

# Sandia Fracture Models for Mixed-Mode Brittle Fracture

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# Overview

- Sandia fracture modeling capabilities in SIERRA
- Preliminary work
  - Geometry
  - Model Parametrization
- Element Death
- Phase Field
- SIERRA / FRANC3D Coupling

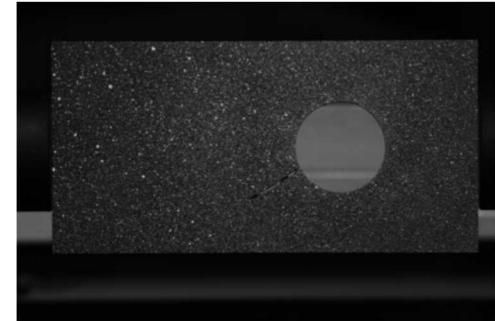
# Sandia Capabilities

- SIERRA finite element code (Sandia National Laboratories)
  - Implicit & explicit integration
  - Fully parallelized for clusters, HPC
  - Finite strain formulation
  - Robust explicit & implicit contact
  - Verification & Validation
  - Multiphysics solutions
- Brittle Failure Strategies in SIERRA:

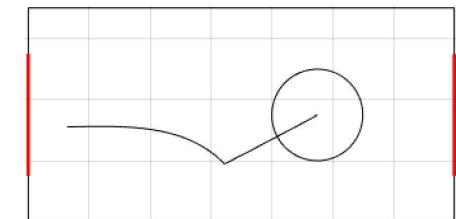
Capability	Status
→ Element Death	Production
XFEM	Production / Development
Peridynamics	Research
RKPM	Research
Cohesive Elements	Production
Localization Elements	Production
→ Phase Field	Research
→ FRANC3D Coupling	Production

# Geometry

- **Geometry:**
  - **Nominal geometry**
    - Use nominal dimensions:
      - Specimen: 140 mm x 70 mm x 10 mm
      - Hole: 30 mm diameter, 25 mm off-center
      - Notch: 35 mm long from hole center, 30° from X axis
    - Use provided imagery:
      - Threshold at critical gray value
      - Measure notch width: estimated 1mm wide
  - **Sculpted geometry**
    - SCULPT (Sandia) – meshes voxelized imagery
    - Input: thresholded image, background mesh (without hole, crack)
    - More expensive, but more accurate
  - **Meshing**
    - Several mesh densities of each
- **Boundary conditions:**
  - Left – fixed X, fixed Y
  - Right – prescribed displacement X (0.1 mm/min), fixed Y
  - Back (symmetry) – fixed Z



