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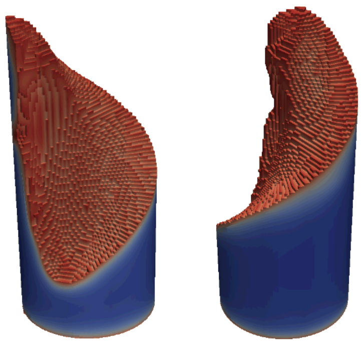 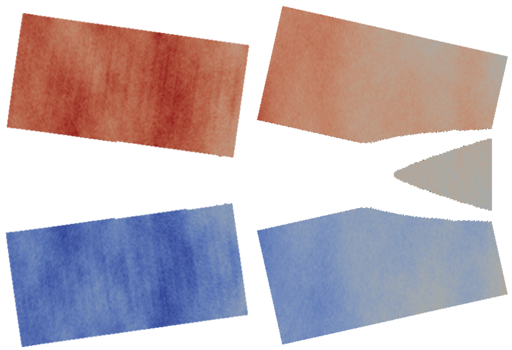 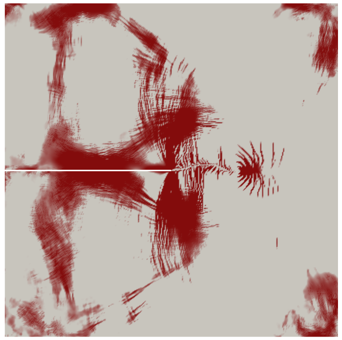

# Inverse methods for fracture based on a parabolic regularization of brittle cohesive laws

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U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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# Fracture Renaissance

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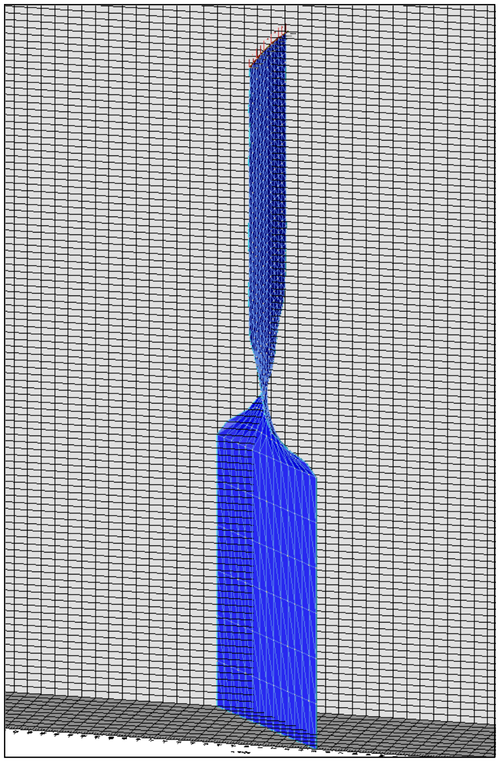
- Several promising new fracture methods have emerged in recent years

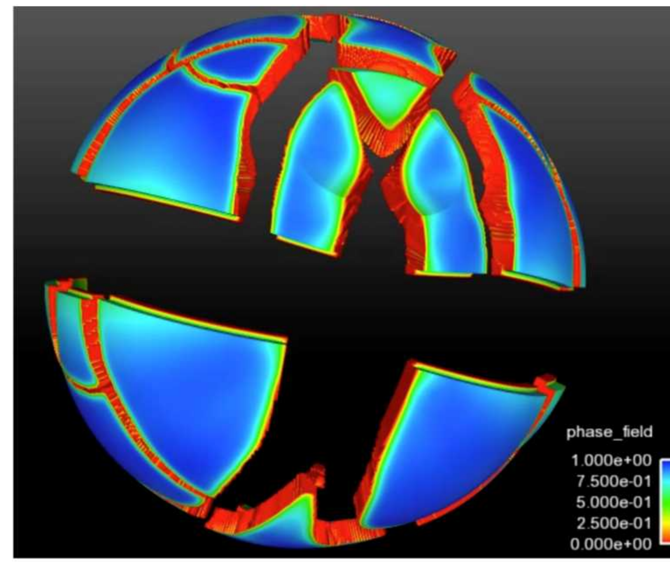


Duarte 2011

GFEM / XFEM

Tupek 2014

Peridynamics




Dolbow, Stevens 2015

Phase field

# Inverse methods for fracture

- Most fracture method focus on predictions
- This remains a significant challenge!
- However, predictions by themselves aren’t that interesting

*“Computers are useless, they can only give you answers.”*

-Pablo Picasso

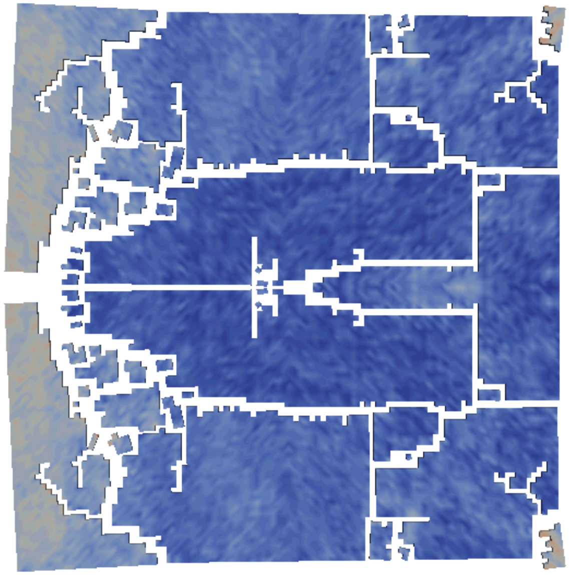
- Predictive simulations should guide decision making

**inverse = predictions ⟶ decisions**

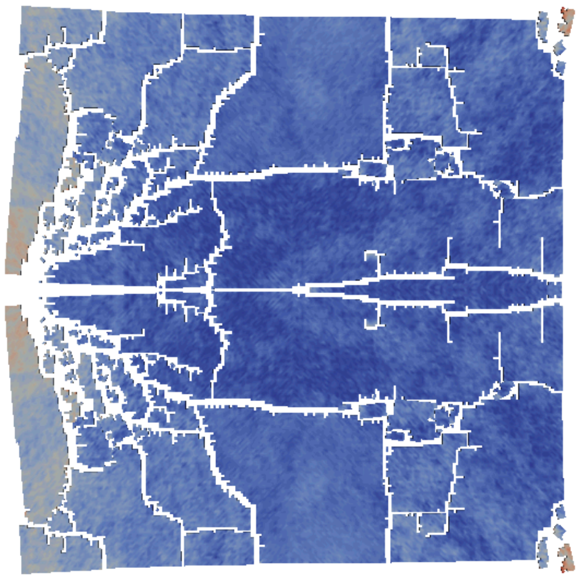
# Classical damage models: ill-posed

- 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

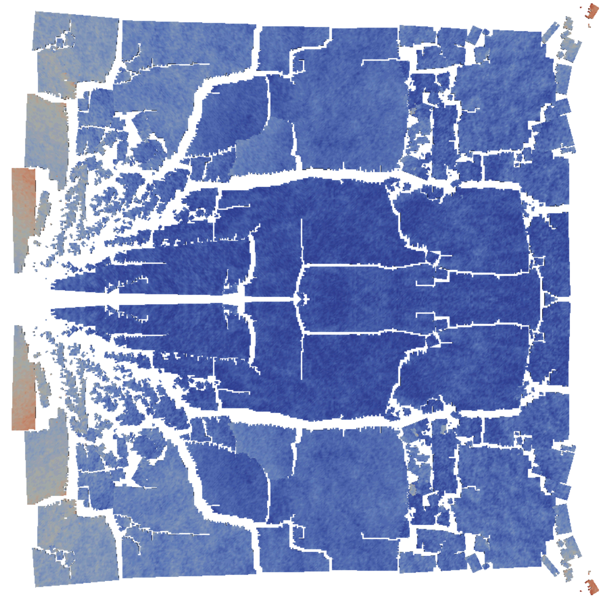
Max principal stress criterion with element death shows significant mesh dependence



Coarse mesh



Medium mesh



Fine mesh

# Reintroducing the Lorentz model

- An elliptic regularization of a cohesive zone model.
- Has a natural critical strain energy criterion.
- Decouples the regularization length scale from the process zone size (though Lorentz argues on physical grounds that the regularization length scale must be smaller than the process zone size).
- Added the now standard decomposition into positive and negative strain energies.
- Irreversibility introduces via $\dot{\phi} \geq 0$.
- However, VERY expensive to solve a nonlinear inequality constrained elliptic PDE, especially for explicitly integrated transient dynamics.

