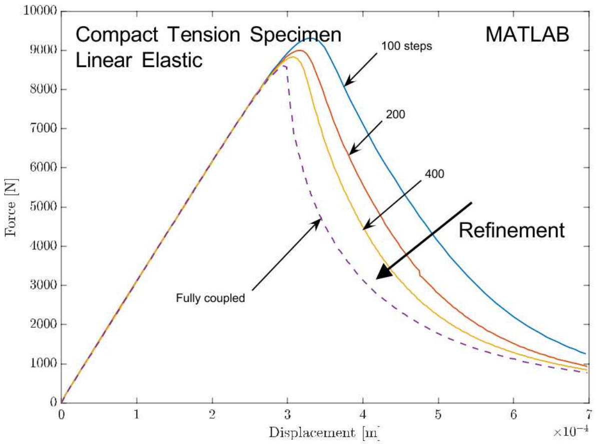
Recent Efforts

- Original coupling scheme:
  - Options: monolithic –or- staggered solution scheme ("alternate minimization")



Coupled Solve Schematic

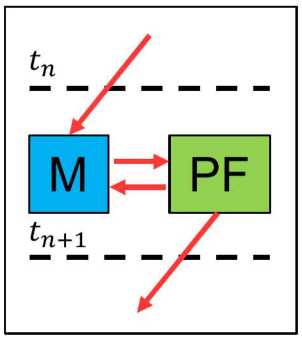




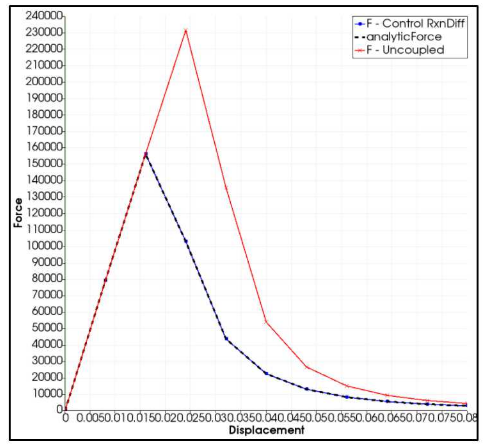
  - Implemented mechanics/PF staggered solution
  - No easy access in SIERRA to implement monolithic solve
  - Initially, no iteration of mechanics/PF solve within timestep
  - Lack of iteration leads to acceptance of *unconverged* solutions at each time step
  - Leads to strong temporal sensitivity, toughness overpredicted

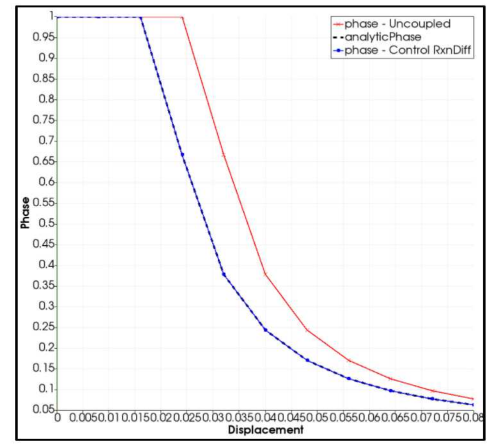
Recent Efforts

- Modified coupling scheme:
  - Implement iteration between Mechanics & PF solves within timestep



Coupled Solve Schematic

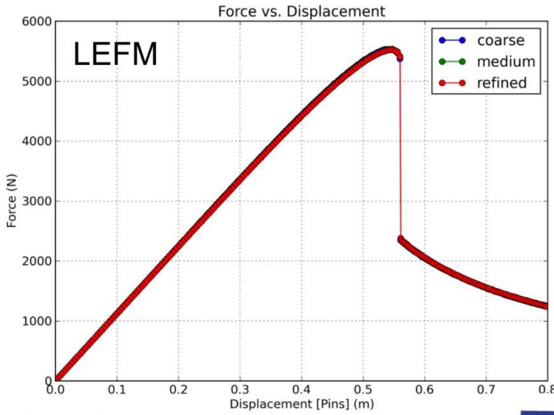


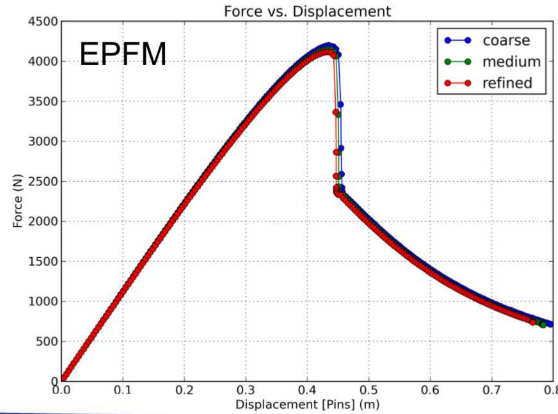


  - Solve mechanics, solve damage, compute M residual
  - Convergence metric: mechanical residual < tolerance
  - Better metric?
    - Phase field solve = linear system → trivial PF residual
    - Combined energy residual?
    - Phase field relative residual between iterations?

