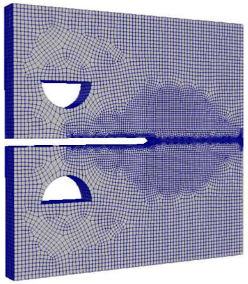
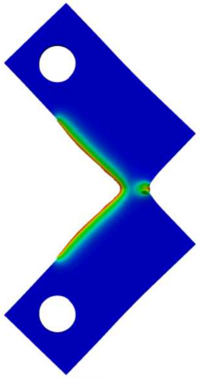
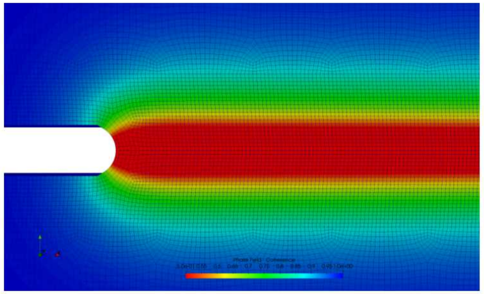
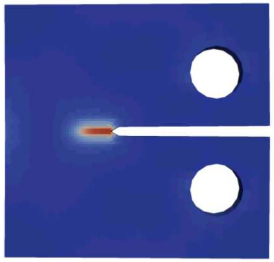
This paper describes objective technical results and analysis. Any subjective views or opinions that might be expressed in the paper do not necessarily represent the views of the U.S. Department of Energy or the United States Government.

SAND2019-6372C









# Ductile Fracture Representation using the Phase-Field Model in SIERRA

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

Sandia National Laboratories / California

CFRAC 2019; Braunschweig, DE; June 12-14, 2019

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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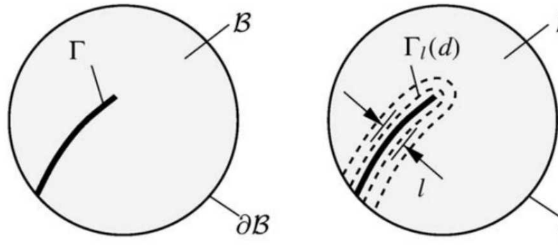
# Phase field approach to fracture

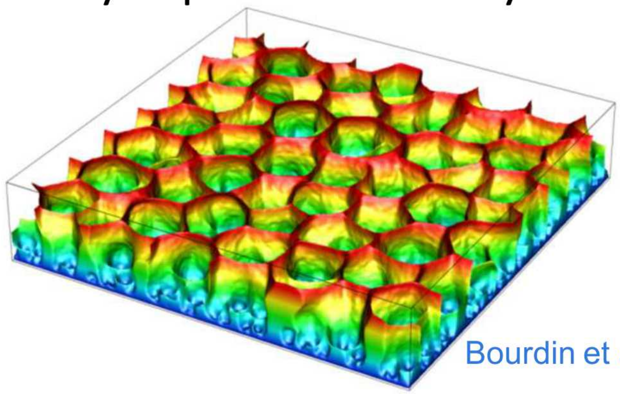
- Cracks represented as smeared field



a) sharp crack b) diffusive crack

Miehe et al (2011)

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



Bourdin et al (2014)

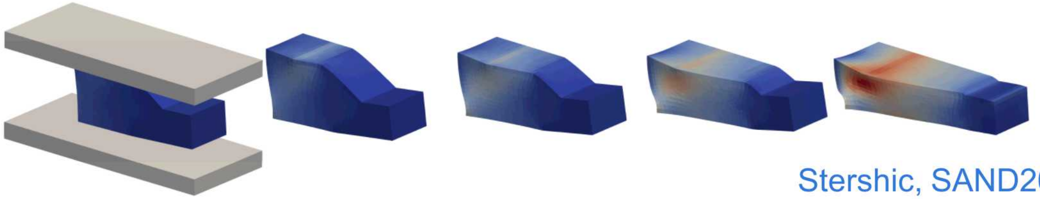
- Genesis in linear elastic brittle fracture
- Approaches for ductile failure have started appearing and are under development

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
  - Classical, “AT-2”
  - Threshold, “AT-1”
- Phase Field Implementation
- Recent Efforts
  - Iterated staggered solution
  - Temporal / Spatial Convergence
- Experimental Comparison
  - Moving to cohesive model
- 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
  - $\Gamma$-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

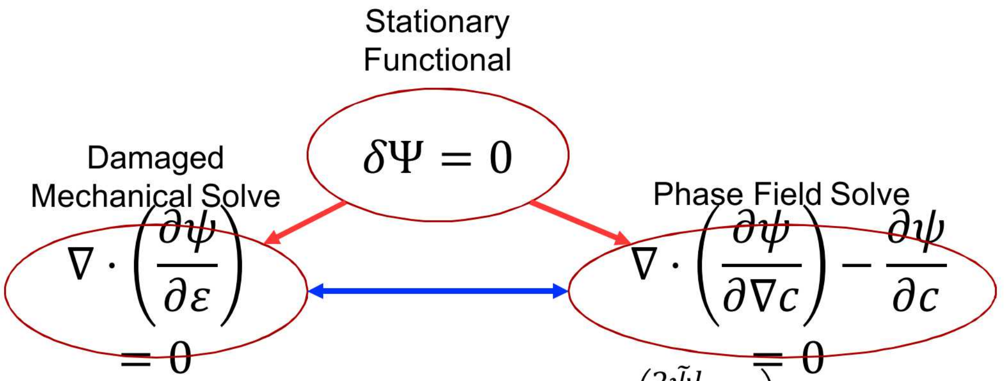
$$\psi = \mathrm{c}^2 * \left(\tilde{\psi}^{\mathrm{e}}(\varepsilon^e) + \tilde{\psi}^p(\varepsilon^p)\right) + 2\psi_{crit}\left((1-c) + l^2|\nabla c|^2\right)$$