# Improved forward modeling of crack propagation in brittle materials

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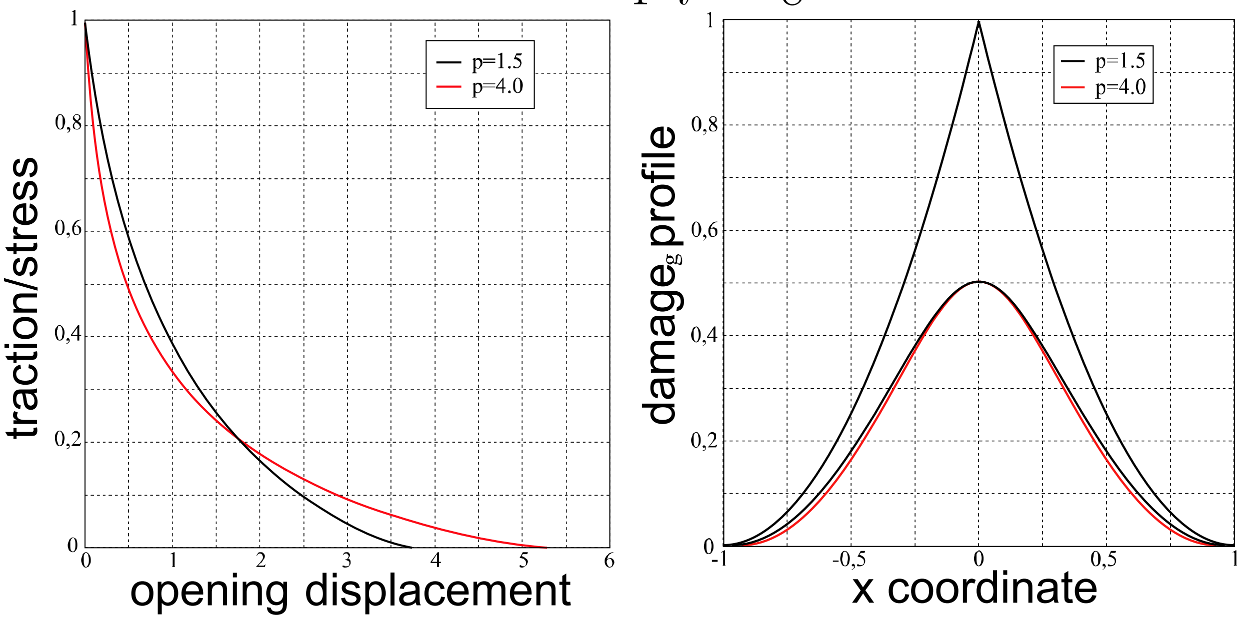
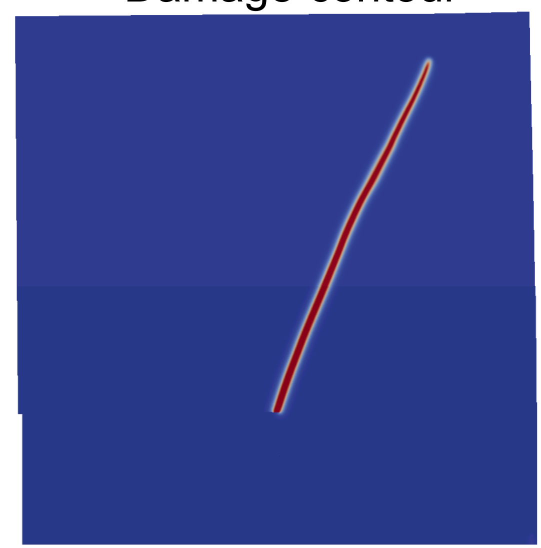
- Developed an explicitly integrated phase-field/gradient-damage model which avoids the usual nonlinear equation solve at each time step (>10 x better performance)
- Extension of the damage model by Lorentz, et al. 2011, which was shown to converge to a cohesive zone model as the lengthscale approaches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

Damage contour



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

# Cohesive gradient damage model

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- Regularized gradient damage model by Lorentz, et al. 2011
- Shown to converge to cohesive zone model as $L \to 0$

$$\rho \ddot{\mathbf{u}} = \nabla \cdot \boldsymbol{\sigma}, \quad \boldsymbol{\sigma} = g(\phi)\frac{\partial \psi_e^+}{\partial \boldsymbol{\varepsilon}} + \frac{\partial \psi_e^-}{\partial \boldsymbol{\varepsilon}}$$

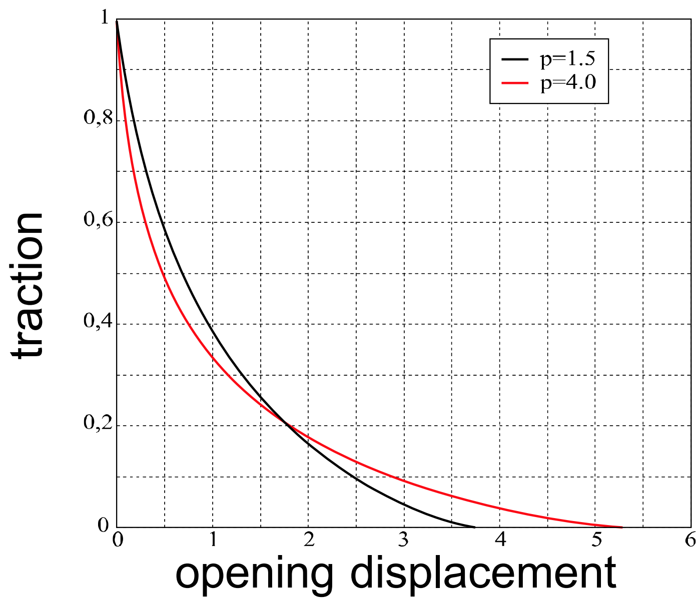
Momentum balance

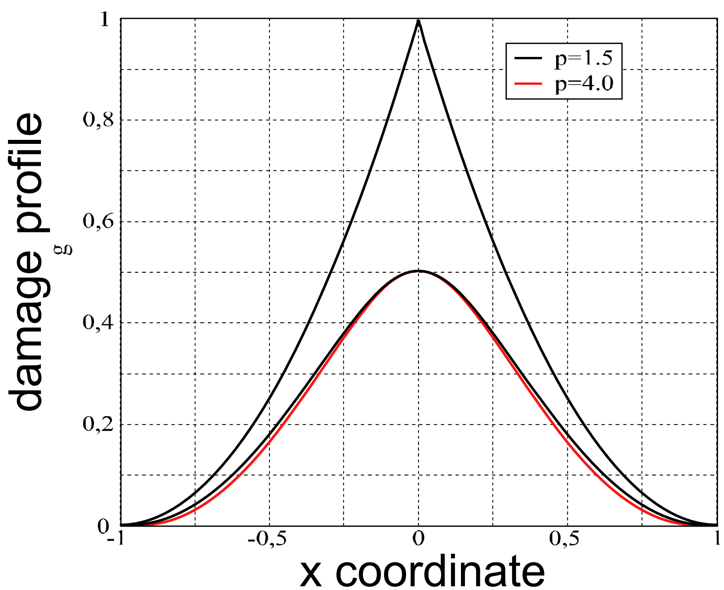
$$g'(\phi)\psi_e^+ + k = c\nabla^2\phi$$

Phase field equation

$$g(\phi) = \frac{(1-\phi)^2}{1+(m-2)\phi+(1+pm)\phi^2}$$

Thermodynamically consistent, derivable from a phase potential



# Parameters of damage model

Depends on cohesive fracture parameters:

$$k = \frac{3}{4}\frac{G_c}{L} \quad c = \frac{3}{8} L G_c \quad m = \frac{3}{2}\frac{E G_c}{\sigma_c^2 L}$$

Note: the fracture energy, $G_{c,}$ is ignored in most damage models

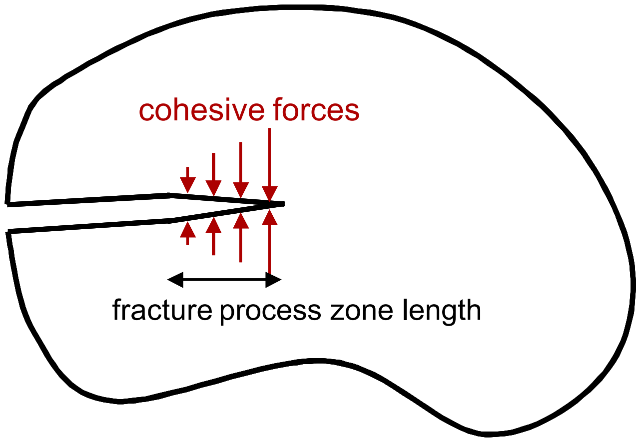
Physically justified constraints on the parameters ensures

- Regularization lengthscale resolves fracture process zone

$$L < \frac{3}{2(p+2)} \frac{E G_c}{\sigma_c^2}$$

- Monotonic stress decay

$$p \geq 1$$



# Parabolic regularization

- For explicitly integrated dynamic problems, solving a nonlinear phase field equation is VERY expensive
- Add a viscous regularization (e.g., Miehe 2010)

