SAND2016-2984C

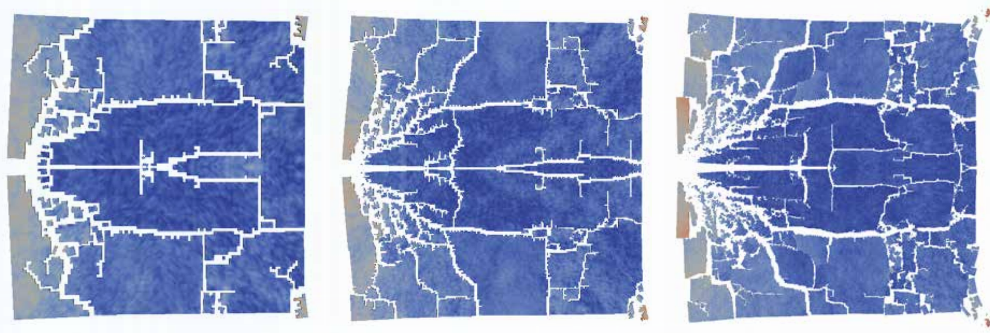
A PDE Constrained Optimization Approach for Crack Inversion Based on Phase-Field Regularization

Michael Tupek, Computational Solid Mechanics and Structural Dynamics

The State of Fracture Modeling

- Fracture modeling is critical to predicting the performance and reliability of many Sandia components and systems
- Many fracture models used at Sandia (and elsewhere) are ill-posed and non-convergent

Max principal stress criterion with element death shows significant mesh dependence

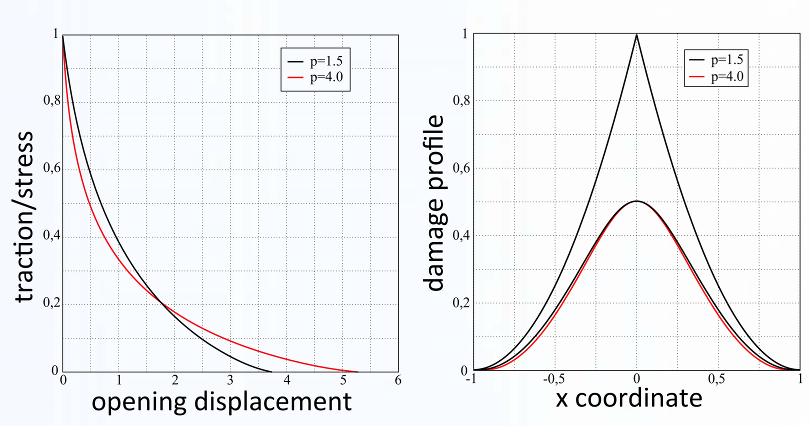


Coarse mesh *Medium mesh* *Fine mesh*

Improved Forward Modeling of Crack Propagation in Brittle Materials

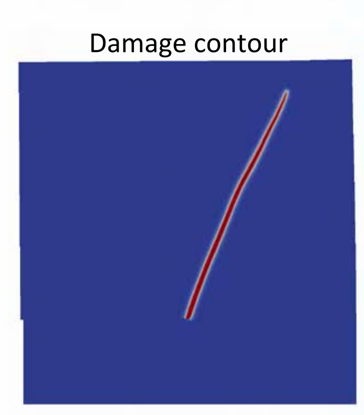
- Developed an explicitly integrated phase-field/gradient-damage model which avoids the usual nonlinear equation solve at each time step (>10 x better performance)
- Extension of the damage model by Lorentz, et al. 2011, which was shown to converge to a cohesive zone model as the length scale approaches 0

$$\eta \dot{d} = h(d)\psi(\boldsymbol{\sigma}) - \frac{3}{4}\frac{G_c}{l} + \frac{3}{8}G_c l \nabla \cdot \nabla d \qquad \rho \ddot{\mathbf{u}} = \nabla \cdot \boldsymbol{\sigma}(\boldsymbol{\epsilon}, d)$$



Cohesive phase-field traction separation law (left) and through 'crack' damage profile (right), p is a parameter of the model.

Adapted from Lorentz, et al. 2011.