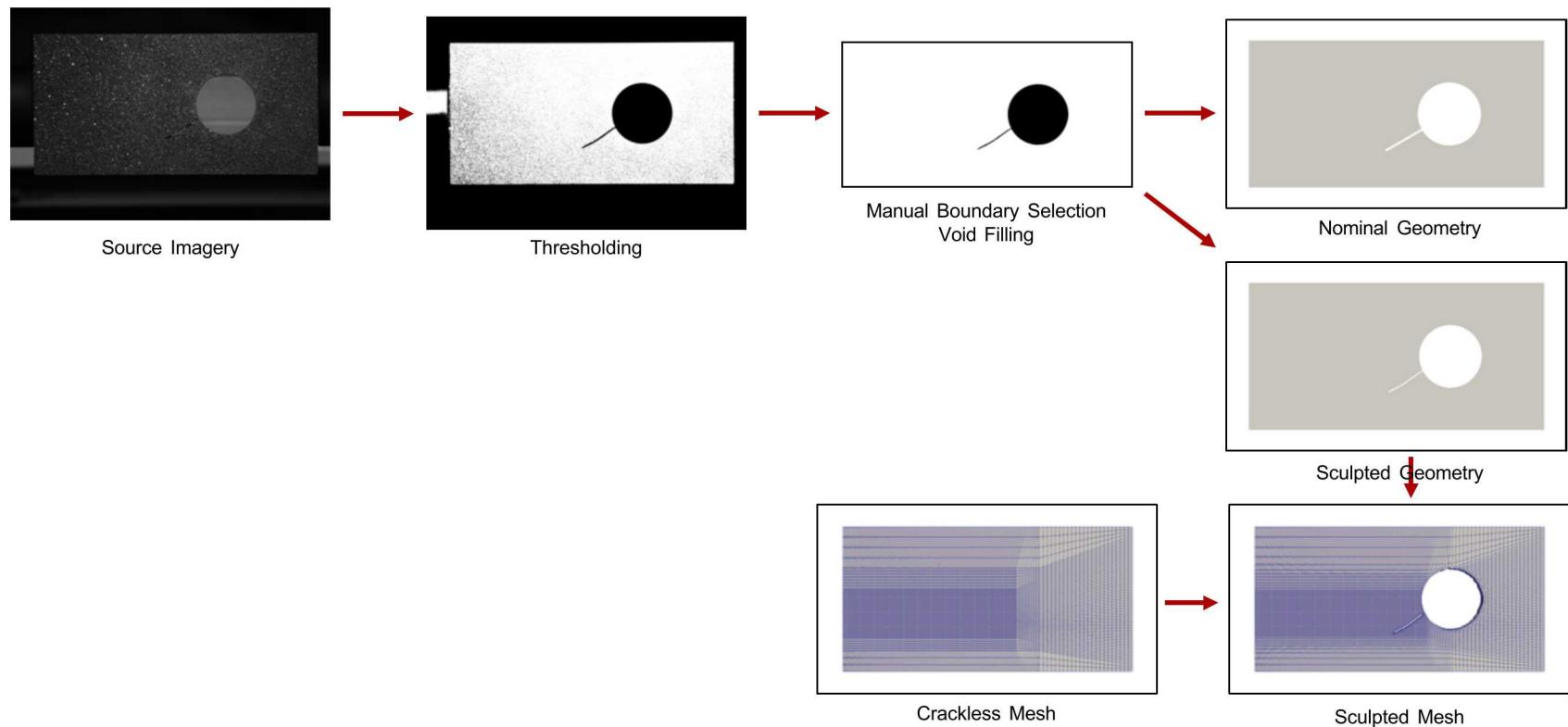
Source Imagery



Nominal Geometry,  
BCs highlighted

# Geometry

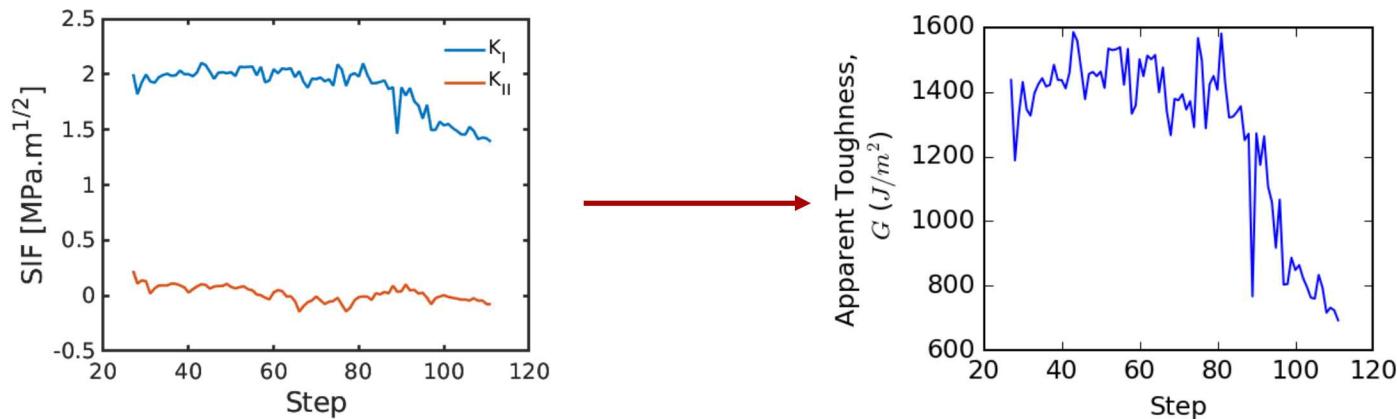
- Geometry:
  - Processing flow-chart:



# Model Parametrization

- Model parametrization
  - Provided data from benchmark specification (Young's modulus, Poisson's ratio)
  - Online references (density, fracture strength)
  - Post-processing of provided data (toughness / fracture energy  $G_c$ )

$$G = \frac{K_I^2}{E'} + \frac{K_{II}^2}{E'} \text{ where } E' = \frac{E}{1-\nu^2}$$



→ Estimate  $G_c \approx 1400 \text{ J/m}^2$

# ELEMENT DEATH

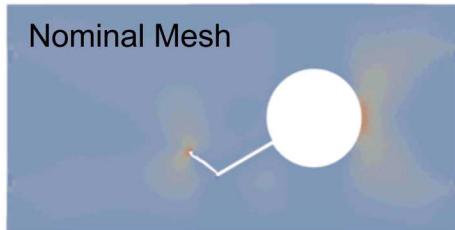
Andrew Stershic



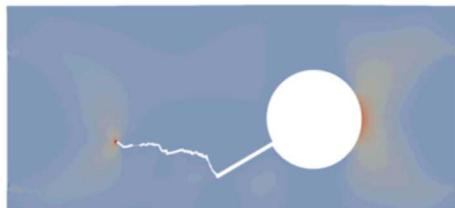
# Element Death

- Approach:
  - Kill elements when maximum principal stress exceeds critical value:  $\sigma_I > \sigma_c$
- Concerns:
  - Mesh sensitivity: crack propagation length & direction, energy dissipation, stability