  - 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

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

Euler-Lagrange:




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

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

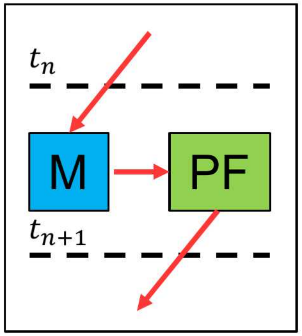
Phase Field Solve

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

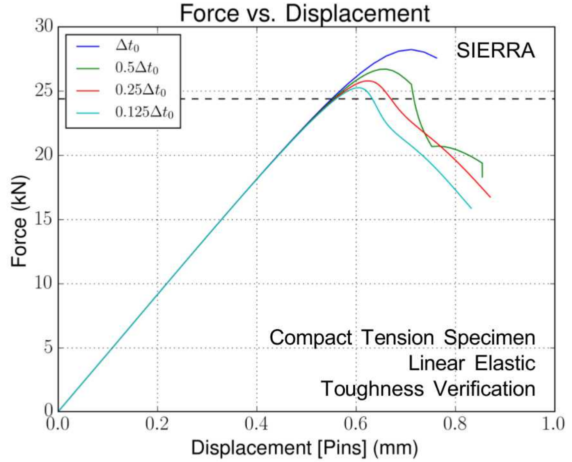
- Augmented Lagrangian approach using Inequality-constrained PDE solve
  - Difficult to implement in Sierra framework, but interested to explore

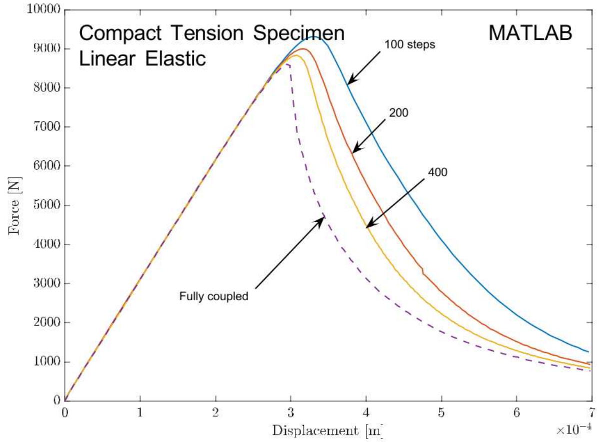
# Phase Field Implementation

- Coupling scheme:
  - Options: monolithic –or- staggered solution scheme (“alternate minimization”)




Coupled Solve Schematic

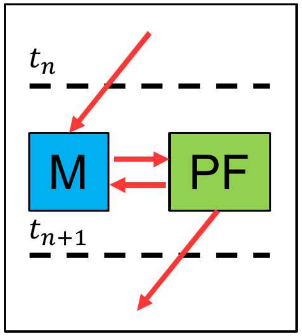


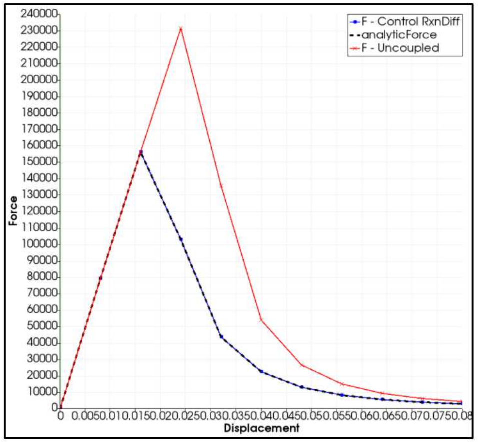

  - Implemented mechanics/PF staggered solution
  - No easy access in SIERRA to implement monolithic solve
  - Initially, no iteration of mechanics/PF solve within timestep
  - Lack of iteration leads to acceptance of *unconverged* solutions at each time step
  - Leads to strong temporal sensitivity, toughness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