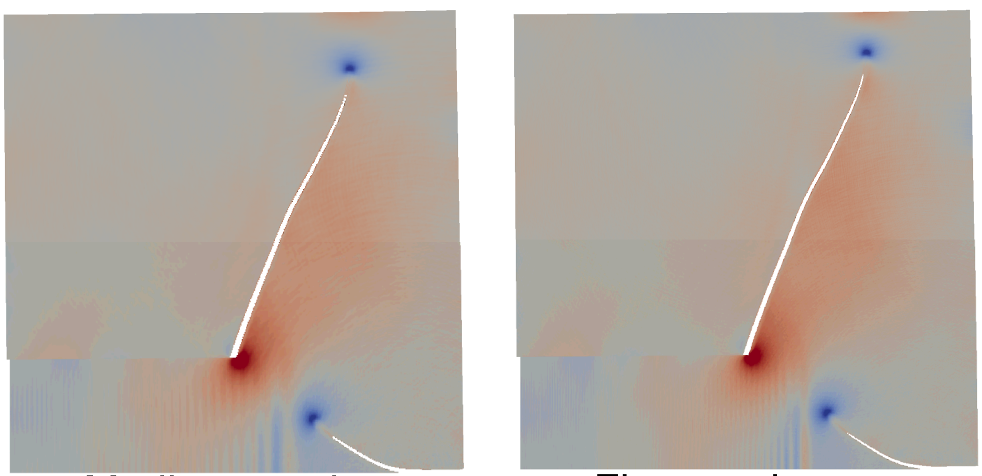
$$\eta\dot{\phi} = -g'(\phi)\psi_e^+ - k + c\nabla^2\phi, \quad \dot{\phi} \geq 0$$

- Choose to integrate this parabolic equation explicitly!
- Hyperbolic timestep constraint: $\Delta t \leq \frac{1}{s}\Delta x$
- Parabolic timestep constraint: $\Delta t \leq \frac{\eta}{c}(\Delta x)^2$
- Use the hyperbolic timestep if: $\eta \geq \frac{c}{s\Delta x}$

# Brittle fracture physics and mesh convergence

- $G_c$ is essential for predicting crack branching
- Mesh insensitive due to introduction of a physical length scale results in observed convergence rate for dissipated energy of ~0.5 when changing length scale
- Can get 1st order convergence for fixed length scale

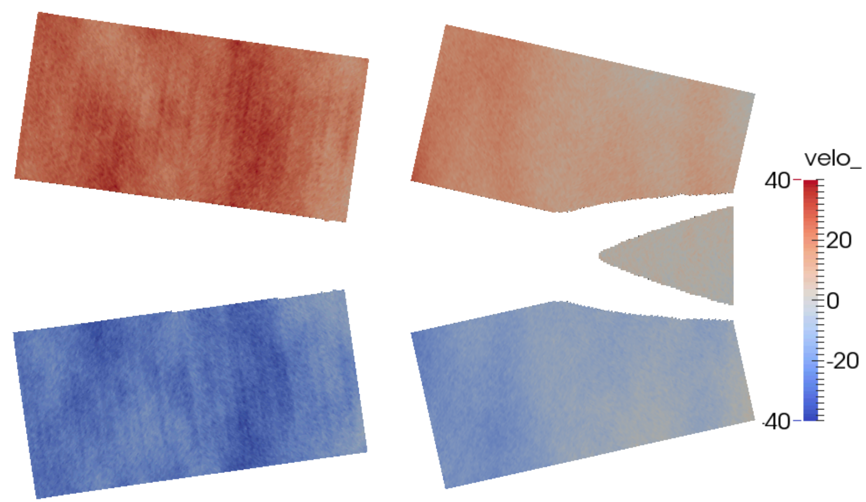
Pressure contours for dynamic crack propagation