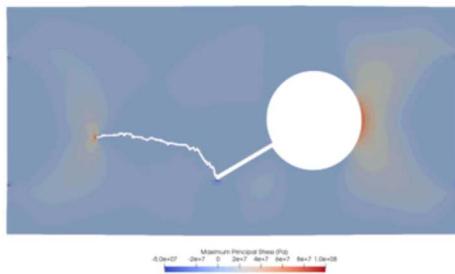
Coarse



Medium

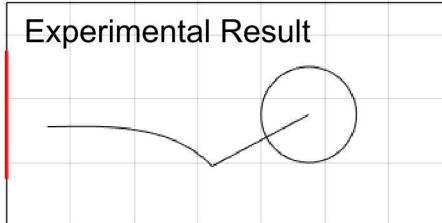


Fine



- Results:

- Element death does decently at capturing the crack path
- Still evidence of mesh dependence in crack length & direction
- Perhaps the global stability of the problem (monotonic F/D even with crack) assists here



# PHASE FIELD

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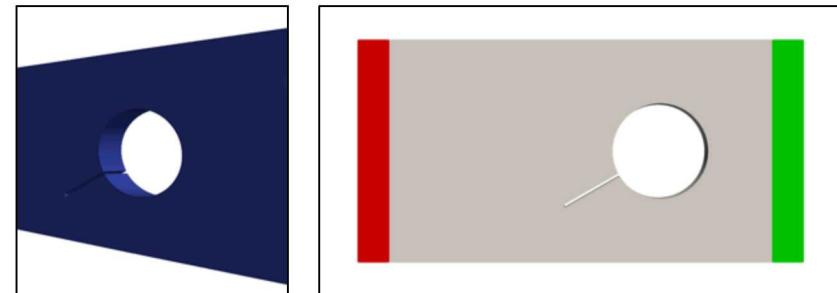
# Phase Field

- Overview of approach:

- Solve fracture problem by minimizing global energy functional
- Approximate surficial fracture energy with volumetric energy

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

- $\Gamma$ -convergent: expressions equivalent in limit  $l \rightarrow 0^+$
- Similar formulation to gradient-damage model



- Details:

- Phase field fracture model:

- Threshold model, "AT-1":  $\psi_{frac} = 2\psi_{crit}((1 - c) + l^2|\nabla c|^2)$ ,  $\psi_{crit} = \frac{3G_c}{16l}$

Damage caused by  
stress conc. at BC

Geometry for phase field model with  
unbreakable blocks

- Model parametrization

- Set  $\psi_{crit}$  &  $l$  based on tensile failure strength ( $\sigma_c \approx 50 \text{ MPa}$ ):  $\psi_{crit} = \frac{\sigma_c^2}{2E} \rightarrow l = \frac{3G_c E}{8\sigma_c^2}$

- Inserting "unbreakable" blocks at boundary conditions

- Prevents damage that arises due to idealization of boundary conditions

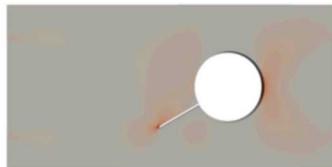
# Phase Field

- Details (continued):
  - Mixed-mode fracture – only want tensile components to contribute to damage
    - Typically, full strain energy considered:  $\tilde{\psi} = \frac{1}{2} \sigma_{ij} \varepsilon_{ij} = \frac{\lambda}{2} \text{tr}(\varepsilon)^2 + \mu \text{tr}(\varepsilon^2)$
    - Consider other energy decompositions:  $\Psi = \int_{\Omega} g(c) \tilde{\psi}_{act} + \tilde{\psi}_{pas} + f(c, \nabla c, l) G_c \, d\Omega$
    - Other energy decompositions implemented for this benchmark

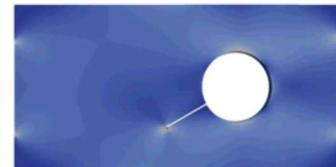
Decomposition	$\tilde{\psi}_{act}$	$\tilde{\psi}_{pas}$	$\sigma$
Full	$\frac{\lambda}{2} \text{tr}(\varepsilon)^2 + \mu \text{tr}(\varepsilon^2)$	0	$g(c)(\lambda \text{tr}(\varepsilon)I + 2\mu\varepsilon)$
→ Spectral	$\frac{\lambda}{2} \text{tr}(\varepsilon_+)^2 + \mu \text{tr}(\varepsilon_+^2)$	$\frac{\lambda}{2} \text{tr}(\varepsilon_-)^2 + \mu \text{tr}(\varepsilon_-^2)$	$g(c)(\lambda \text{tr}(\varepsilon_+)I + 2\mu\varepsilon_+) + (\lambda \text{tr}(\varepsilon_-)I + 2\mu\varepsilon_-)$
Volumetric/ Deviatoric	$\frac{\lambda}{2} \text{tr}(\varepsilon_{vol,+})^2 + \mu \text{tr}(\varepsilon_{dev}^2)$	$\frac{\lambda}{2} \text{tr}(\varepsilon_{vol,-})^2$	$g(c)(\lambda \text{tr}(\varepsilon_{vol,+})I + 2\mu\varepsilon_{dev}) + \lambda \text{tr}(\varepsilon_{vol,-})I$
→ Volumetric/ Deviatoric Spectral	$\frac{\lambda}{2} \text{tr}(\varepsilon_{vol,+})^2 + \mu \text{tr}(\varepsilon_{dev,+}^2)$	$\frac{\lambda}{2} \text{tr}(\varepsilon_{vol,-})^2 + \mu \text{tr}(\varepsilon_{dev,-}^2)$	$g(c)(\lambda \text{tr}(\varepsilon_{vol,+})I + 2\mu\varepsilon_{dev,+}) + (\lambda \text{tr}(\varepsilon_{vol,-})I + 2\mu\varepsilon_{dev,-})$