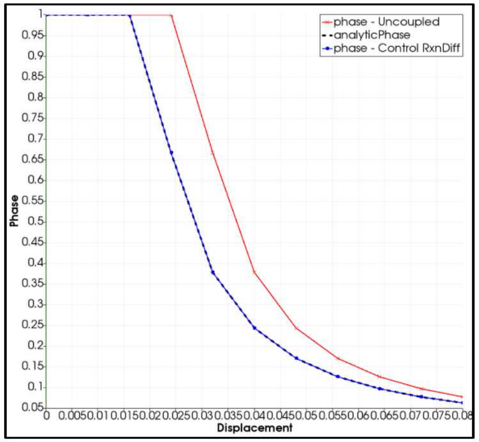
# Recent Efforts

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




Coupled Solve
Schematic

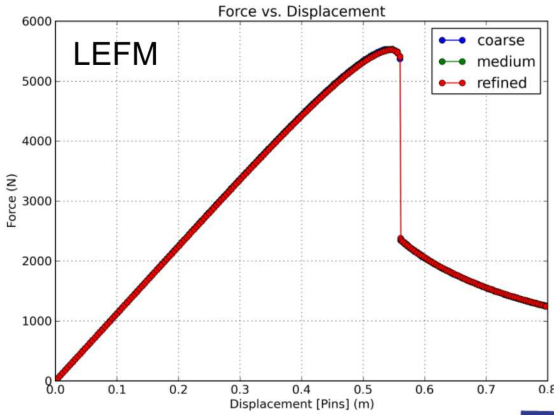


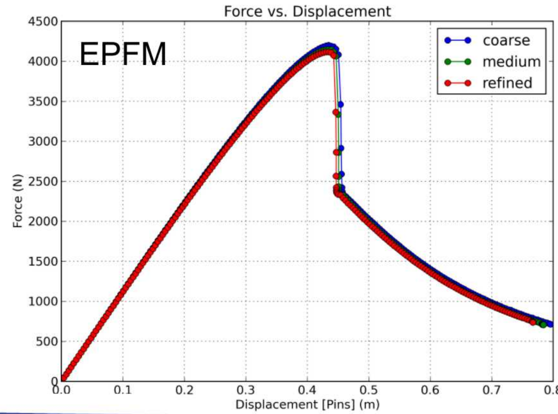




  - Solve mechanics, solve damage, compute M residual
  - Convergence metric: mechanical residual < tolerance
  - Better metric?
    - Phase field solve = linear system → trivial PF residual
    - Combined energy residual?
    - Phase field relative residual between iterations?