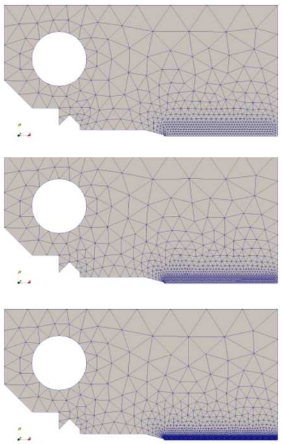
Recent Efforts

- Coupling scheme:
  - Implement iteration between Mechanics & PF solves within timestep
  - Spatial convergence:

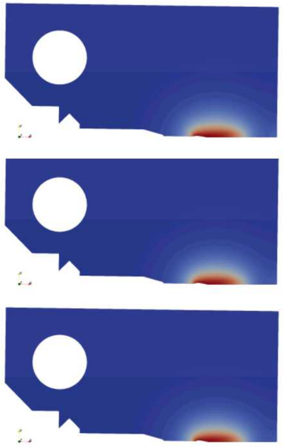




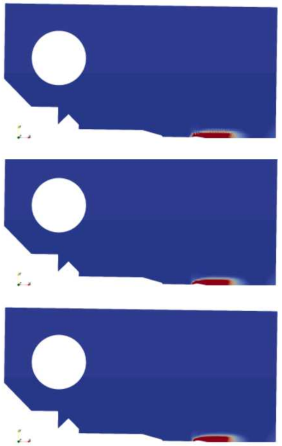
Compact Tension Specimen Meshes