# Phase Field

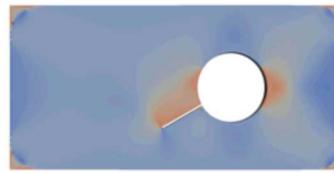
- Preliminary results:
  - Full energy does not crack in correct direction (expected)
  - Spectral decompositions crack in correct direction (expected)



Max. Principal Stress

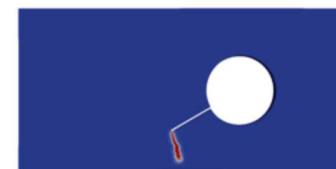


Von Mises Stress

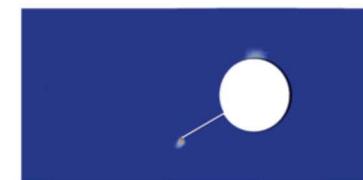


Triaxiality

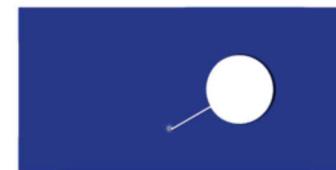
SIERRA



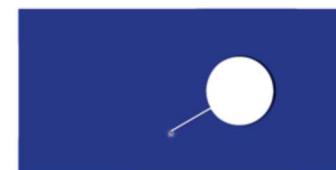
MOOSE



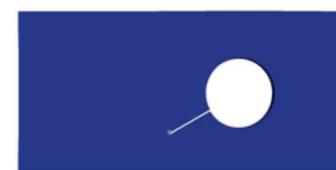
Full



Strain  
Spectral



Vol-Dev



Vol-Dev  
Spectral

- Performed qualitative verification by comparing to MOOSE framework

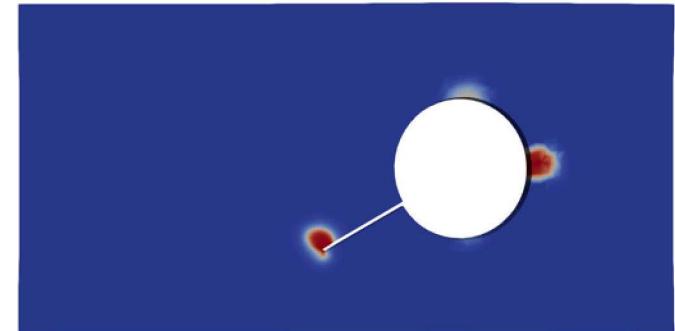
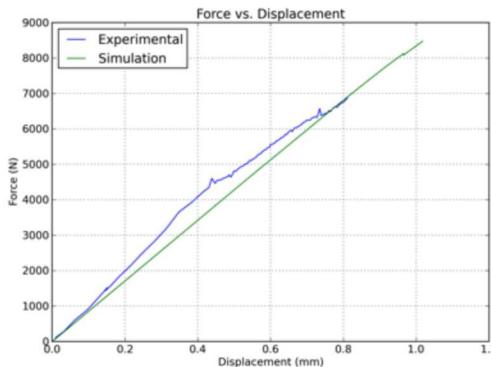
- Same trends for all energy decompositions
- Results do differ slightly in magnitude:

– SIERRA & MOOSE have different solution schemes: staggered vs. monolithic

# Phase Field

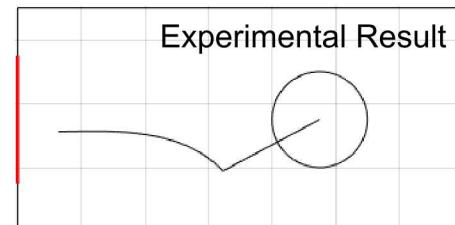
- Results:

- Best answer (volumetric/deviatoric spectral, overloaded)
  - Predicts tensile crack development, but also has cracks growing from hole
  - Notched crack grows in correct direction, but not far enough
  - Force/displacement plot much more linear
    - Stiffness does decrease with damage growth, but much later