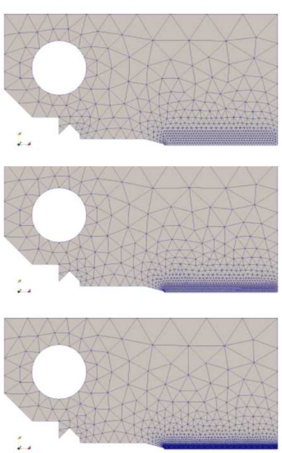
# Recent Efforts

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

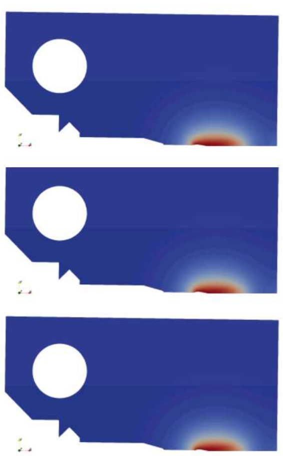


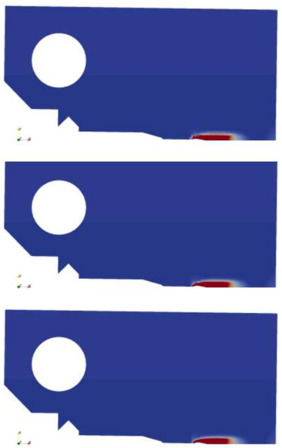

Compact Tension Specimen Meshes



Phase Field

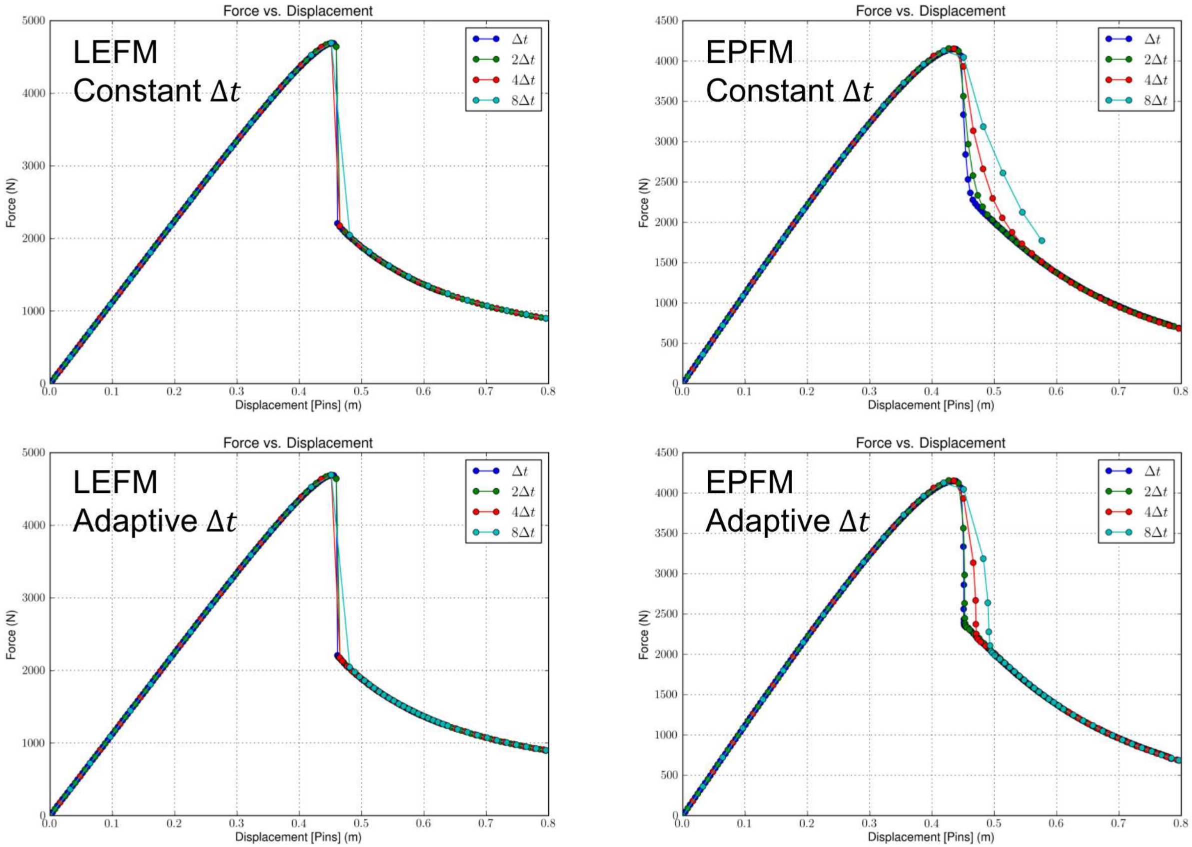


EQPS



# 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

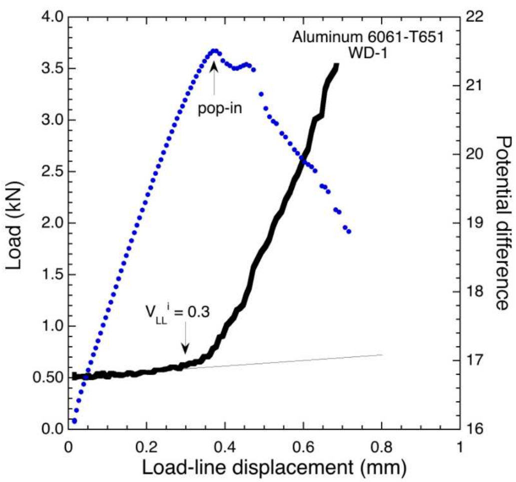
  - Spatially convergent ✓
  - Temporally convergent ✓

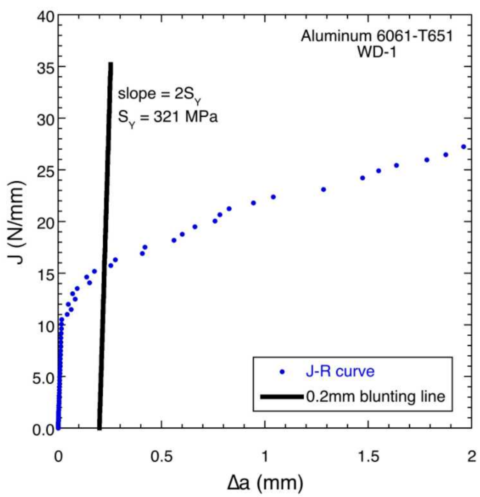
  - When the crack is growing, convergence is poor & slow
  - Loose tolerances needed for "convergence" & timestep completion
  - Tighter tolerances can't always be reached with 100 iterations, even with timestep refinement

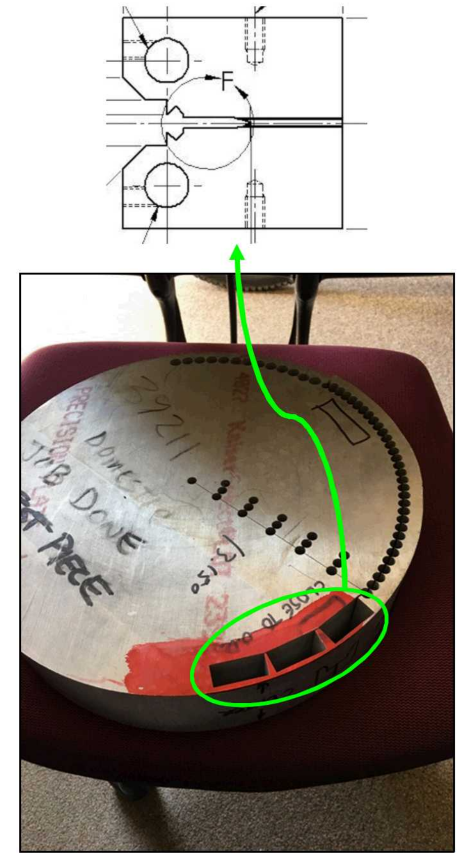
  - Consequence of using 'alternate minimization'?
    - Solving without benefit of off-diagonal terms
  - Consequence of using history variable?
    - Corrupted usage of variational principle, energies no longer consistent