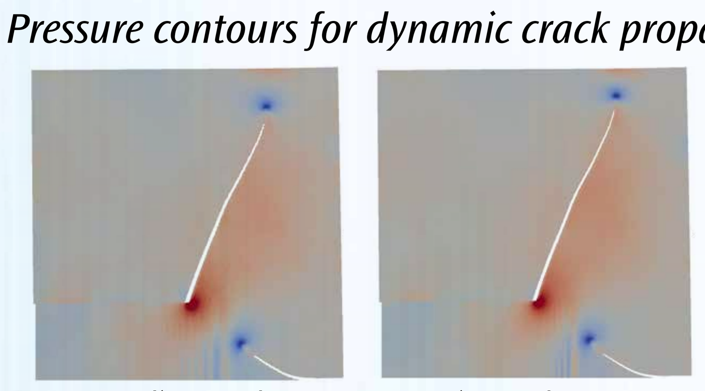


Kalthoff validation problem achieves the expected crack propagation angle: ~70°

Brittle Fracture Physics and Mesh Convergence

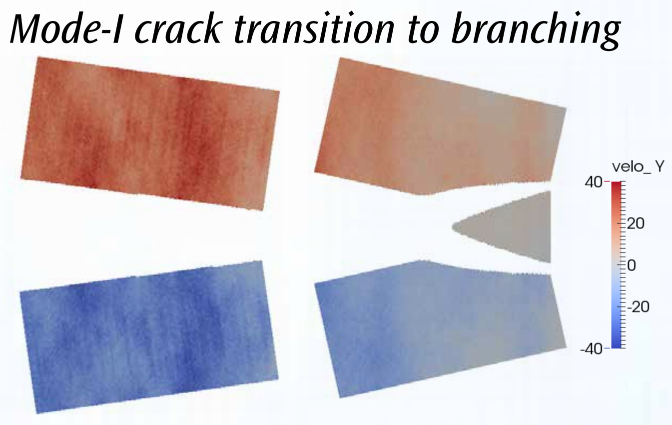
- Crack propagation in brittle materials is characterized primarily by a critical stress σ_c and critical energy release rate G_c (energy dissipated per crack area)
- Many brittle damage material models include σ_c, but G_c is often ignored
- However, G_c is essential for predicting crack branching and introducing a physical length scale to get mesh insensitive results
- Observed convergence rate for dissipated energy: ~0.7

Pressure contours for dynamic crack propagation



Medium mesh: 250k elements *Fine mesh: 1,000k elements*

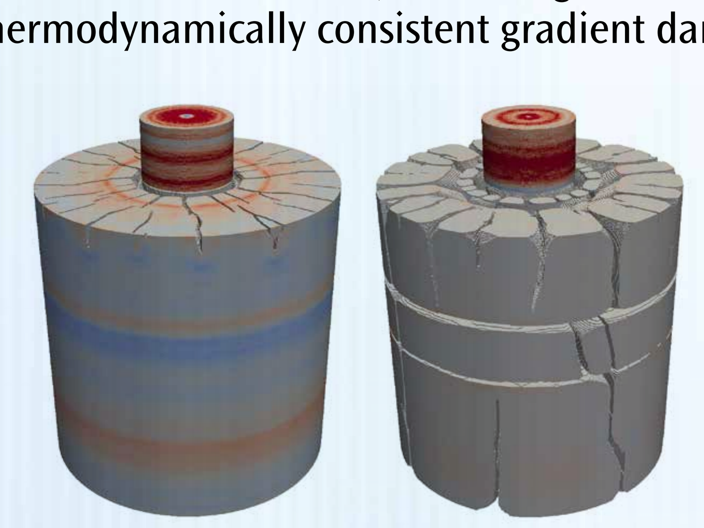
Mode-I crack transition to branching



High G_c *Low G_c*

Extension to 3D in Sierra-SM

- Capable of capturing complex 3D crack patterns without explicitly representing crack geometry
- Predicts crack initiation, branching and coalescence all from a single thermodynamically consistent gradient damage model



Ceramic impact

Brittle torsion fracture

Fracture Inverse Problems

- Most analyses today are forward problem solves: simulate what happens in a given scenario
- However, what is often truly desired is the solution to the corresponding inverse problem
- Example fracture inverse problems:
  - Crack detection/non-destructive evaluation: determine the existence and locations of cracks in a structure
  - Crack forensics: find the loadings applied to a structure which result in the observed failure pattern
  - Material design: optimize the properties and geometry of a structure to resist crack initiation and propagation
- These last examples require accurate fracture prediction

General inverse problem statement as a PDE constrained optimization problem

$$\min_{\boldsymbol{\theta}} g(\mathbf{u}, \boldsymbol{\theta}) \quad \text{s.t.} \; \mathcal{L}(\mathbf{u}, \boldsymbol{\theta}) = \mathbf{0}.$$

$\mathbf{u}$ *:state variables*
$\boldsymbol{\theta}$ *:design parameters*
$\mathcal{L}$ *:differential operator*
g *:quantify of interest*