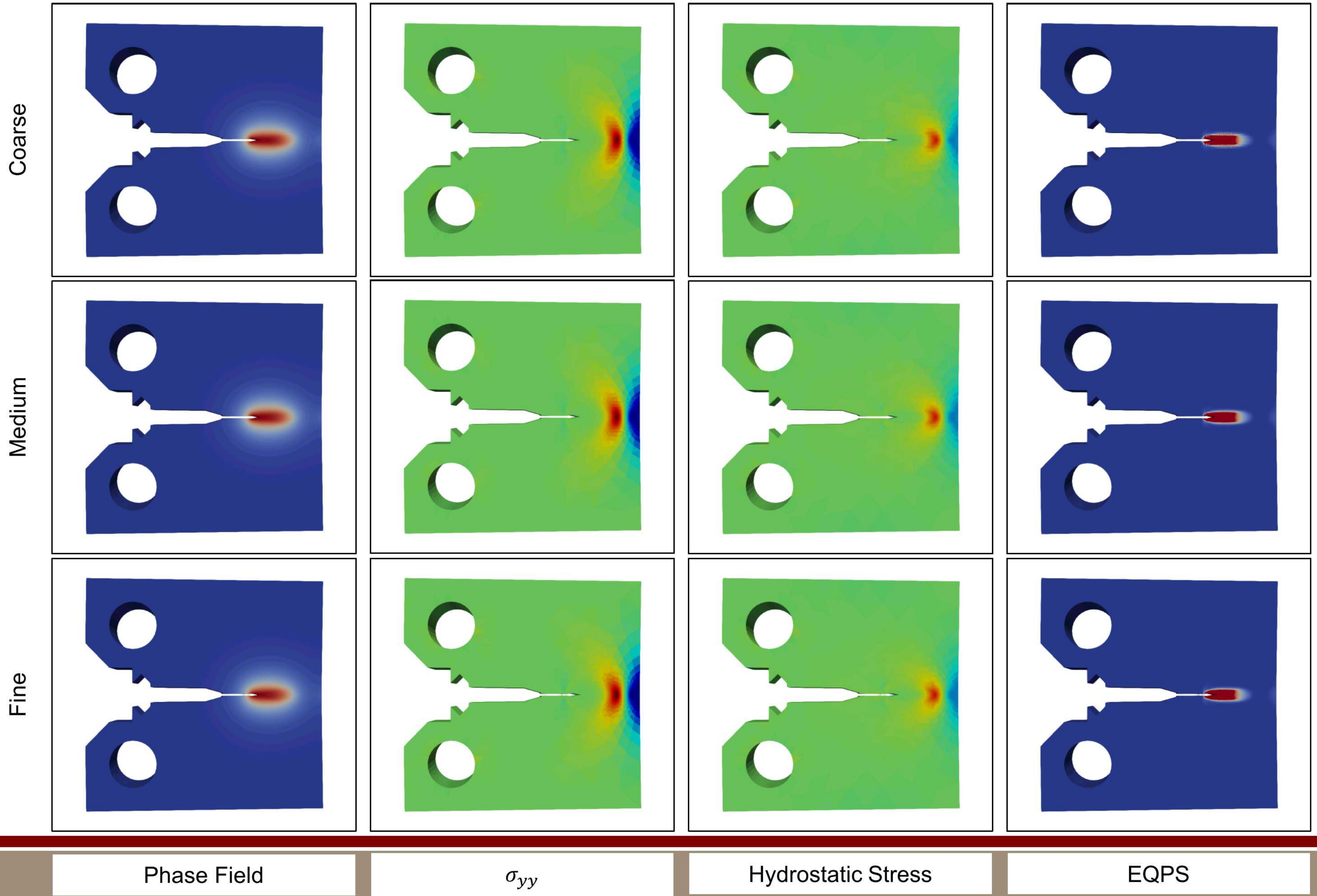
Phase Field



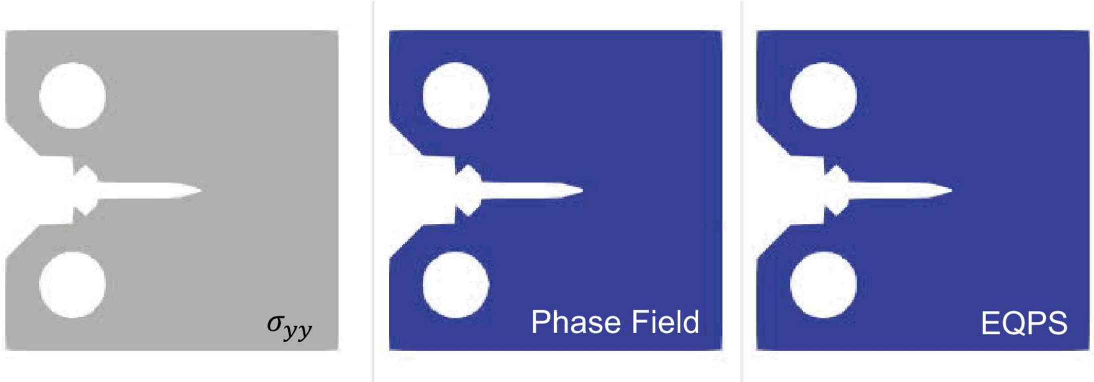
EQPS

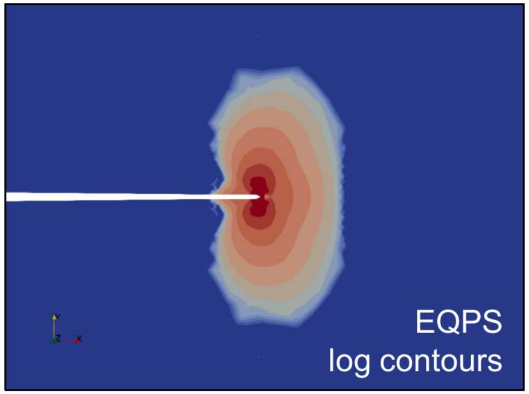


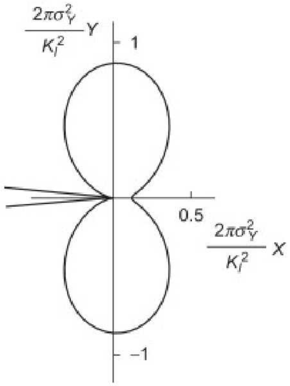
Spatial Convergence (UL-Qtet10)



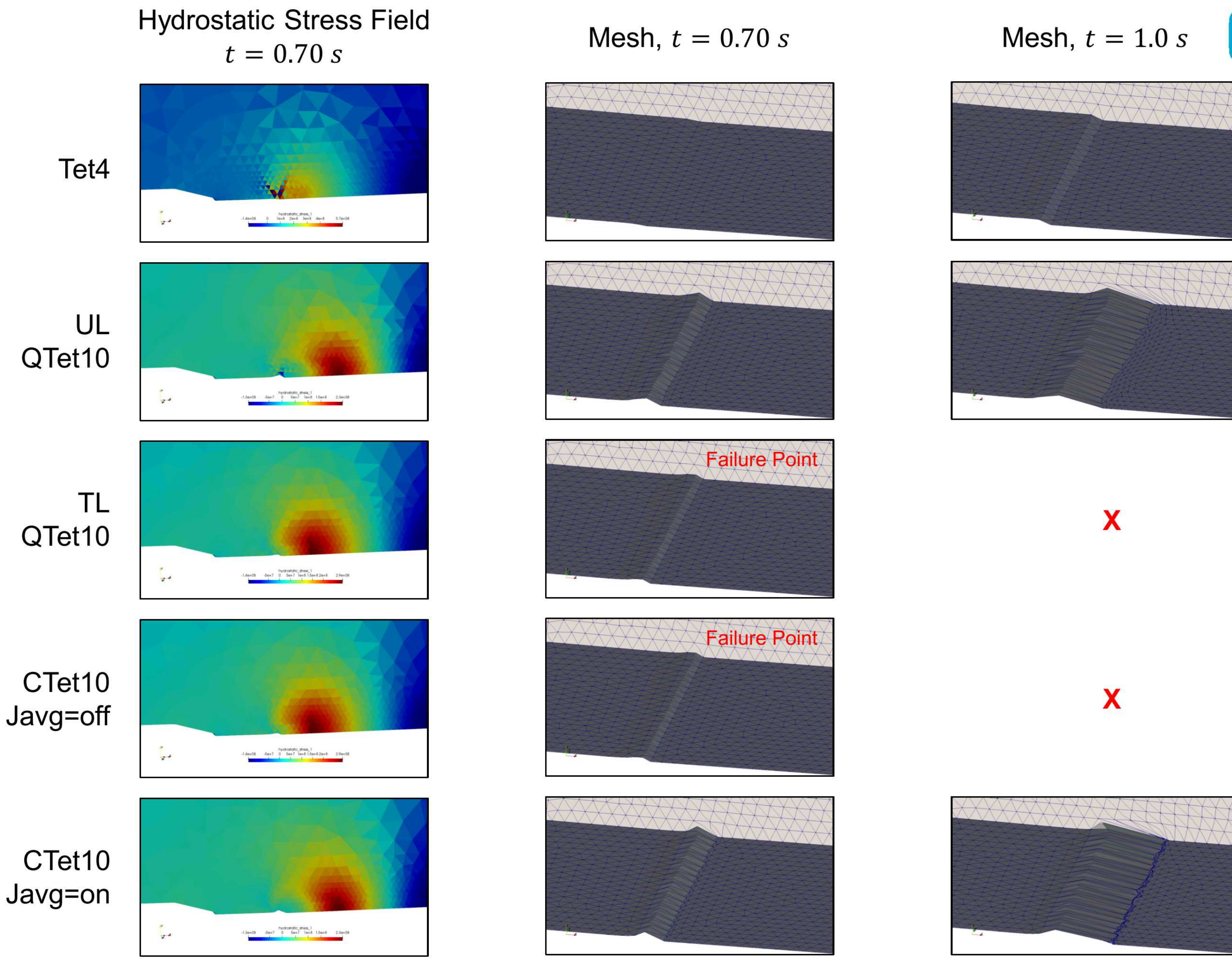
Plasticity Results (UL QTet10, fine)