Medium mesh: 250k elements

Fine mesh: 1,000k elements

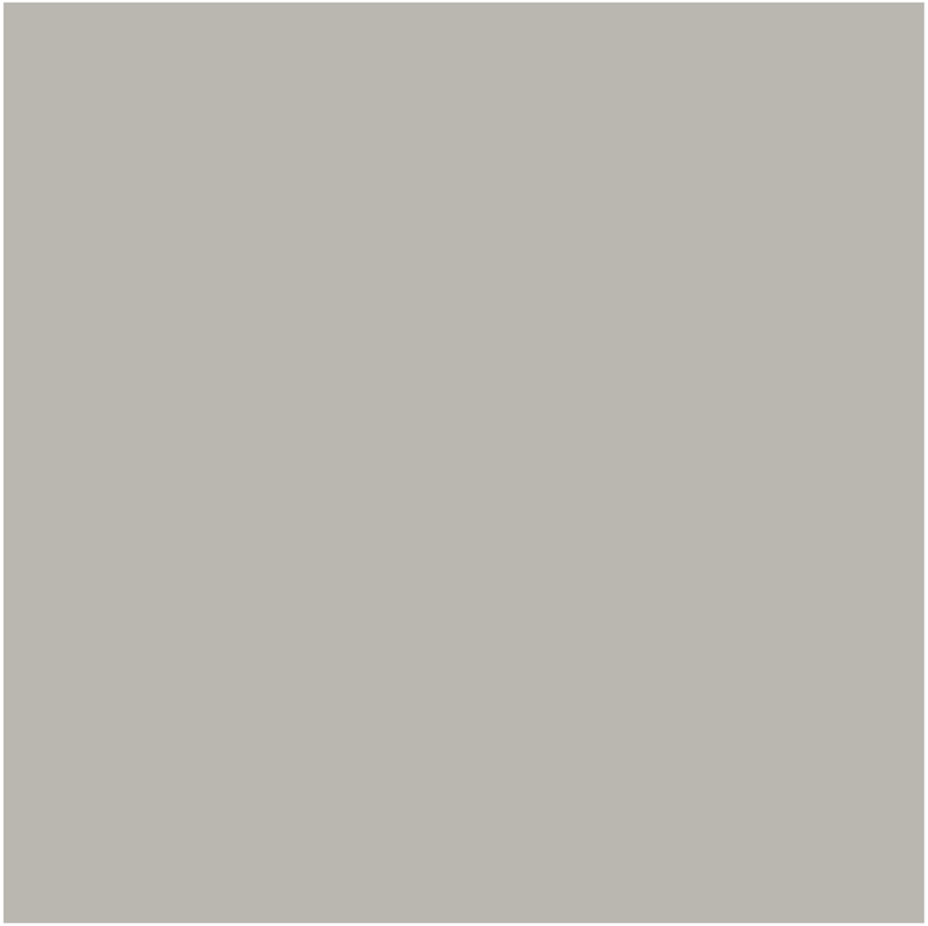
Mode-I crack transition to branching




High $G_c$

Low $G_c$

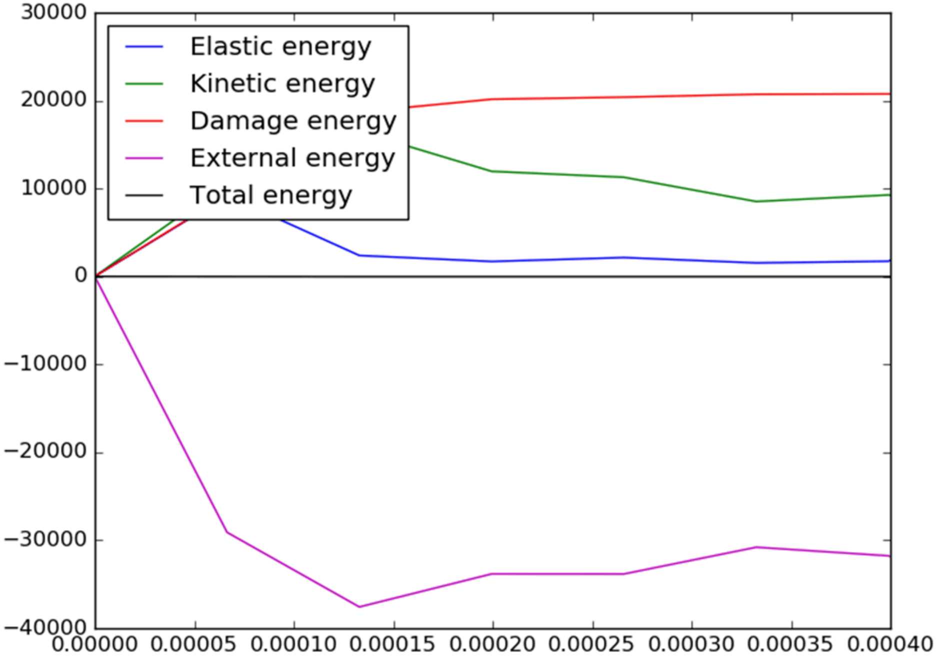
# High fracture energy release rate



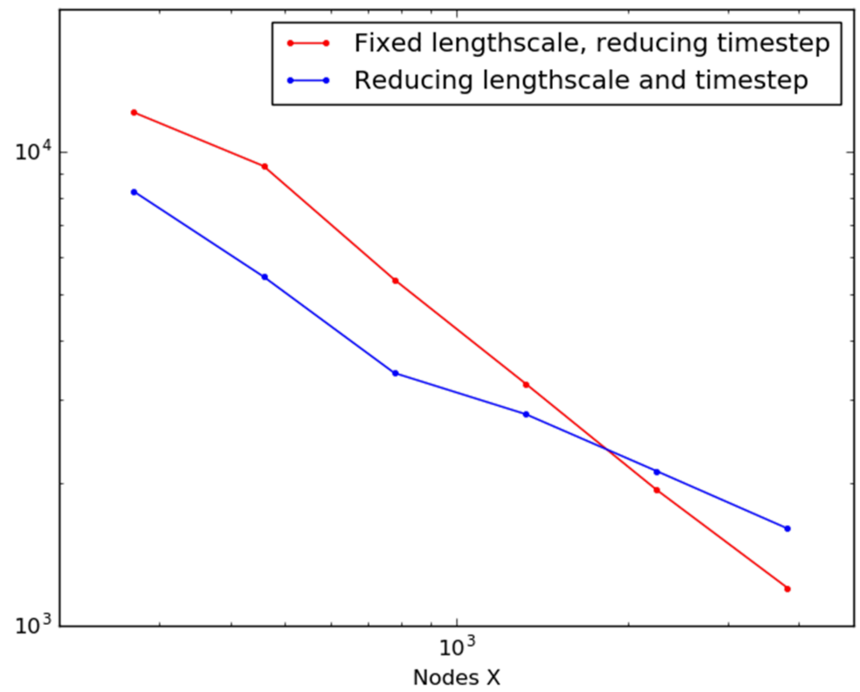
# Low fracture energy release rate

# Accuracy

Total numerical energy is preserved

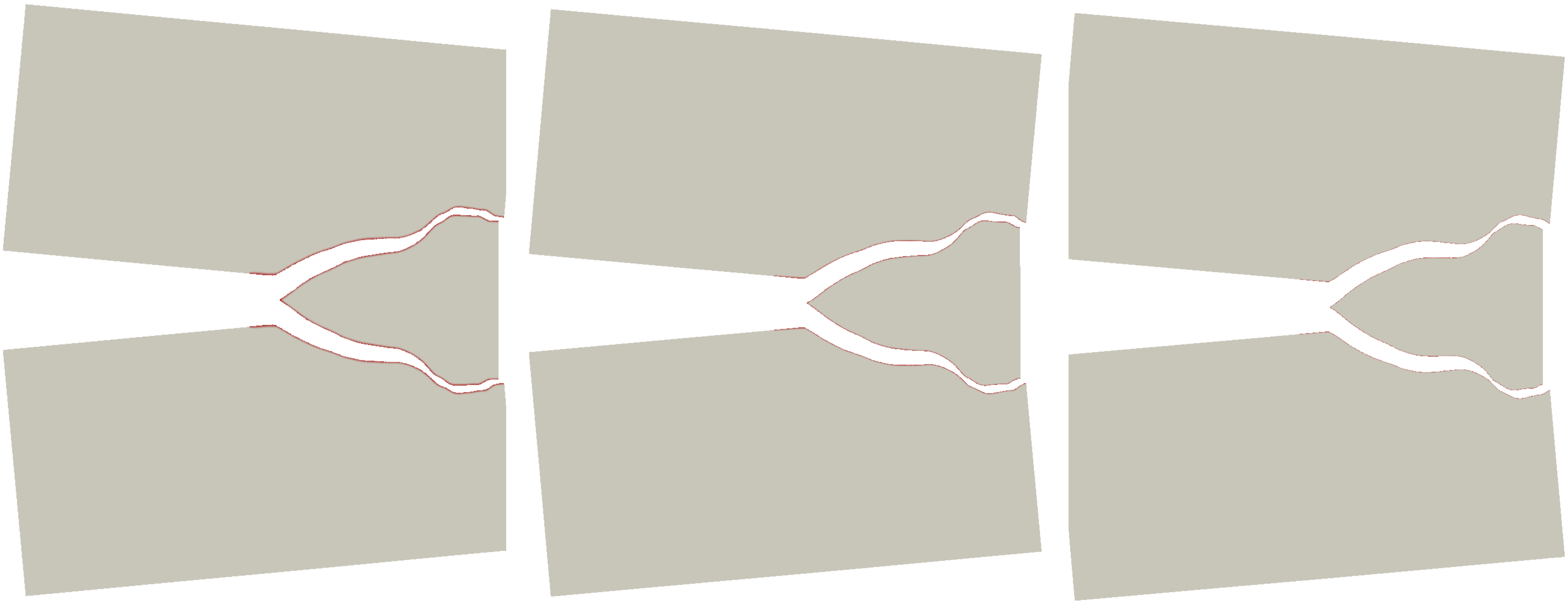



Dissipated fracture energy error




- Convergence rate of ~1 for fixed lengthscale
- Convergence rate of ~0.5 otherwise
- Dissipation due to viscous regularization dominates error

# Branching: mesh insensitivity



2.8 million elements | 9 million elements | 29 million elements

Runs in ~12 hours

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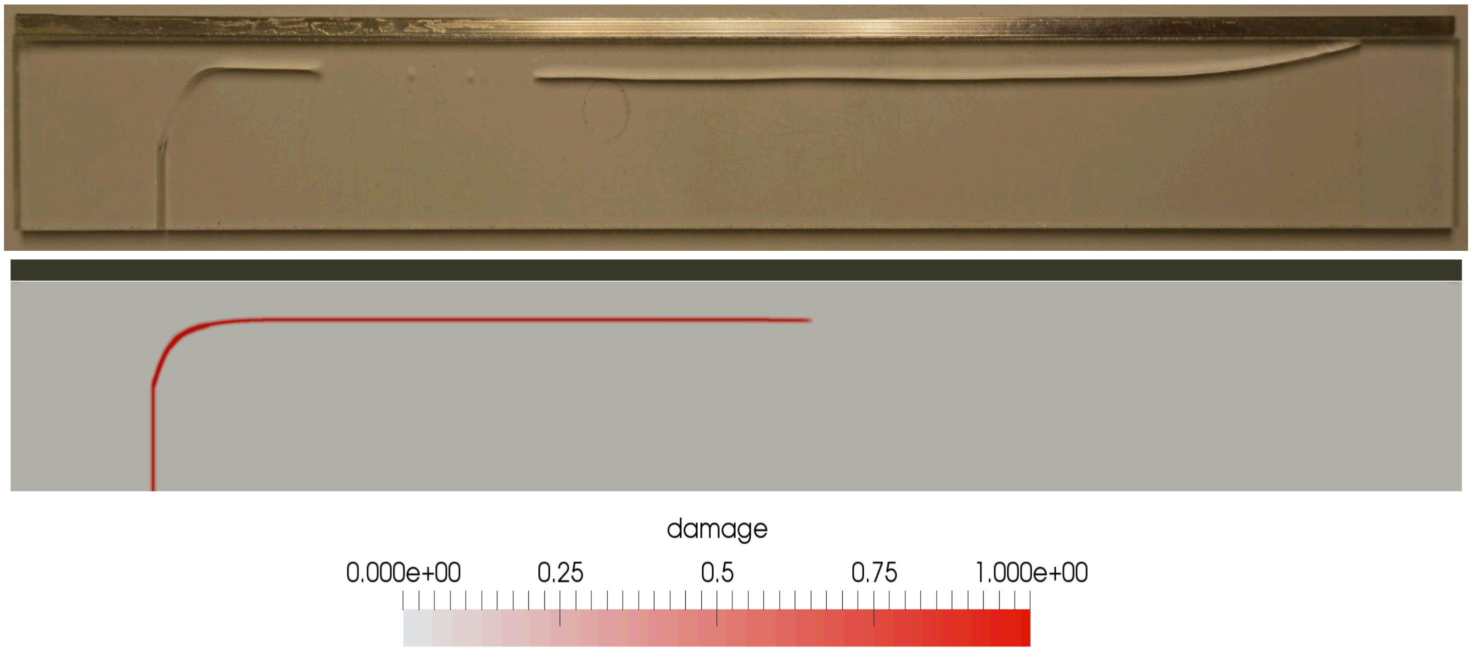
# Thermally loaded glass-metal interface




- Experimentally observed crack path for a glass to metal seal demonstration problem (top figure). The loading is driven by a temperature drop, which causes the metal on top to contract relative to the glass below. An initial vertical crack on the left first propagates upward, and then turns to run parallel to the glass-metal interface. The simulation contains 1.5 million elements and runs in 6 hours on a single GPU (bottom figure).