# Model Validation

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



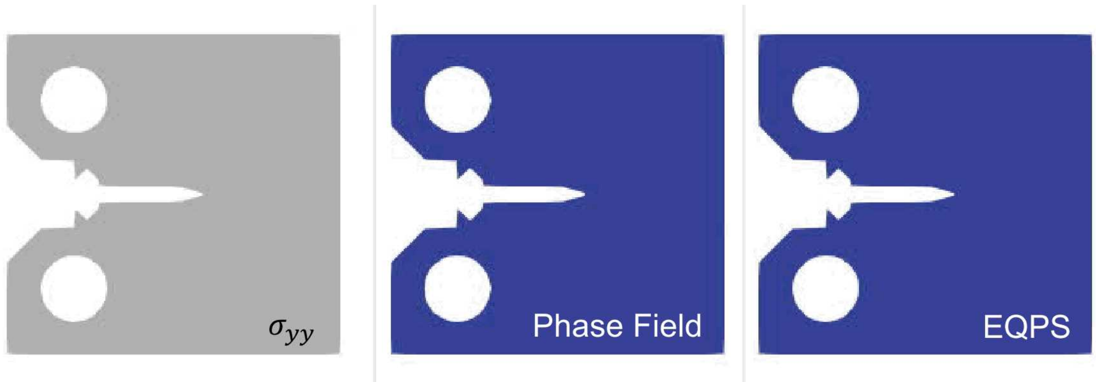



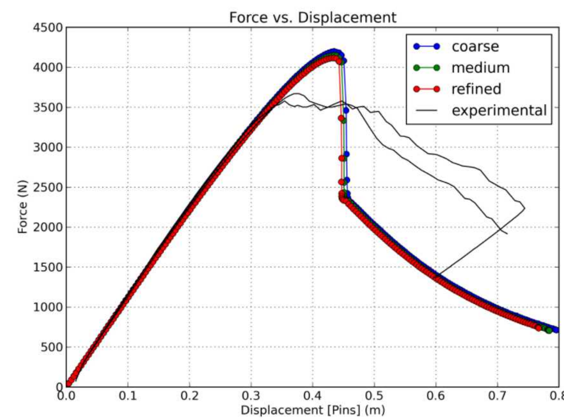




→ Seek to compare model to experimental data

# Model Validation

- Parametrizations:
  - Elasticity & Plasticity – calibrated from tensile specimen
  - Fracture:
    - Toughness $G_c = 12\ kJ/m^2$ from Matweb (corresponds to experimental $J_0$)
    - Length scale chosen arbitrarily for plastic response, $\tilde{\psi}_{crit} \approx 4\tilde{\psi}(\sigma_y)$




- Validation caveats
  - Geometry is 3-D but plane strain → need to allow for thickness-direction deformation
  - More thoughtful selection of length scale needed
  - 3-D geometry needs to have side grooves added

→ more work to be done!

# Model Validation

- Parametrizations:
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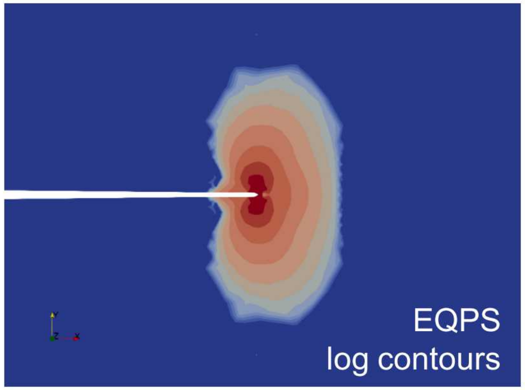
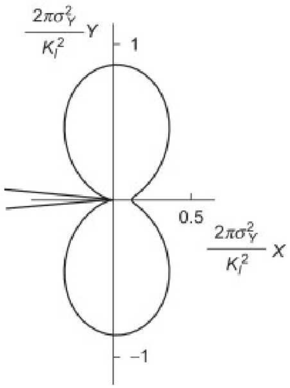


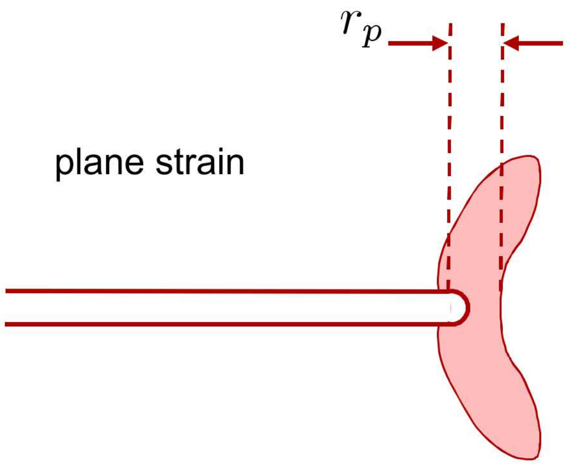

From Sun & Jin, *Fracture Mechanics* (2012)

- Validation caveats
  - Geometry is 3-D but plane strain → need to allow for thickness-direction deformation
  - More thoughtful selection of length scale needed
  - 3-D geometry needs to have side grooves added

→ more work to be done!