- Takeaways:

- More work needed!
- Alternative selection of length scale?
- Eager to learn best practices



# SIERRA / FRANC3D

Scott Grutzik

John Emery

<http://www.fracanalysis.com> (FRANC3D)



# SIERRA / FRANC3D

- Overview of approach:
  - Discrete fracture representation
  - Coupling of SIERRA (Sandia) & FRANC3D (Fracture Analysis Consultants, Inc.)
    - SIERRA handles solid mechanics solve
    - FRANC3D performs mesh cutting & remeshing
    - FRANC3D uses “M-integral” calculate stress intensity factors
    - FRANC3D uses SIFs to compute crack extension distance & direction
- Details:
  - Solution in multiple steps. In each:
    - Compute physics (*entire displacement*)
    - Compute SIFs
    - Update geometry
  - Fatigue-like formulation
    - Solved in linear fashion
    - Crack growth proportional to SIF magnitudes:  $\Delta a \sim K_I^2$
    - SIF ratios → crack growth direction
    - No concept of  $K_{IC}$ ; no effort to ensure that  $K_i \leq K_{ic}$  at all points (nonlinear)

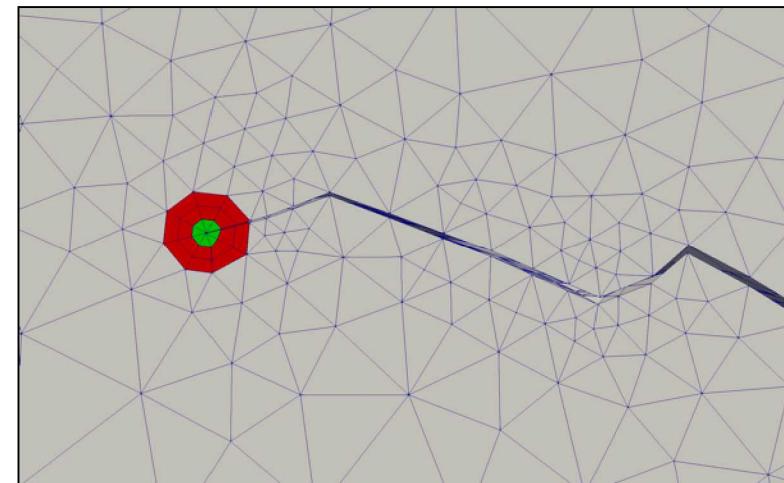
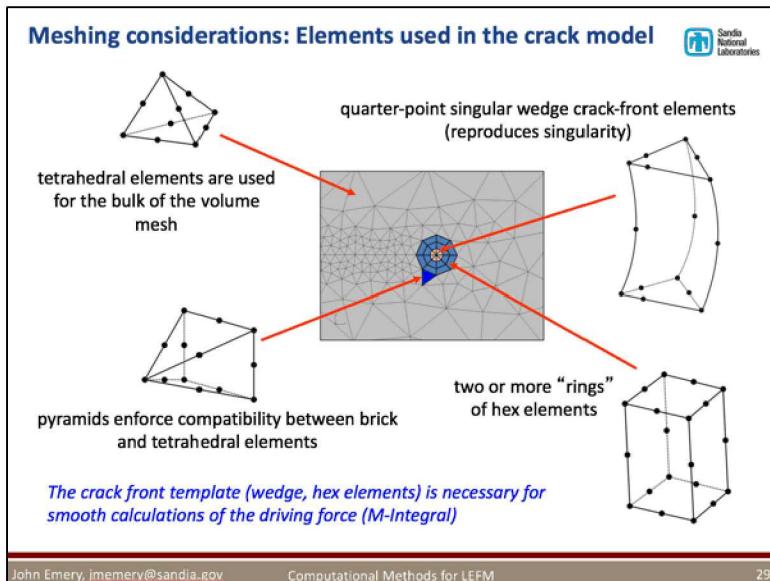


Illustration of FRANC3D mesh template placed at crack tip

# SIERRA / FRANC3D

- Overview of approach:
  - Details of mesh template & SIF calculation



Option 1

**Displacement correlation methods with 1/4-point elements**



$$v_{upper} - v_{lower} = [4(v_b - v_d) + v_e - v_c] \sqrt{\frac{r}{l}} + [4(v_b - v_d) + 2(v_c - v_e)] \frac{r}{l}$$

Evaluate

$$v = \frac{K_L}{\mu} \left[ \frac{r}{2\pi} \right]^{1/2} \sin \frac{\theta}{2} \left[ 2 - 2\nu - \cos^2 \frac{\theta}{2} \right]$$

for  $\theta = \pm 180^\circ$

$$v_{upper} - v_{lower} = \frac{2K_L}{\mu} \sqrt{\frac{r}{2\pi}} (2 - 2\nu)$$

Solve for  $K_I$

$$K_I = \frac{2\mu\sqrt{2\pi}}{\sqrt{l}(2-2\nu)} [4(v_b - v_d) + v_e - v_c]$$

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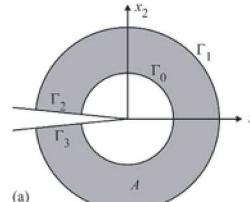
Computational Methods for LEFM