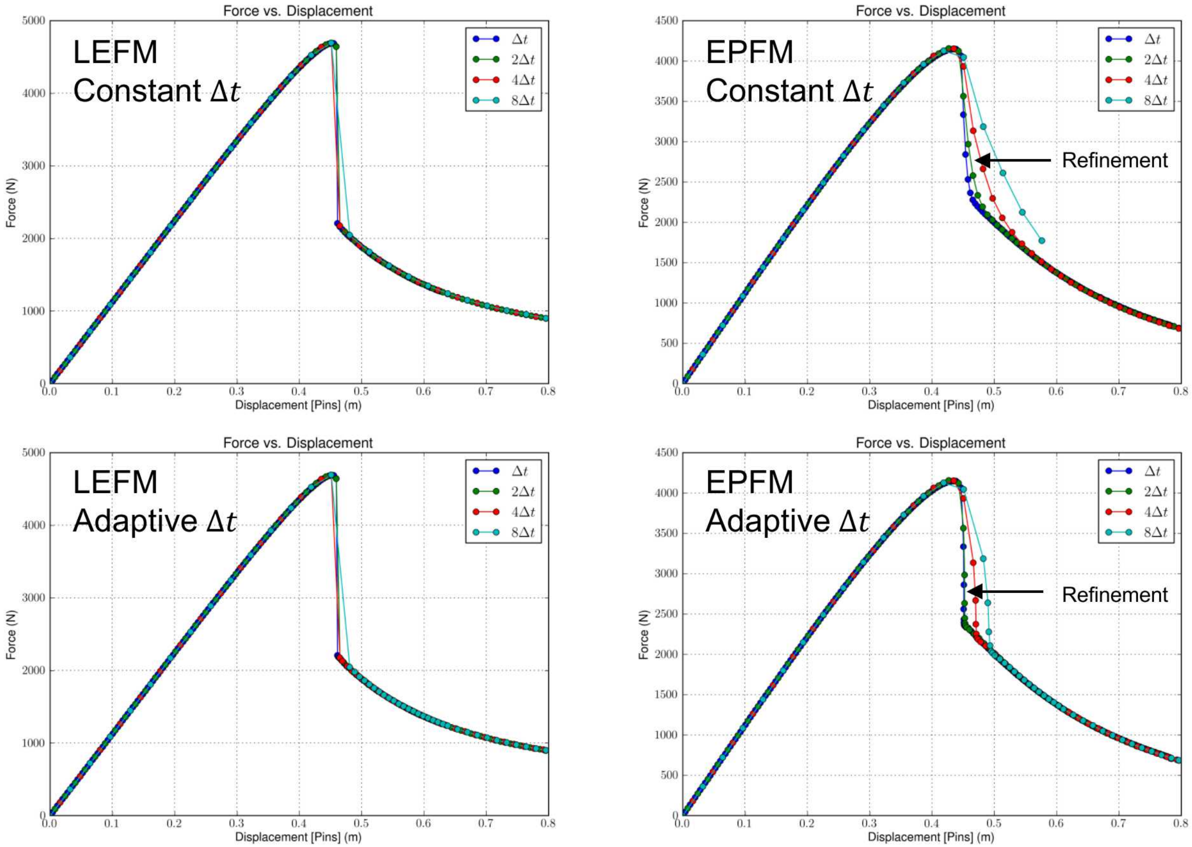


From Sun & Jin, *Fracture Mechanics* (2012)