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

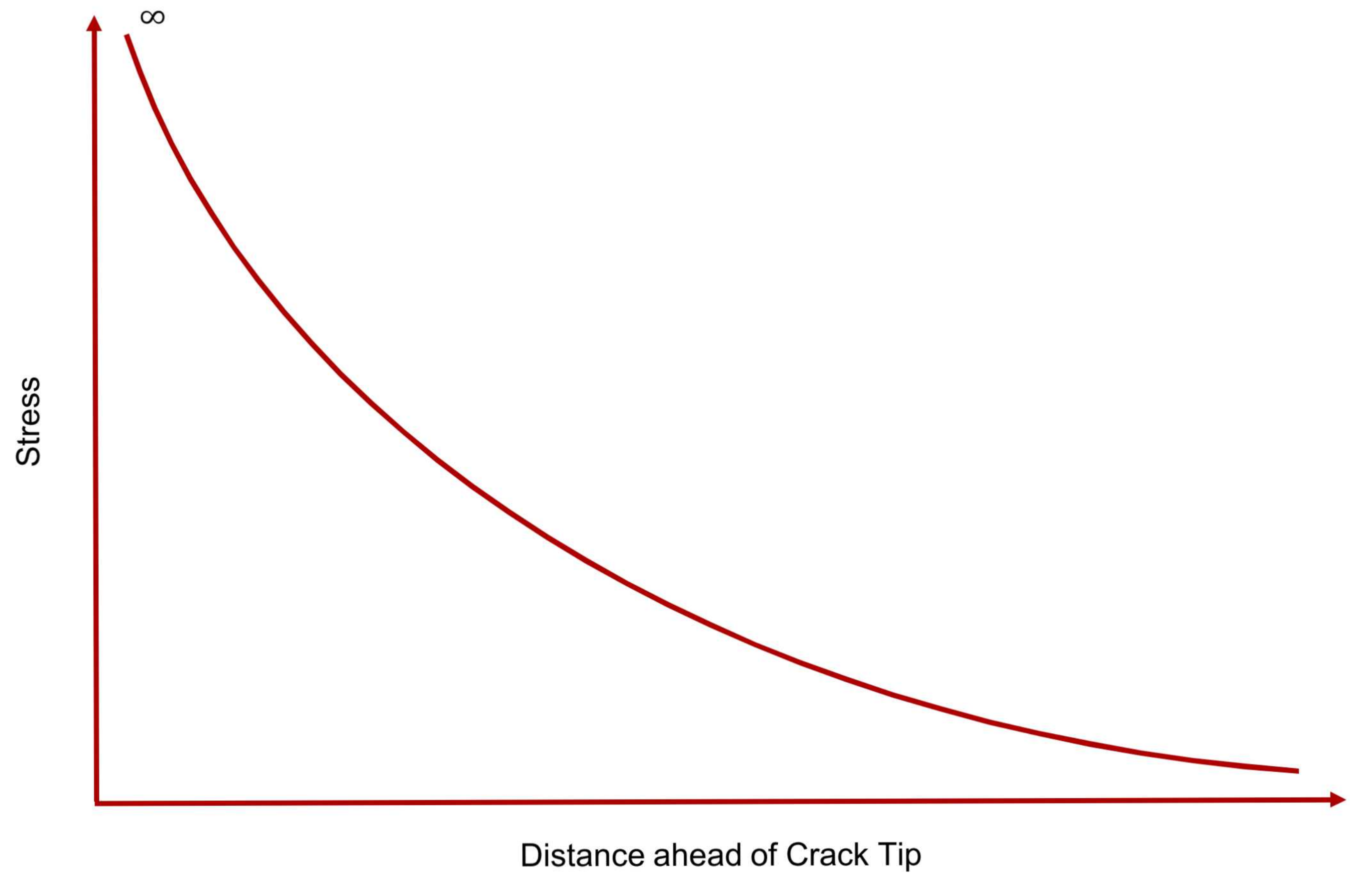
  - Regularization length scale $l$ cannot be chosen with reference only to the geometry
  - Ratio of $l/r_p$ should be meaningful in terms of crack growth resistance (approximating a physical J-R curve)
  - Motivation to move toward cohesive/Lorentz-type model

# Future Directions

- Model:
  - Implement 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
- Validation effort:
  - Fully 3-D mesh with side grooves added
  - Compare apparent J-R curve produced by phase field model
  - Explicit dynamics validation