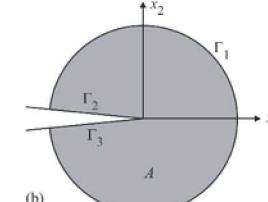
27

Option 2

**The J-Integral (2-D): Area Version**



(a) 

(b) 

$$\bar{J} = \int_A \left[ \sigma_{ij} \frac{\partial u_i}{\partial x_j} - W \delta_{ij} \right] \frac{\partial q_j}{\partial x_i} dA$$

where  $\delta$  is the Kronecker delta and  $q$  is a weighting function defined over the domain of integration. Physically,  $q$  can be thought of as the displacement field due to a virtual crack extension.

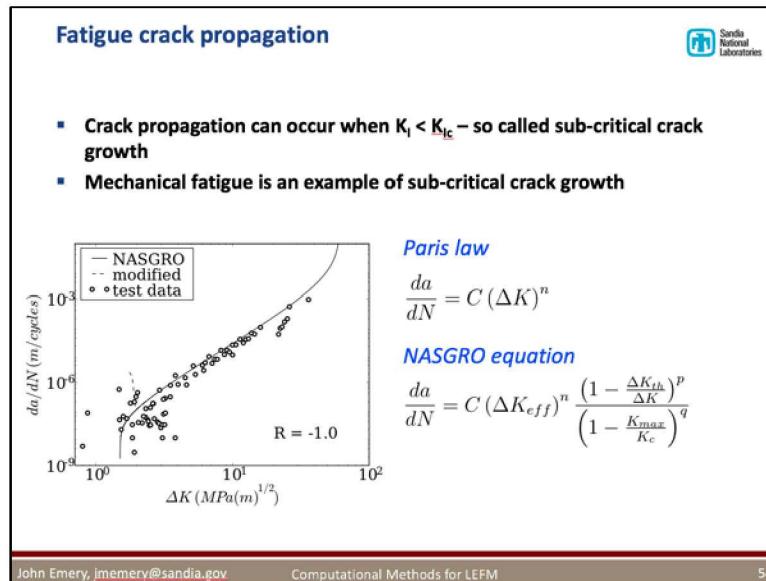
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Computational Methods for LEFM

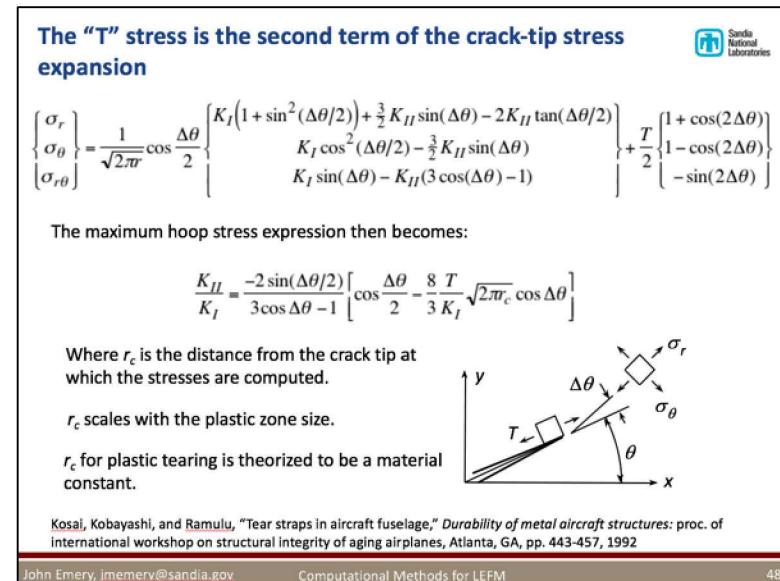
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# SIERRA / FRANC3D

- Overview of approach:
  - Details of crack extension & direction calculation:



Crack extension compute as fatigue crack

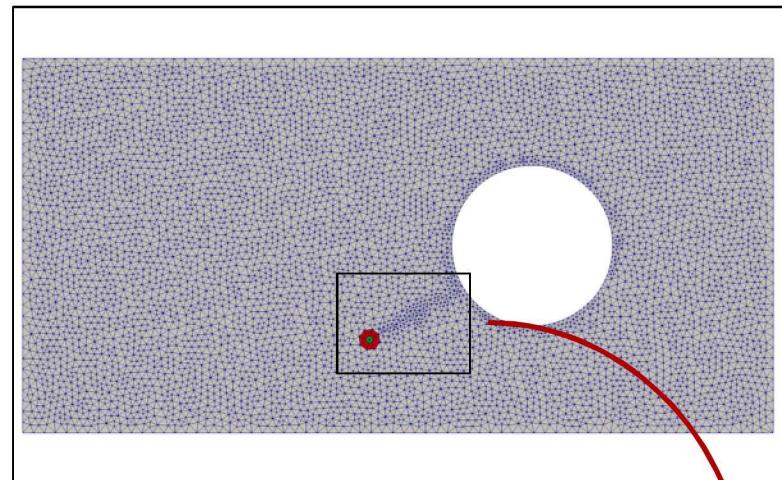


Crack direction determined by minimizing hoop stress  $\sigma_\theta$ :  $\frac{\partial \sigma_\theta}{\partial \theta} = \sigma_{r\theta} = 0$

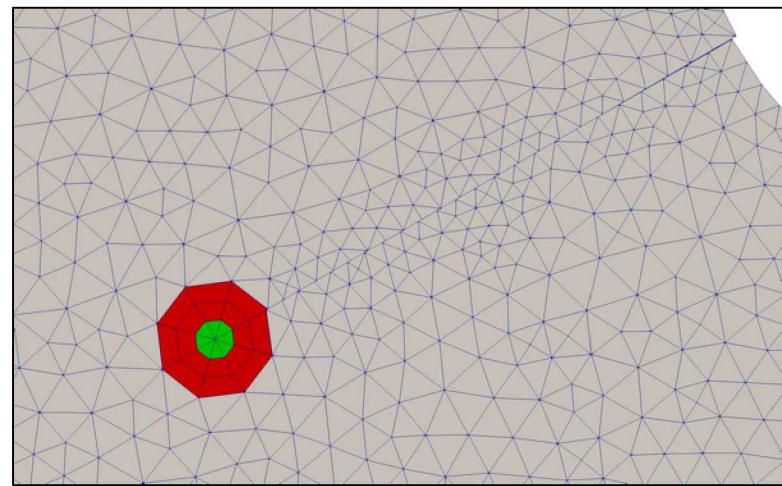
# SIERRA / FRANC3D

- Strategy:
  - Geometry:
    - Nominal geometry & zero-thickness pre-crack
  - Analysis:
    - Total Lagrange quadratic Tet10 elements
    - Apply quasistatic displacement of 1 mm
    - Analyze over many steps, until crack extension becomes “sufficiently small”
    - 13 steps in this case, could go further
- Post-Processing:
  - $K_{Ic}$  correction:
    - $\sigma$  &  $K_i$  linear functions of applied displacement
    - Assume that the crack extends at  $K_I = K_{Ic}$
    - Scale simulation displacement (1 mm) by  $\frac{K_{Ic}}{K_I}$  ratio to estimate actual displacement required to reach  $K_I = K_{Ic}$

$$u_{actual} = \frac{K_{Ic}}{K_{I,simulation}} u_{simulation}$$



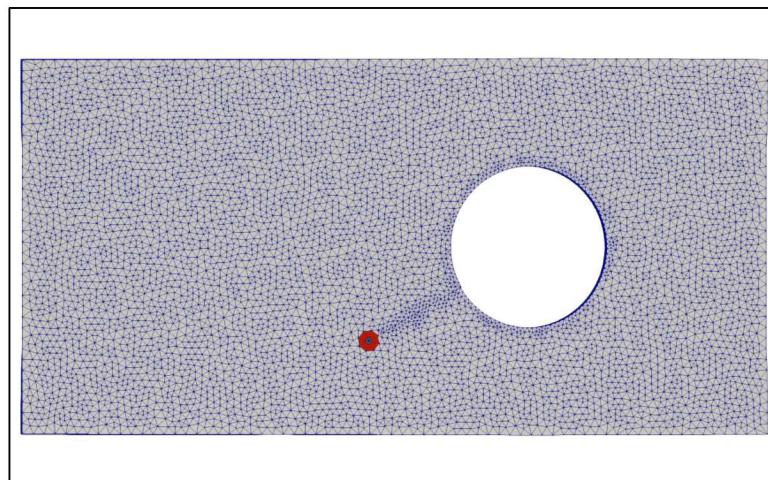
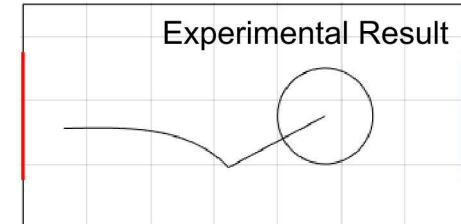
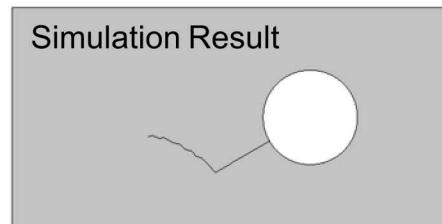
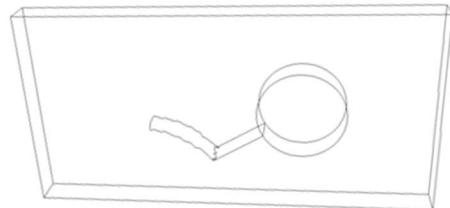
Initial Mesh – nominal geometry with zero-thickness crack