Hydrostatic Stress Field
$t = 0.70\ s$
Mesh, $t = 0.70\ s$
Mesh, $t = 1.0\ s$
Tet4
UL
QTet10
TL
QTet10
CTet10
Javg=off
CTet10
Javg=on
Failure Point
Failure Point
X
X

Recent Efforts

- Coupling scheme:
  - Implement iteration between Mechanics & PF solves within timestep
  - Temporal convergence:



Recent Efforts

- Coupling scheme:
  - Implement iteration between Mechanics & PF solves within timestep

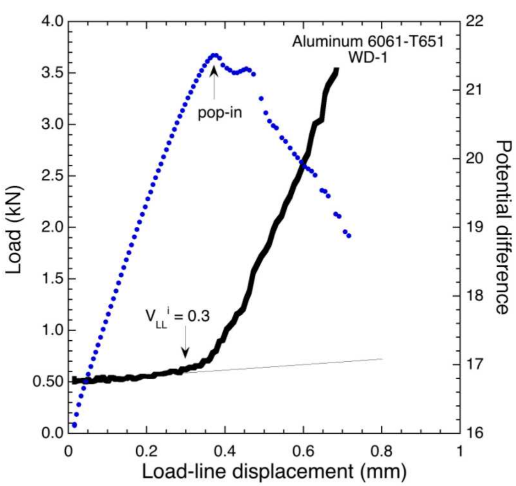
  - Spatially convergent ✓
  - Some element formulations are more robust to damage/softening than others…
  - Temporally convergent ✓

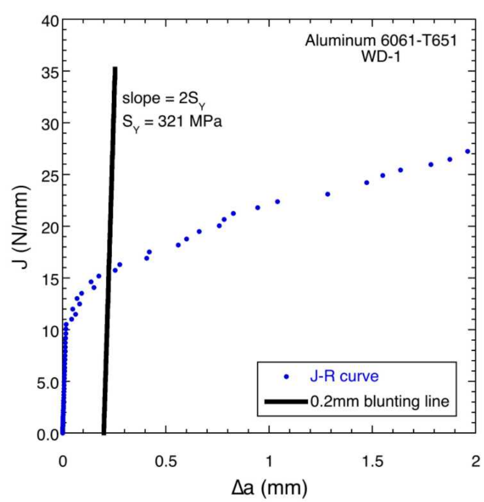
  - When the crack is growing, convergence is poor & slow
  - Loose tolerances needed for “convergence” & timestep completion
  - Tighter tolerances can’t always be reached with 100 iterations, even with timestep refinement

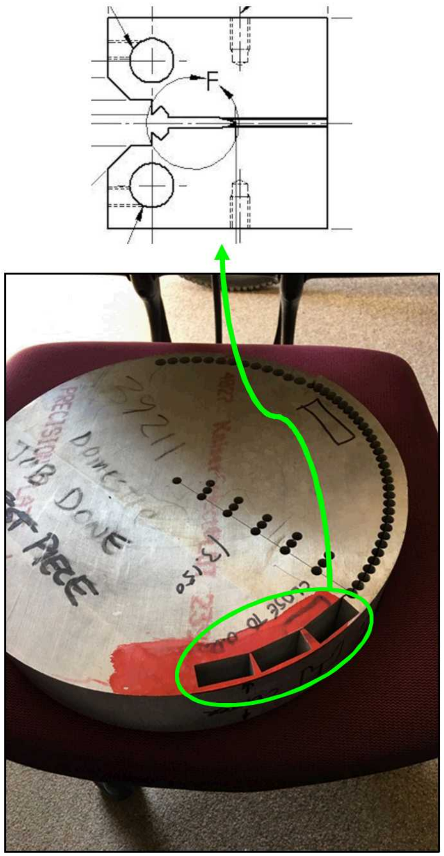
  - Consequence of using ‘alternate minimization’?
    - Solving without benefit of off-diagonal terms
  - Consequence of using history variable?
    - Corrupted usage of variational principle, energies no longer consistent

Model Validation

- Experimental test data, compact tension specimen:
  - Experiment partner: Chris San Marchi (Sandia)
  - Al 6061-T651
  - Force/displacement, J-R curves







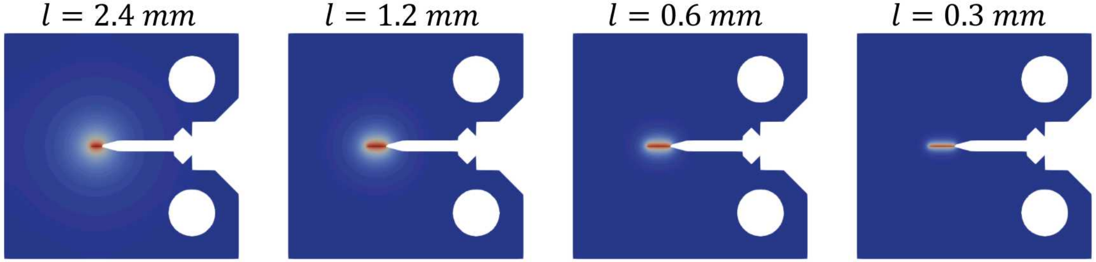
→ Seek to compare model to experimental data