Library for Efficient Computation of Parameter Sensitivities

- A C++ library has been developed which simplifies the implementation and testing of adjoint sensitivities for explicit dynamic simulations
- Users define the state u (e.g. the nodal displacements), and the input parameters θ (e.g. each element's material damage), and the following time step update rules and quantify of interest operators:

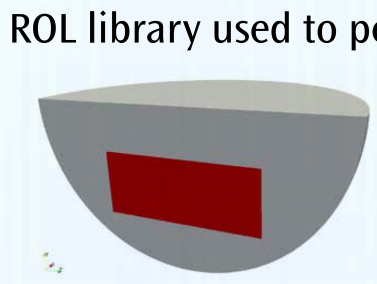
$$\mathbf{u}^{n+1} = \mathbf{f}(\mathbf{u}^n, \boldsymbol{\theta}) \qquad \frac{\partial \mathbf{f}(\mathbf{u}^n, \boldsymbol{\theta}) \cdot \boldsymbol{\mu}}{\partial \mathbf{u}^n} \qquad \frac{\partial \mathbf{f}(\mathbf{u}^n, \boldsymbol{\theta}) \cdot \boldsymbol{\mu}}{\partial \boldsymbol{\theta}}$$

$$\text{q.o.i.} = g(\mathbf{u}^N, \boldsymbol{\theta}) \qquad \frac{\partial g(\mathbf{u}^N, \boldsymbol{\theta})}{\partial \mathbf{u}^N} \qquad \frac{\partial g(\mathbf{u}^N, \boldsymbol{\theta})}{\partial \boldsymbol{\theta}}$$

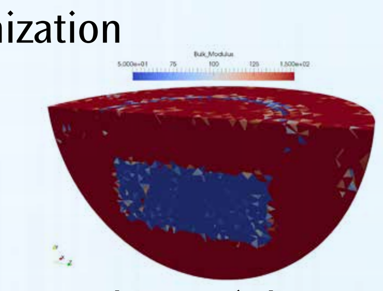
- From this definition of the physics, the sensitivity $\frac{dg(\mathbf{u}^N, \boldsymbol{\theta})}{d\boldsymbol{\theta}}$ is automatically computed by the library
- Computes 1,000 – 1,000,000 parameter sensitivities with O(10) times the cost of a forward solve

Phase-field Inversion Examples

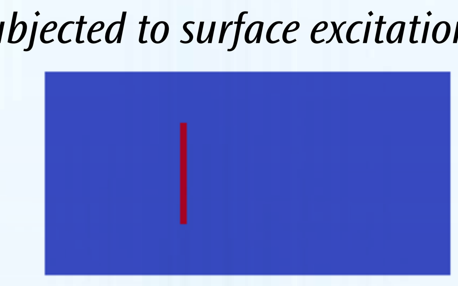
- Minimize discrepancy between observed displacements and simulated displacements by varying phase (volume fraction) element by element
- Sandia's ROL library used to perform the optimization



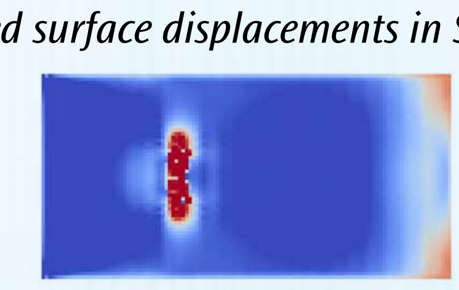
Initially unknown hidden tunnel subjected to surface excitation



Reconstructed material properties due to observed surface displacements in Sierra-SD



Initial crack/damage in specimen



Reconstructed crack based on observed displacements due to acoustic excitation

Work in Progress

- Collaborating with Sandia analysts to validate phase-field models for lab relevant 3D problems
- Applying the new inverse framework to the new phase-field crack propagation model in order to solve unprecedented crack inverse problems
- SANDIA reports and journal articles:
  - Brittle fracture phase-field modeling of a short-rod specimen (published SANDIA report)
  - A parabolic regularization of cohesive fracture for explicit dynamic crack propagation (to be submitted for peer review)
  - A C++ library for efficient adjoint sensitivities and automatic checkpointing in nonlinear explicit dynamic simulations (in progress SANDIA report)
- References:

  - Convergence of a gradient damage model toward a cohesive zone model, E. Lorentz, et al.
  - Minimal repetition dynamic checkpointing algorithm for unsteady adjoint calculation, Q. Wang, et al.
  - Crack identification by 'arrival time' using XFEM and a genetic algorithm, D. Rabinovich, et al.

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.
SAND 2016-XXXXP Sandia Creative Group 284-5637 SL-03-16

Sandia National Laboratories