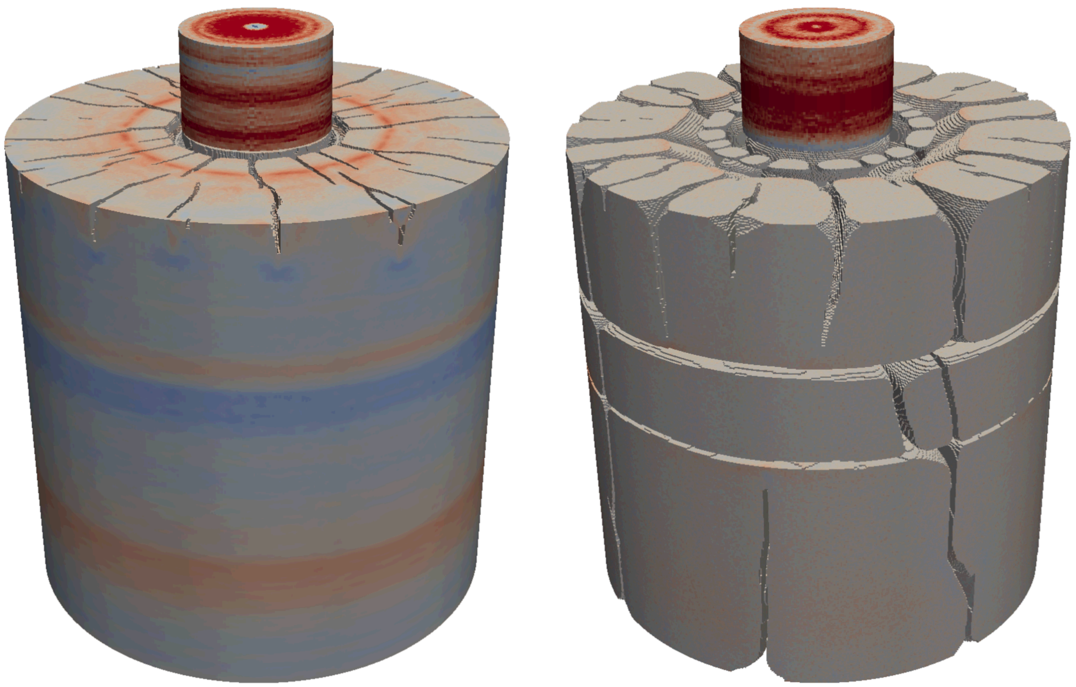
# Parabolic regularization

- Modify the phase-field/gradient damage equations by adding a mobility/viscosity term D_dot = …
- This allows for the option to explicitly integrate the damage equation, VERY minimal overhead!
- On physical grounds, it’s unnatural to have to solve an elliptic PDE for damage, as its well known that brittle cracks propagate at ~0.6 the Rhaile wavespeed.
- We should be able to get away with an explicit time integrator.

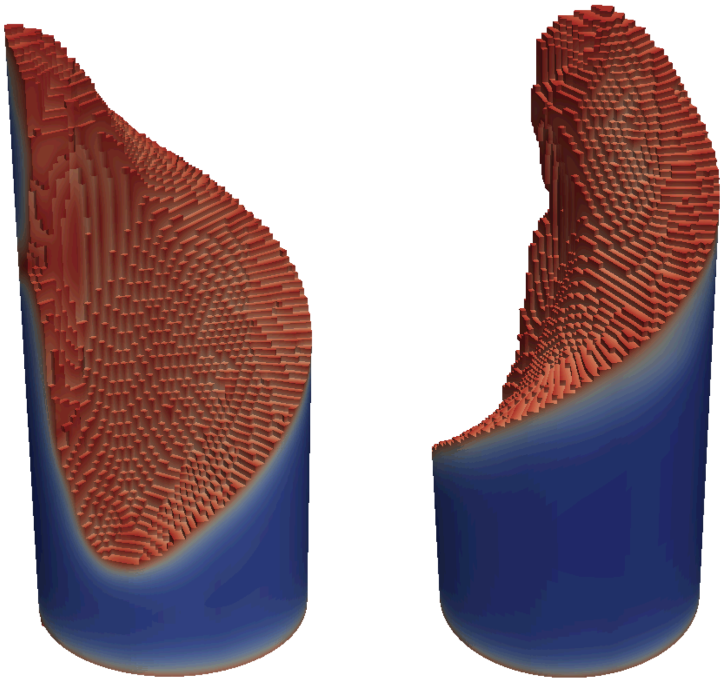
# Comments

- It is well known that explicitly integrating parabolic equations is a poor idea, but lets see what happens.
- Choose to interpret the viscosity as a purely numerical parameter, chosen as large as possible without affecting stability
- Ongoing work with John Dolbow to assess this model in fragment scaling studies.

# Demonstrations in 3D



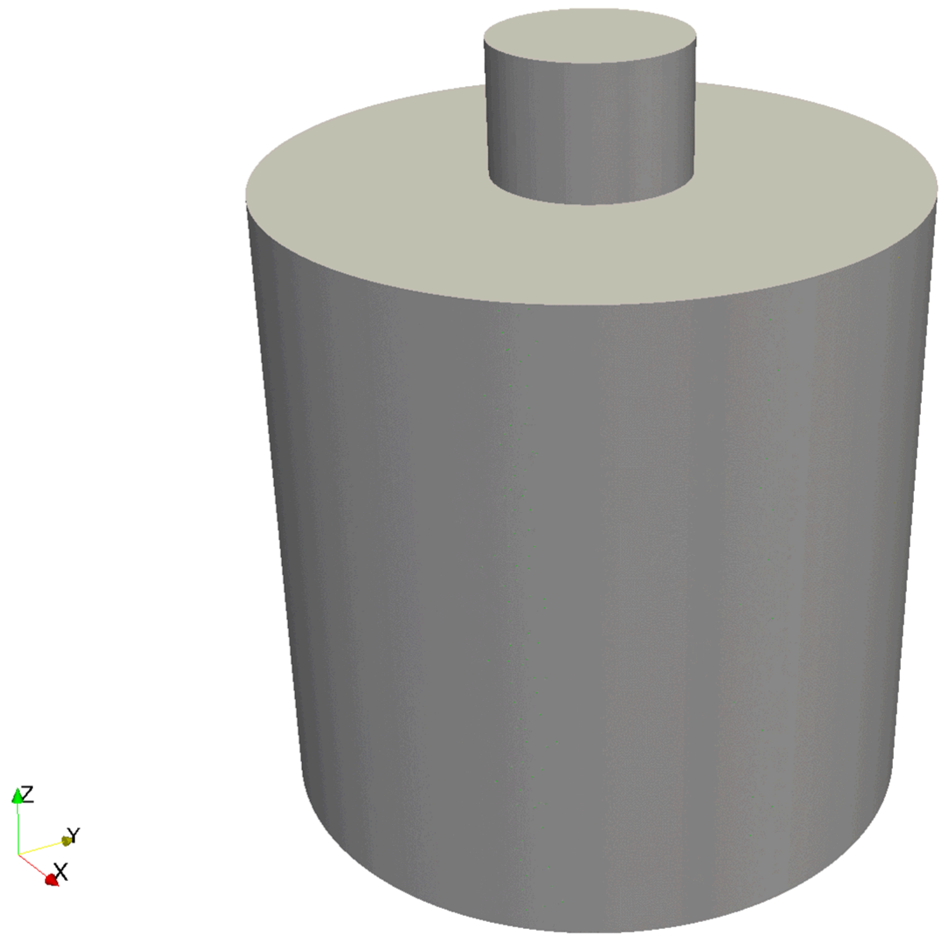
Ceramic impact



Brittle torsion fracture

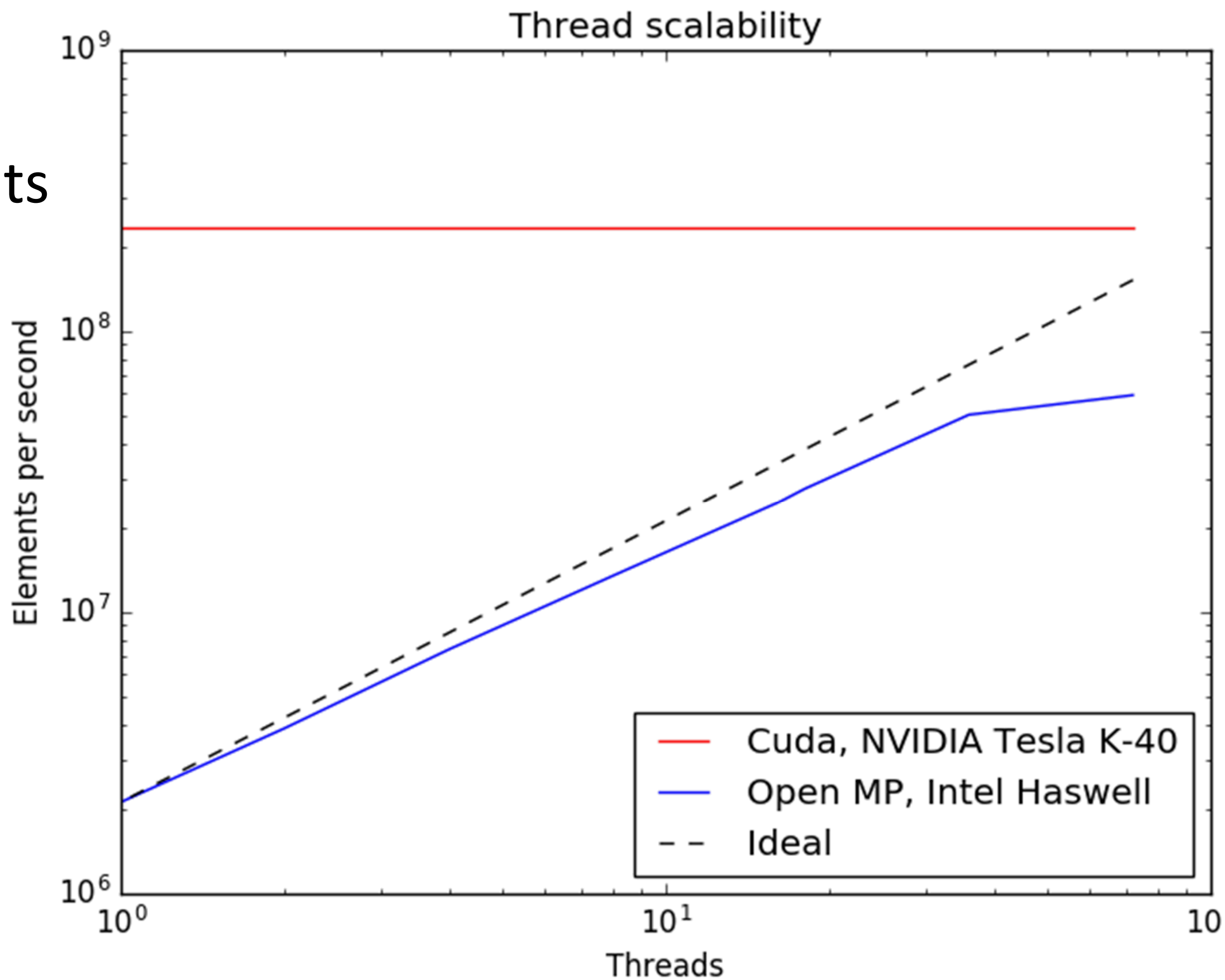
- Capable of capturing complex 3D crack patterns without explicitly representing crack geometry
- Predicts crack initiation, branching and coalescence all from a single thermodynamically consistent gradient damage model