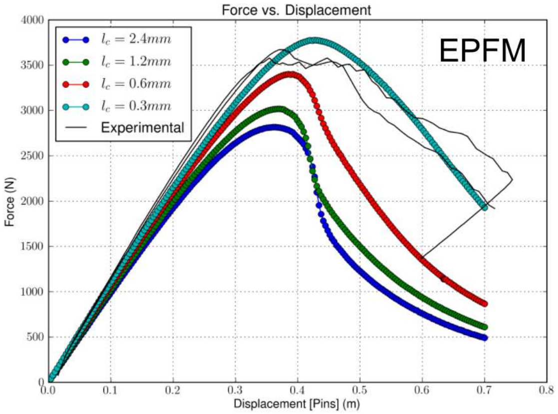
→ Simulation toughness $G_c = 12\ kJ/m^2$ from Matweb (corresponds to experimental J_0)

Model Validation

- Initial phase BC:
  - Intent:
    - Develop phase field around crack to avoid jumps in F/D response
    - BC set to minimize effect on elastic stiffness (must be less than full length)

Initial Phase Field

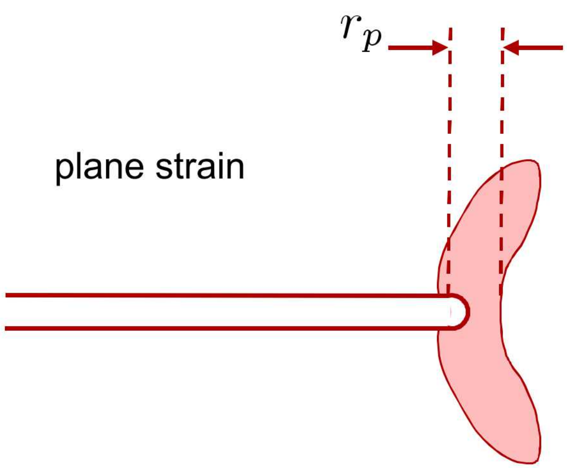




- Results:
  - Appears that choice of l exists that would reasonably approximate F/D curve ~ 0.3mm
  - Desire to confirm that choice of l allows reproduction of J-R curve
  - Robustness still an issue…

Addressing Plasticity

- Plasticity & length scales:
  - The addition of plasticity introduces an additional *physical* length scale



$$r_p = \frac{1}{3\pi}\frac{\bar{E}G_c}{\sigma_0^2}$$

where $\bar{E} = \frac{E}{1-\nu^2}$

- Regularization length scale l cannot be chosen with reference only to the geometry
- Ratio of l/r_p should be meaningful in terms of crack growth resistance (approximating a physical J-R curve)
- Motivation to move toward cohesive/Lorentz-type model
  - Lorentz *et al.* (2011), Geelen *et al.* (2019)

EXPLICIT TIME INTEGRATION

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: $\eta\dot{c} = -\begin{cases} 2\tilde{\psi}c - \frac{G_c}{2l}(1-c) - 2G_c l\Delta c \\ 2\tilde{\psi}c - 2\psi_{crit} - 4\psi_{crit}l^2\Delta c \end{cases}$ & $\dot{c} \leq 0$
  - 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 $(\Delta t)_{\mathrm{M}} \leq (\Delta t)_{PF}$

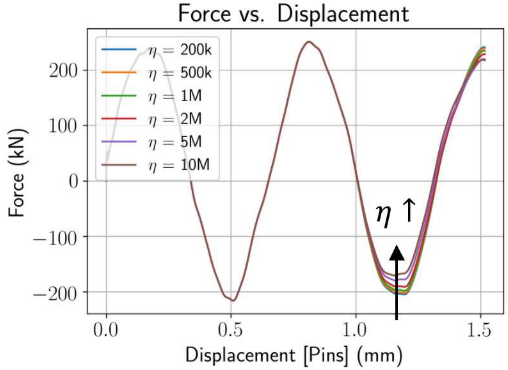
$$\frac{\eta}{(\Delta t)_{PF}} \geq \left\{\frac{2G_c l}{(\Delta x)^2}, \frac{4\psi_{crit}l^2}{(\Delta x)^2}\right\} \rightarrow (\Delta t)_{PF} \leq \left\{\frac{\eta(\Delta x)^2}{2G_c l}, \frac{\eta(\Delta x)^2}{4\psi_{crit}l^2}\right\}, (\Delta t)_M \leq \frac{\Delta x}{v_c}$$