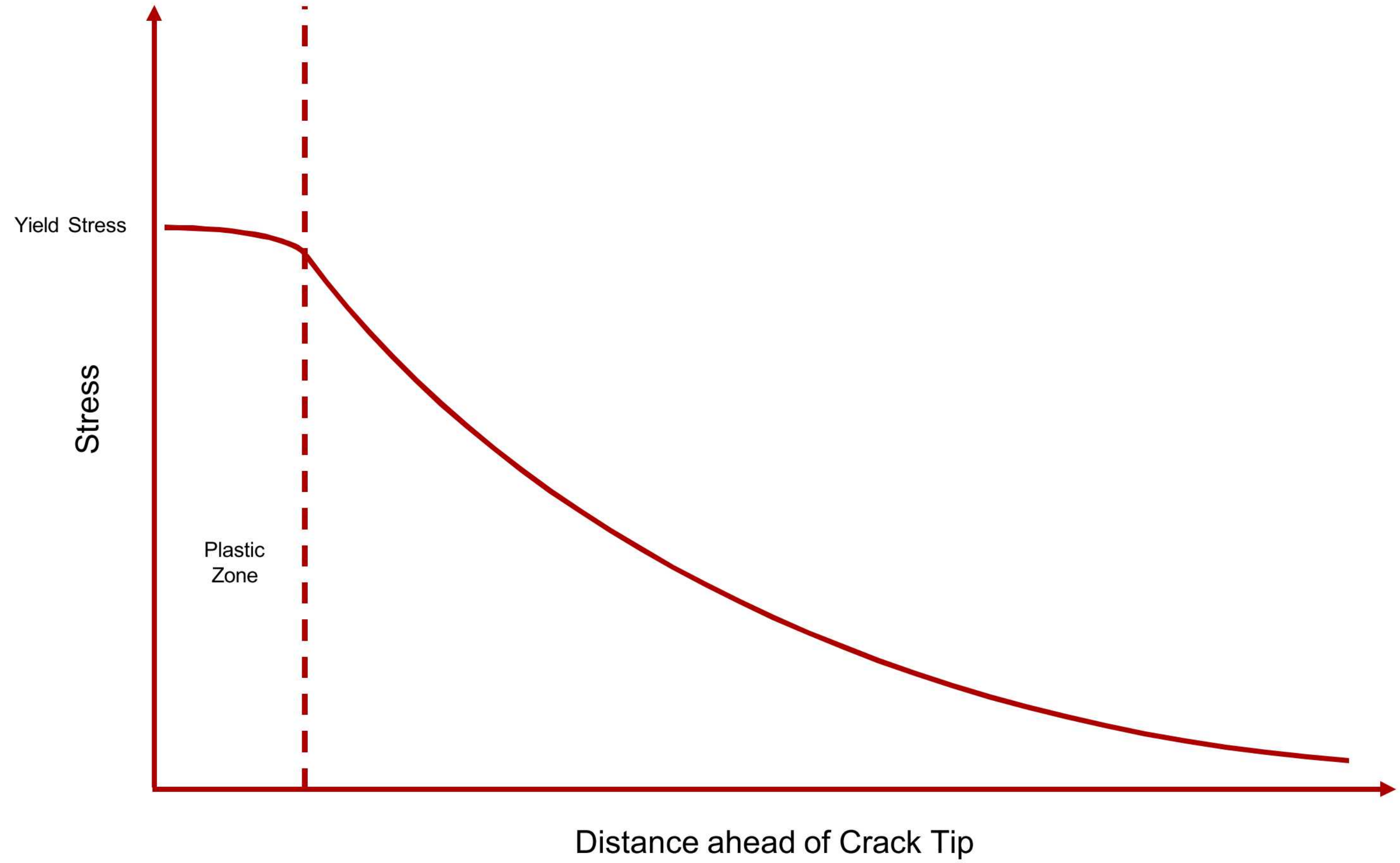
# Stress Profiles

- Brittle Fracture (ideal, LEFM)