# Brittle impact demonstration



# Thread scalable, platform portable

- Sandia's Kokkos library allows cross-platform, thread scalable implementations
- GPU: ~110 X faster
- 250 million elements per second
- OpenMP scales



# Why explicit gradient damage

- It’s trivially massively thread scalable!
- This is critical for future compute architectures
- Mesh modification, data movement and introducing new degrees of freedom on-the-fly is a huge hit to performance today and will get MUCH worse

# Inverse methods

Solve multiple “forward” prediction simulations in order to

- Design
- Calibrate properties
- Match observations/experiments

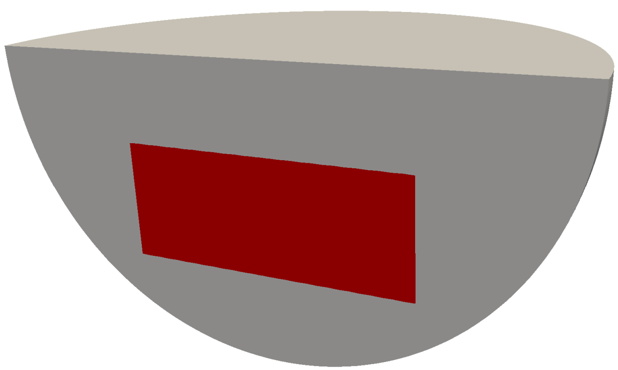
$$\min_{\boldsymbol{\theta}} g(\mathbf{u}, \boldsymbol{\theta})$$

Quantity of interest depends on

- physical solution $\mathbf{u}$
- design parameters $\boldsymbol{\theta}$

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

Constrained by the physics



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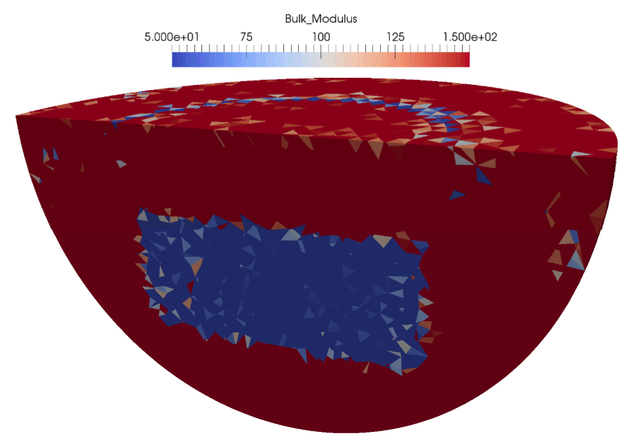


Reconstructed material properties due to observed surface displacements in Sierra-SD

# Why is this hard?

- Quantity must be differentiable function of the input parameters
- In many interesting cases, # of design variables is proportional to mesh resolution

**Fracture inverse examples:**

- **Non-destructive evaluation**: determine the damage at every material point given observations of how waves propagate (unknowns ~ # elements)
- **Crack forensics**: determine what happened to a structure that caused it to damage in an observed way (unknowns ~ # number of BCs time # timesteps)
- **Meta-material design**: how to design composite materials to maximize resistance to crack propagation (unknowns ~ # elements)

- The last two of these involve explicitly integrating nonlinear PDEs
- Without gradient information, these inverse problems are infeasible

# Review of the adjoint method

- Computing finite difference gradients requires many, many solves: O(#design parameter)
- Adjoint method requires just 1 additional solve!

Explicit update rule: $\mathbf{u}^n = \mathbf{h}^n(\mathbf{u}^{n-1};\theta)$

Quantity of interest: $g(\mathbf{u}^N;\theta)$

Desired sensitivities: $\dfrac{dg(\mathbf{u}^N;\theta)}{d\theta}$

$$\mathcal{L}(\mathbf{u},\boldsymbol{\lambda};\theta) = g\left(\mathbf{u}^N;\theta\right) + \sum_n \langle \boldsymbol{\lambda}^n, \mathbf{h}^n(\mathbf{u}^{n-1};\theta) - \mathbf{u}^n\rangle$$

$$\frac{d\mathcal{L}}{d\theta} = g_{,\boldsymbol{\theta}} + \langle g_{,\mathbf{u}}, \mathbf{u}^N_{,\theta}\rangle + \sum_n \langle \boldsymbol{\lambda}^n, \mathbf{h}^n_{,\theta} + \mathbf{h}^n_{,\mathbf{u}}\mathbf{u}^{n-1}_{,\theta} - \mathbf{u}^n_{,\theta}\rangle$$

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$$\frac{d\mathcal{L}}{d\theta} = g_{,\boldsymbol{\theta}} + \langle g_{,\mathbf{u}}, \mathbf{u}^N_{,\theta} \rangle + \sum_n \langle \boldsymbol{\lambda}^n, \mathbf{h}^n_{,\theta} + \mathbf{h}^n_{,\mathbf{u}} \mathbf{u}^{n-1}_{,\theta} - \mathbf{u}^n_{,\theta} \rangle$$

# Adjoint of discrete solution

Final condition: $$\boldsymbol{\lambda}^N = g_{,\mathbf{u}}(\mathbf{u}^N;\theta)$$

Adjoint update: $$\boldsymbol{\lambda}^n = \left(\mathbf{h}^{n+1}_{,\mathbf{u}}\right)^T \boldsymbol{\lambda}^{n+1}$$

Sensitivity: $$\frac{d\mathcal{L}}{d\theta} = g_{,\theta} + \sum_n \langle \boldsymbol{\lambda}^n, \mathbf{h}^n_{,\theta} \rangle$$

**Example:**

Explicit Newmark time integration

$$\begin{aligned}
\mathbf{u}^{n+1} &= \mathbf{u}^n + \Delta t\, \mathbf{v}^n + \tfrac{\Delta t^2}{2}\mathbf{a}^n \\
\mathbf{v}^{n+1/2} &= \mathbf{v}^n + \tfrac{\Delta t}{2}\mathbf{a}^n \\
\mathbf{a}^{n+1} &= \boldsymbol{\pi}^{n+1}(\mathbf{u}^{n+1}) \\
\mathbf{v}^{n+1} &= \mathbf{v}^{n+1/2} + \tfrac{\Delta t}{2}\mathbf{a}^{n+1}
\end{aligned}$$

Explicit adjoint

$$\begin{aligned}
\hat{\mathbf{a}}^{n+1/2} &= \hat{\mathbf{a}}^{n+1} + \tfrac{\Delta t}{2}\hat{\mathbf{v}}^{n+1} \\
\hat{\mathbf{u}}^{n} &= \hat{\mathbf{u}}^{n+1} + \hat{\mathbf{a}}^{n+1/2} \cdot \boldsymbol{\pi}^{n+1}_{,\mathbf{u}} \\
\hat{\mathbf{v}}^{n} &= \hat{\mathbf{v}}^{n+1} + \Delta t\, \hat{\mathbf{u}}^n \\
\hat{\mathbf{a}}^{n} &= \tfrac{\Delta t}{2}\hat{\mathbf{v}}^n
\end{aligned}$$