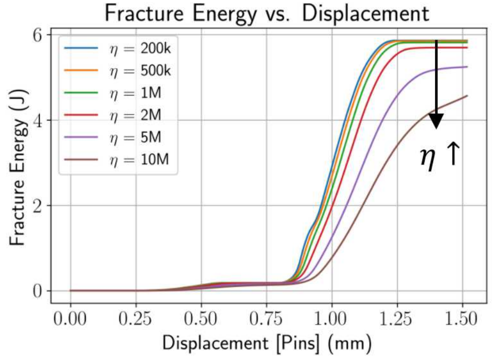
$$\eta \geq \tilde{\eta} = \left\{\frac{2G_c l}{\Delta x\, v_c}, \frac{4\psi_{crit}l^2}{\Delta x\, v_c}\right\}$$

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

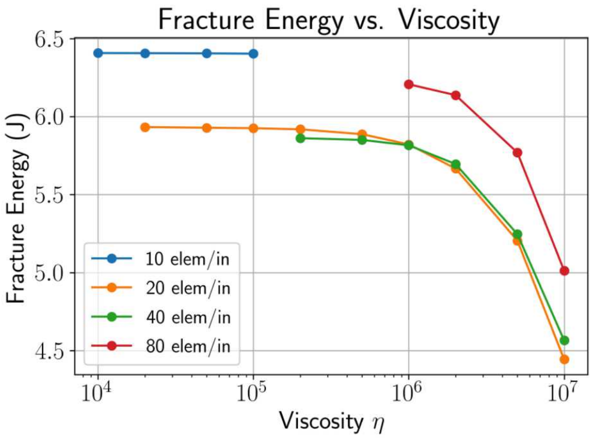
Stability & Viscosity

- Overview:
  - Vary phase viscosity parameter η over wide range to determine:
    - For what values of η are the simulation stable?
    - How does the simulation respond to increasing phase viscosity?



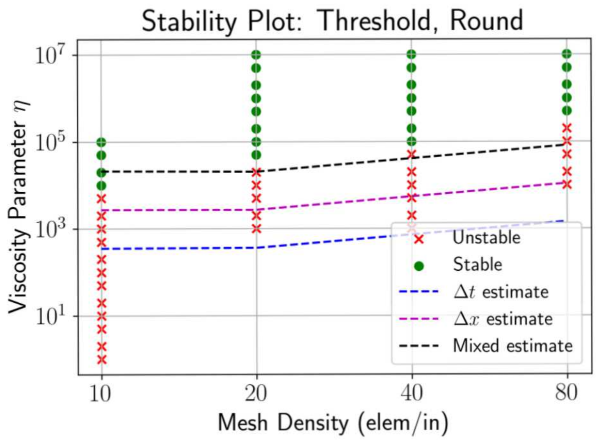


- Global metrics diverge with 'high enough' levels of phase viscosity parameter η
- Evidence of rate dependence (lag) when high phase viscosity

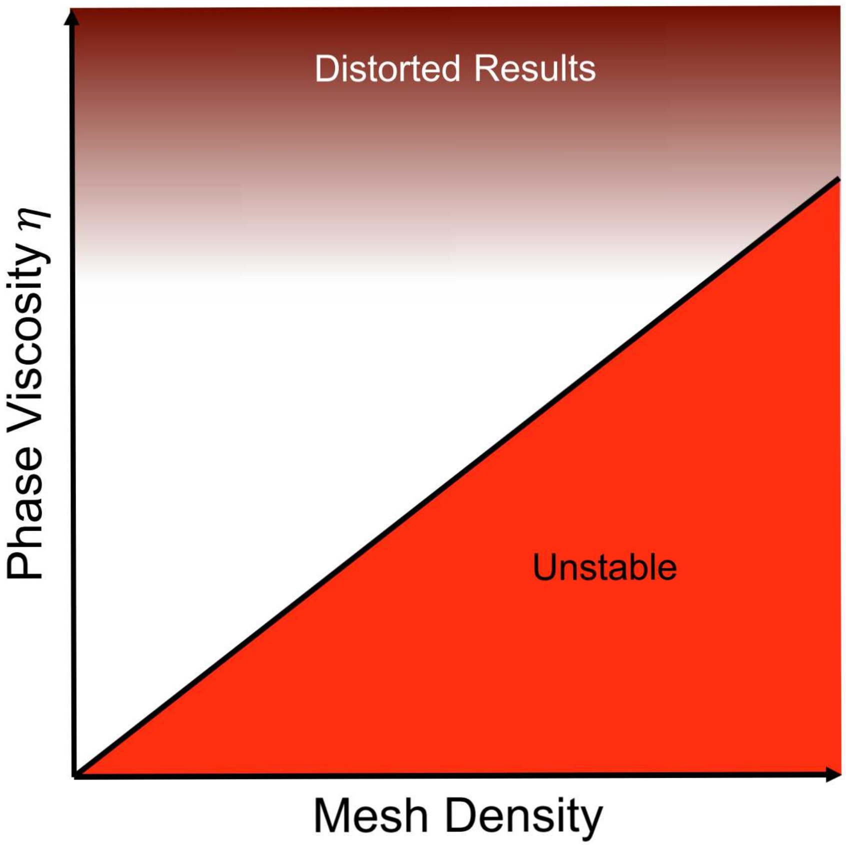


Example: Threshold, sharp tip, 40 elem/in.