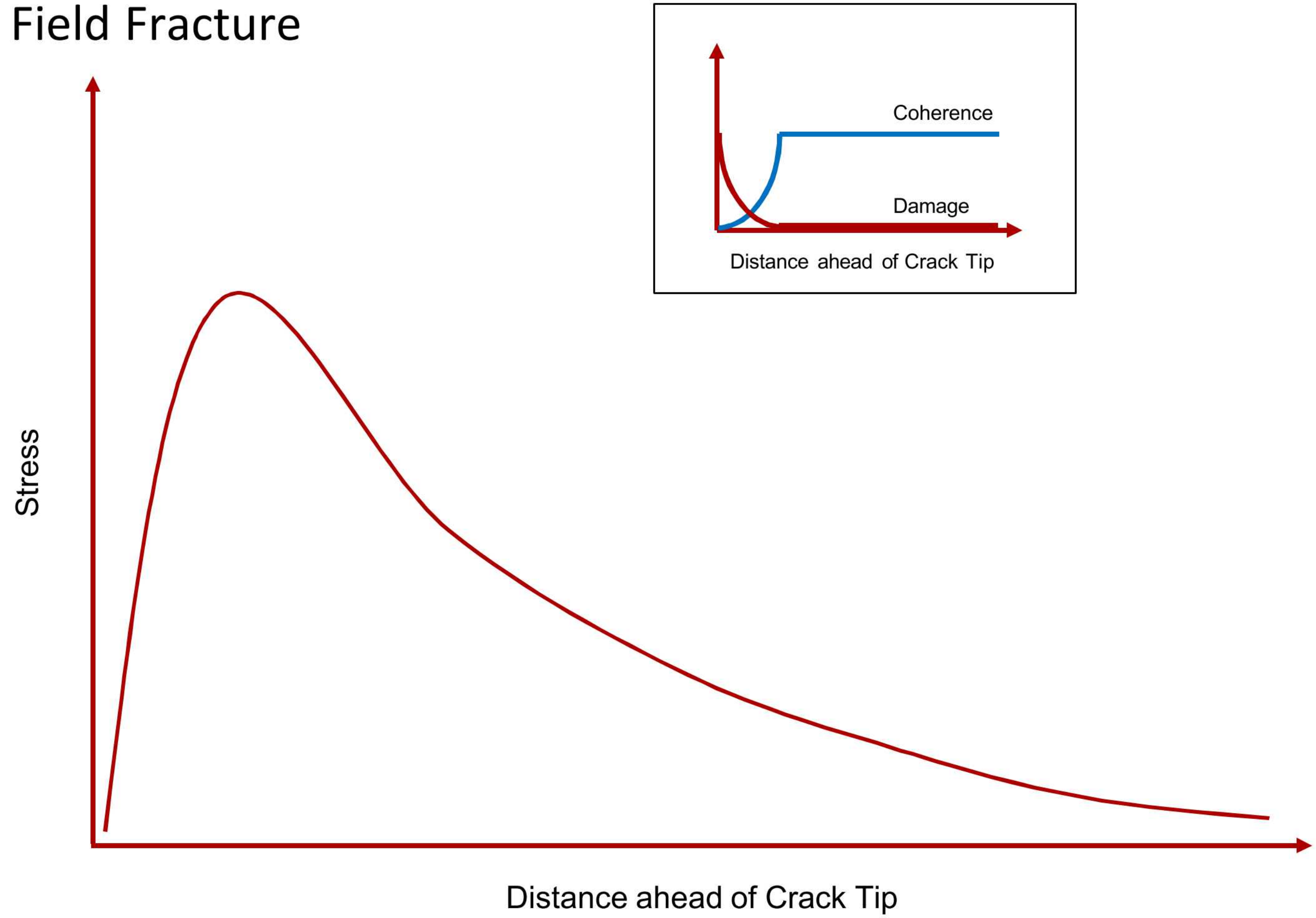
# Stress Profiles

- Ductile Fracture



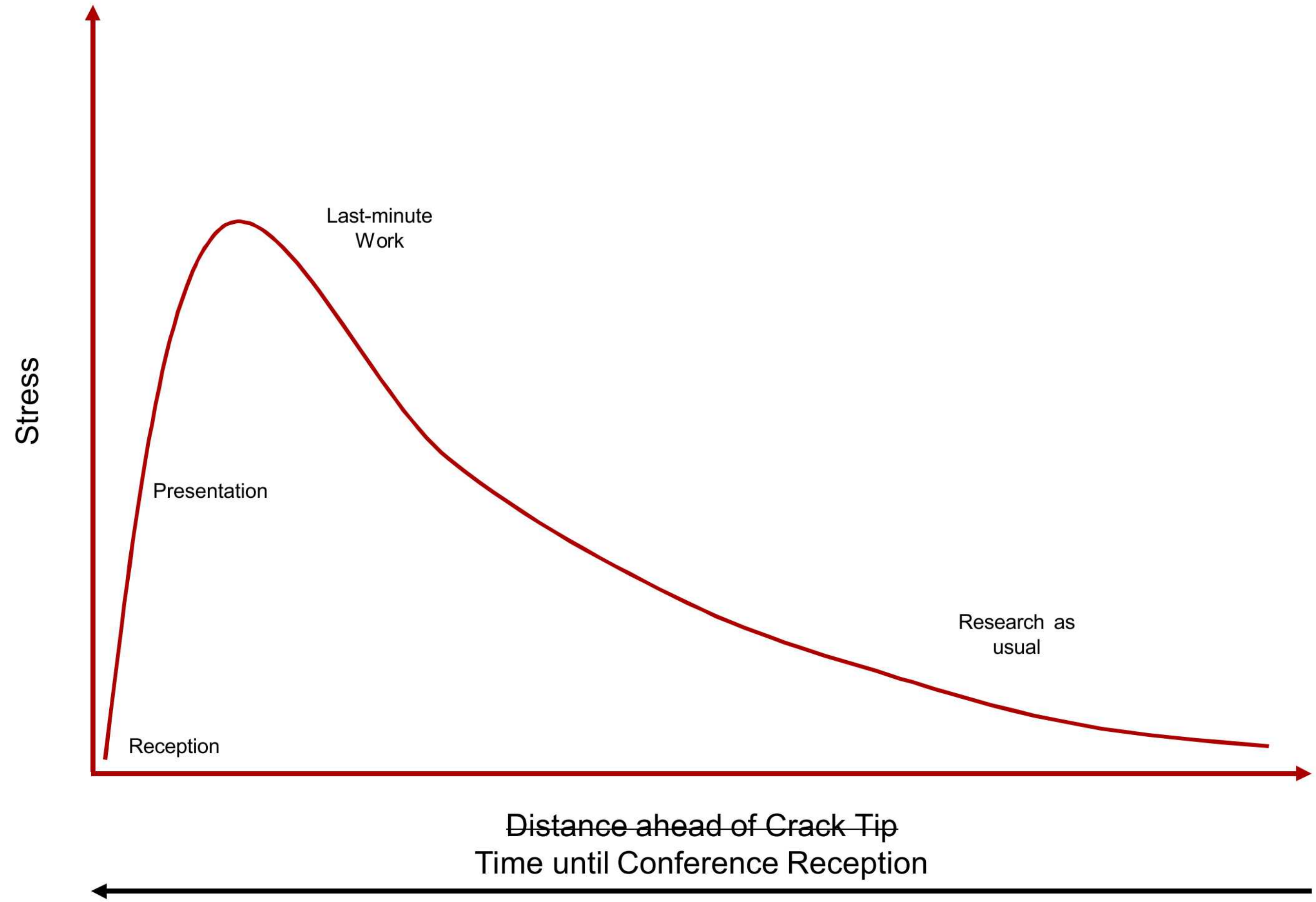
# Stress Profiles

- Phase Field Fracture



# Stress Profiles

- Solid Mechanics Researcher



# Thank you!

Thanks to conference & minisymposia organizers!



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