# 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

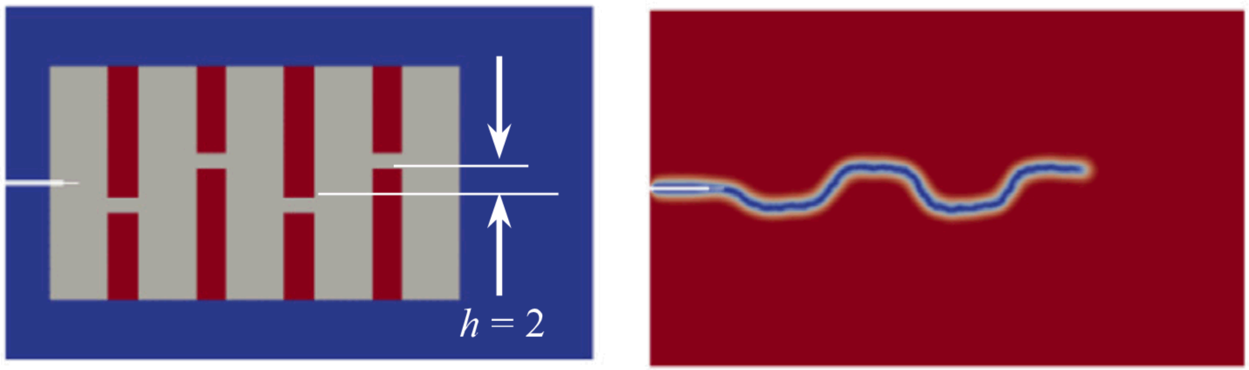
$$\min_{\boldsymbol{\theta}} \; g(\mathbf{u}, \boldsymbol{\theta})$$

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

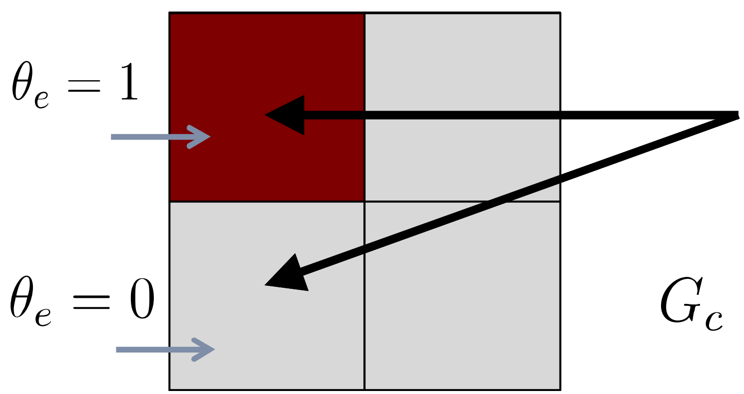
$\mathbf{u}$: state variables
$\boldsymbol{\theta}$: design parameters
$\mathcal{L}$: differential operator
$g$: quantify of interest

# Heterogeneous material design

- Hossain, Hsueh, Bourdin, Bhattacharya 2014 have shown phase field models of heterogeneous materials can exhibit higher toughness that constituent materials alone!