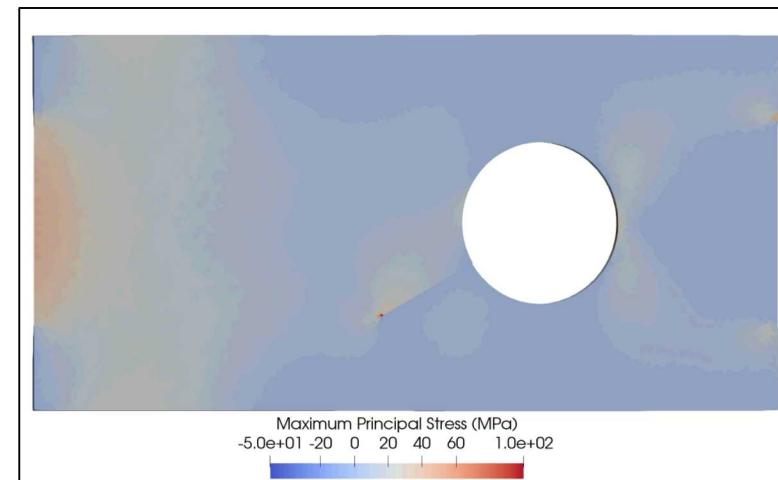
Initial Mesh – close-up of zero-thickness crack and crack tip mesh template

# SIERRA / FRANC3D

- Results:



Mesh Evolution

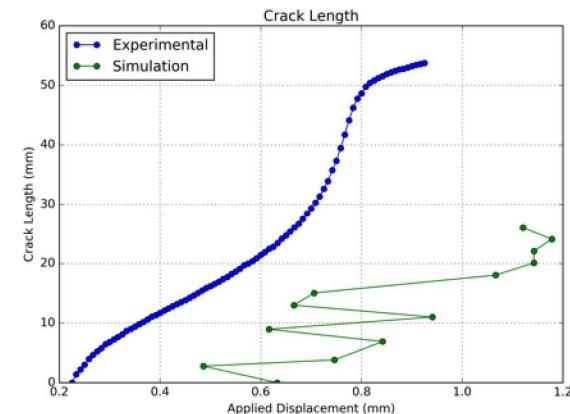
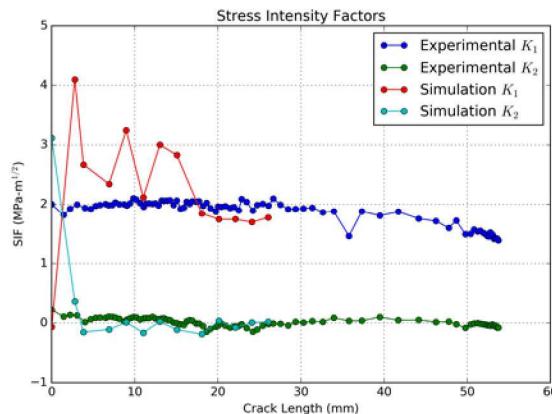
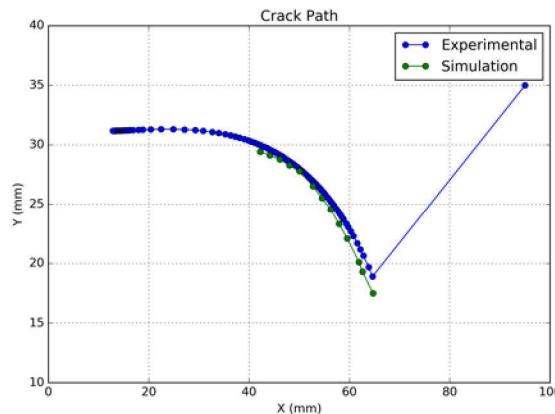


Maximum Principal Stress Evolution

- FRANC3D does well at capturing experimental crack path
- Might get even better result with smaller steps, additional steps, and mesh refinement

# SIERRA / FRANC3D

- Results:
  - Quantitative comparisons to experimental data, post-processed



\*estimated using  $\frac{K_{Ic}}{K_I}$  scaling

- FRANC3D does well at capturing experimental crack path
- Stress intensity factors are similar
- Crack length vs. applied displacement matches less well, but this is based on post-processing ( $\frac{K_{Ic}}{K_I}$  scaling)
- Force/displacement comparison not (yet) available
- Might get even better result with smaller steps, additional steps, and mesh refinement

# Thank you!



Thanks to conference & benchmark organizers!



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