Stability & Viscosity

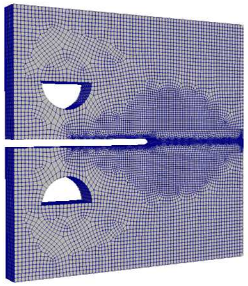


$$\eta \geq \left(\frac{4}{l v_c^2 \Delta t} = \frac{4}{l v_c \Delta x} = \frac{4\,\Delta t}{l(\Delta x)^2} \right)$$

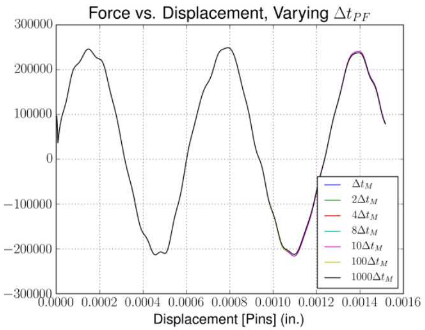


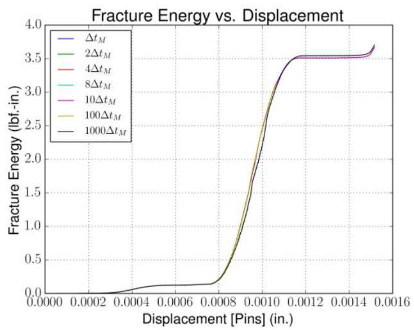
- Explicit (Mechanical) / Explicit (Phase Field) integration with viscous regularization might be more limiting than it is useful
- Explicit (Mechanical) / Implicit (Phase Field) flavor might be more expensive** but lacks quality and stability issues

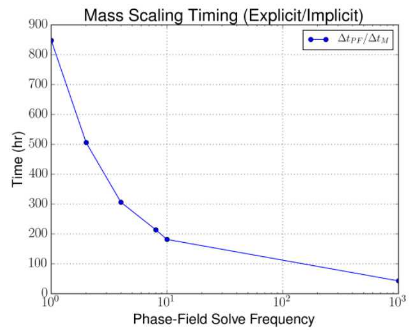
Capabilities – Explicit/Implicit



- Explicit Mechanics / Implicit Phase-Field solve
  - 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





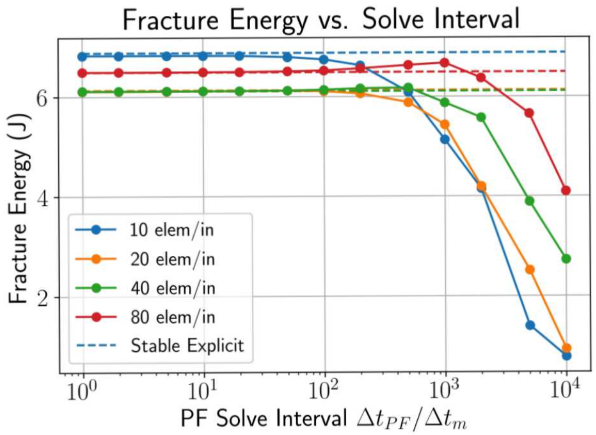


- Very similar force/displacement & fracture energy responses
- Great simulation time savings realized

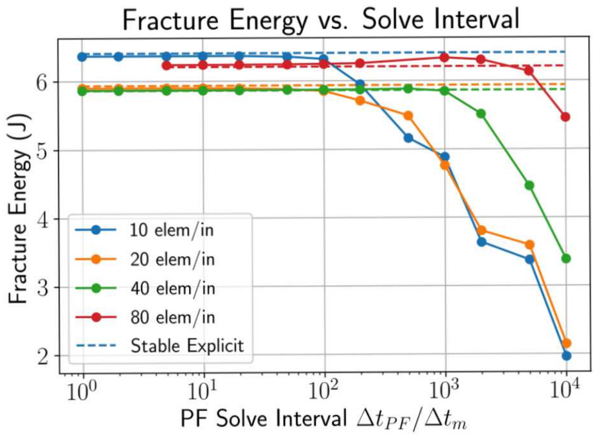
Timing Study

- Results – QoI Convergence:

Rounded Crack Tip



Sharp Crack Tip



- Explicit/Implicit and Explicit/Explicit (stable) results generally agree
- Explicit/Implicit results convergent as solve interval approaches 1
- Deviation observed for larger PF solve intervals (>50)

Future Directions

- Model:
  - Consider inequality-constrained phase field solve
  - Nonlinear PDE solve
    - Allow for cohesive/Lorentz-type phase field model
  - Modularization for use with arbitrary (hyperelastic & hypoelastic) plasticity models
- Verification efforts:
  - “Surfing BC” problem – verify toughness as function of crack length in EPFM (J-R curve)
  - Explicit dynamics – convergence testing
- Validation effort:
  - Compare apparent J-R curve produced by phase field model to experimental
  - Explicit dynamics validation

Thank you!

Thanks to conference & minisymposia organizers!

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