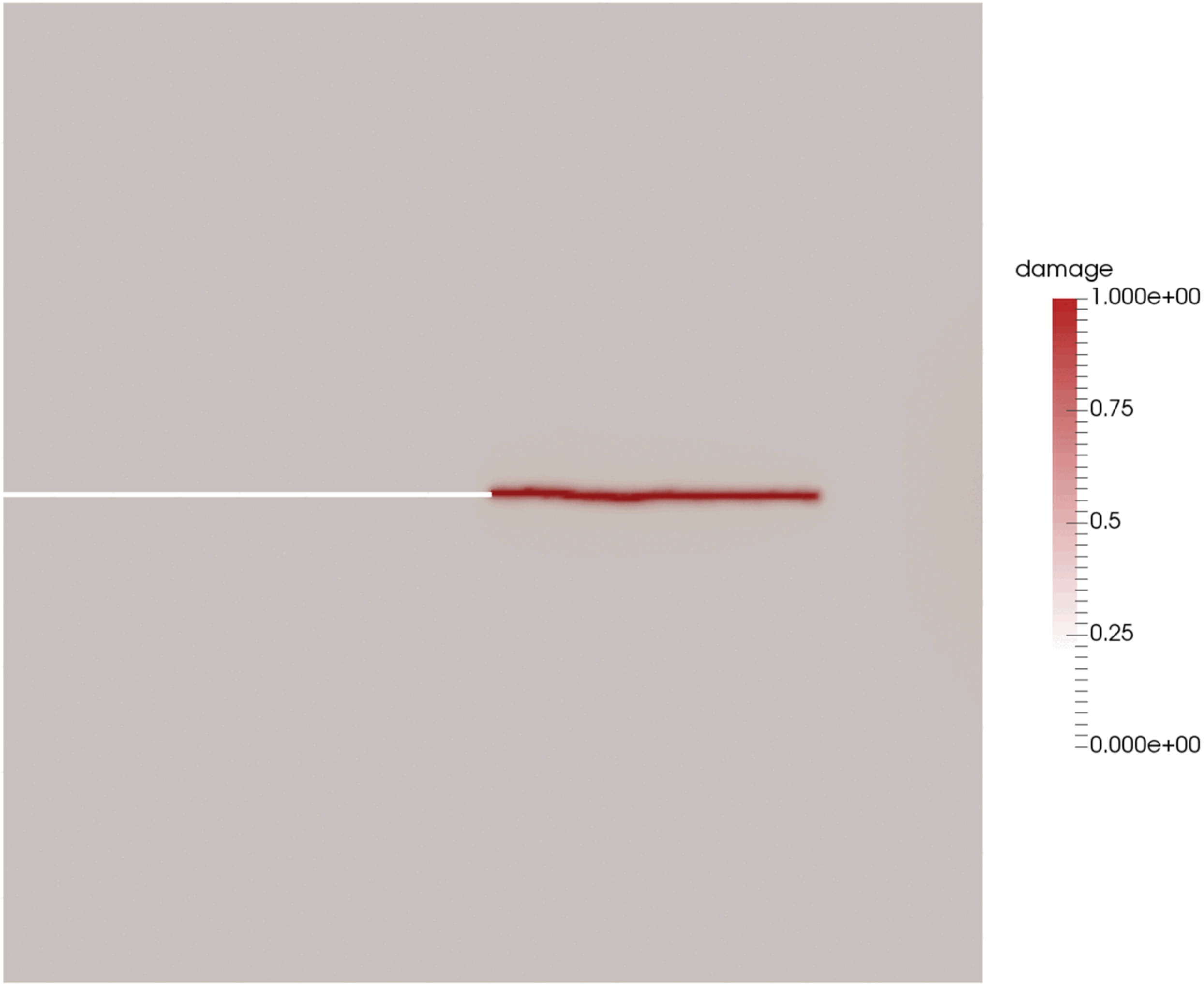

- Use inverse framework to automatically design tougher material



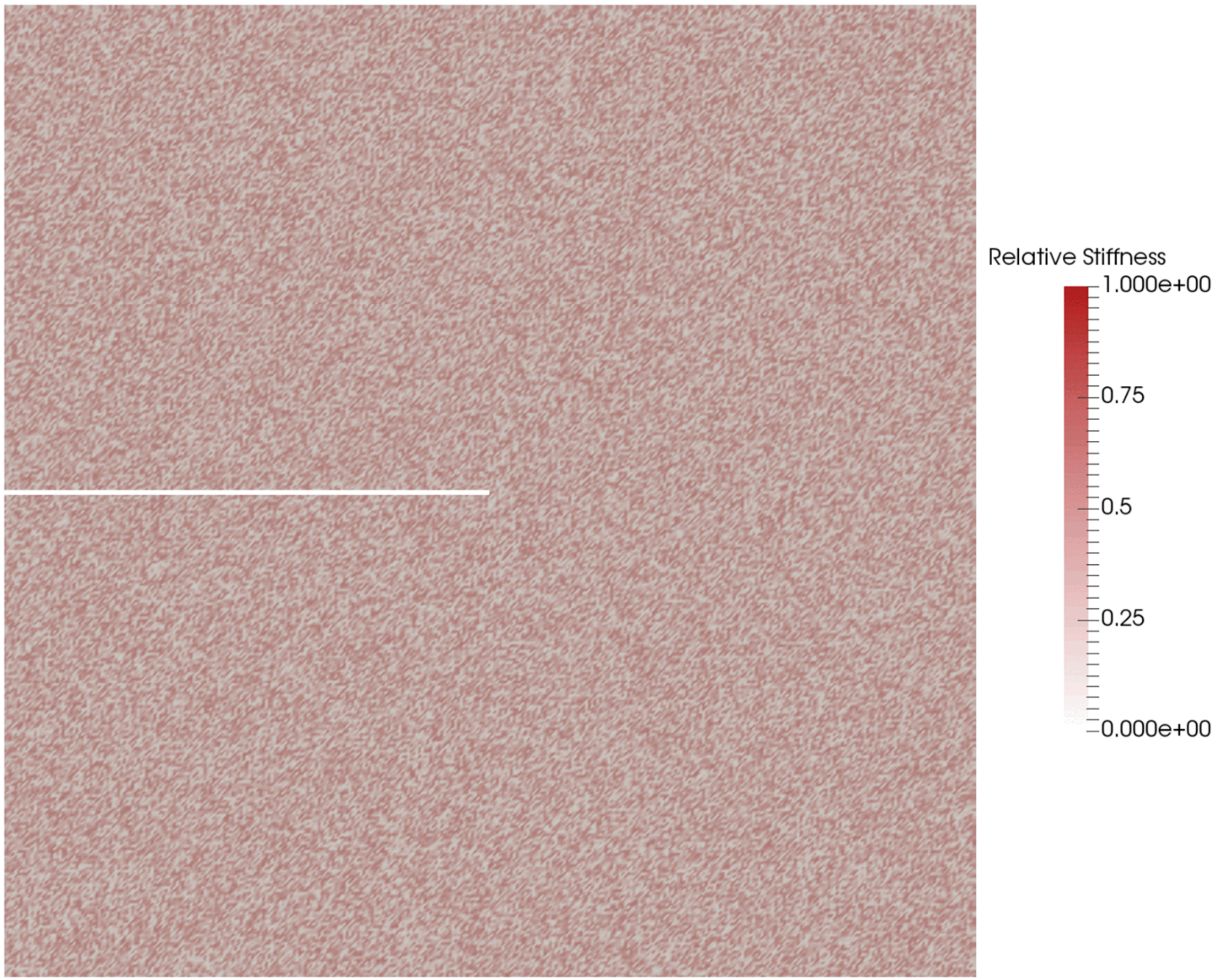

Allow each element to choose to be compliant or stiff : $\theta_e \in [0, 1]$

$$G_c = 4e5 \quad \rho = 8000 \quad E = 47.5e9 \text{ or } 190e9$$

# Minimize crack propagation



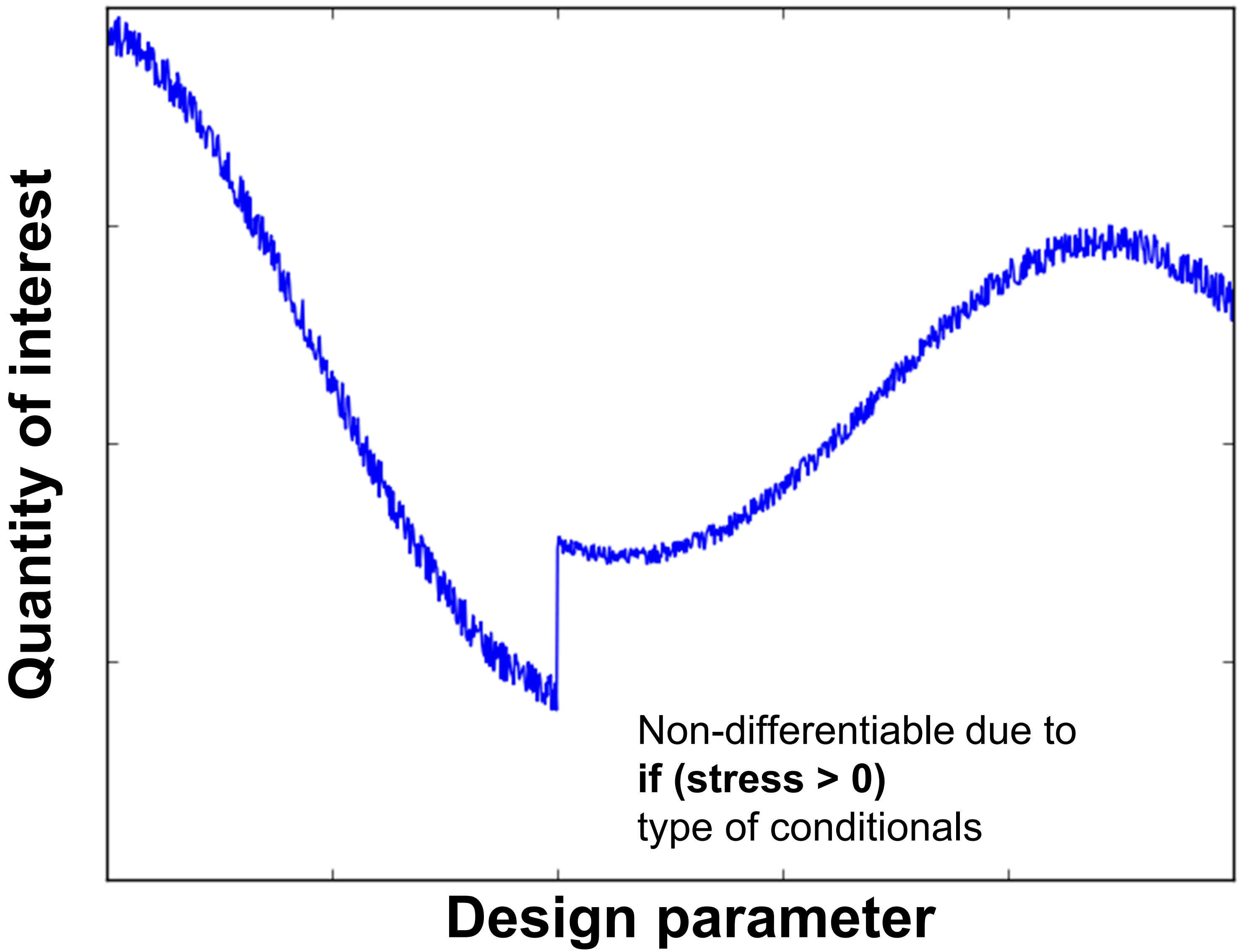
# Finding locally optimal design



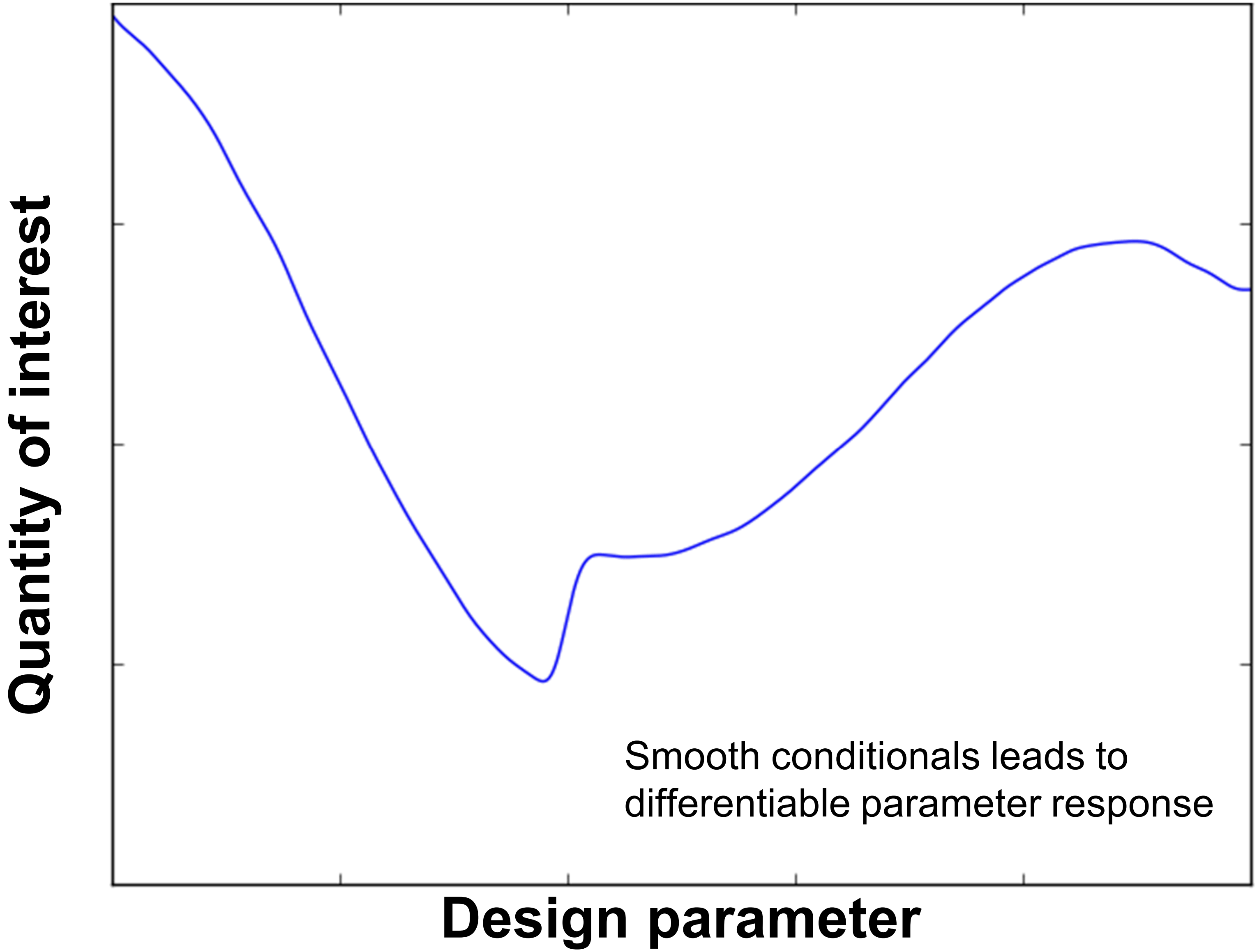

121801 design parameters

121801 gradient computed

# Non-smooth quantity of interest

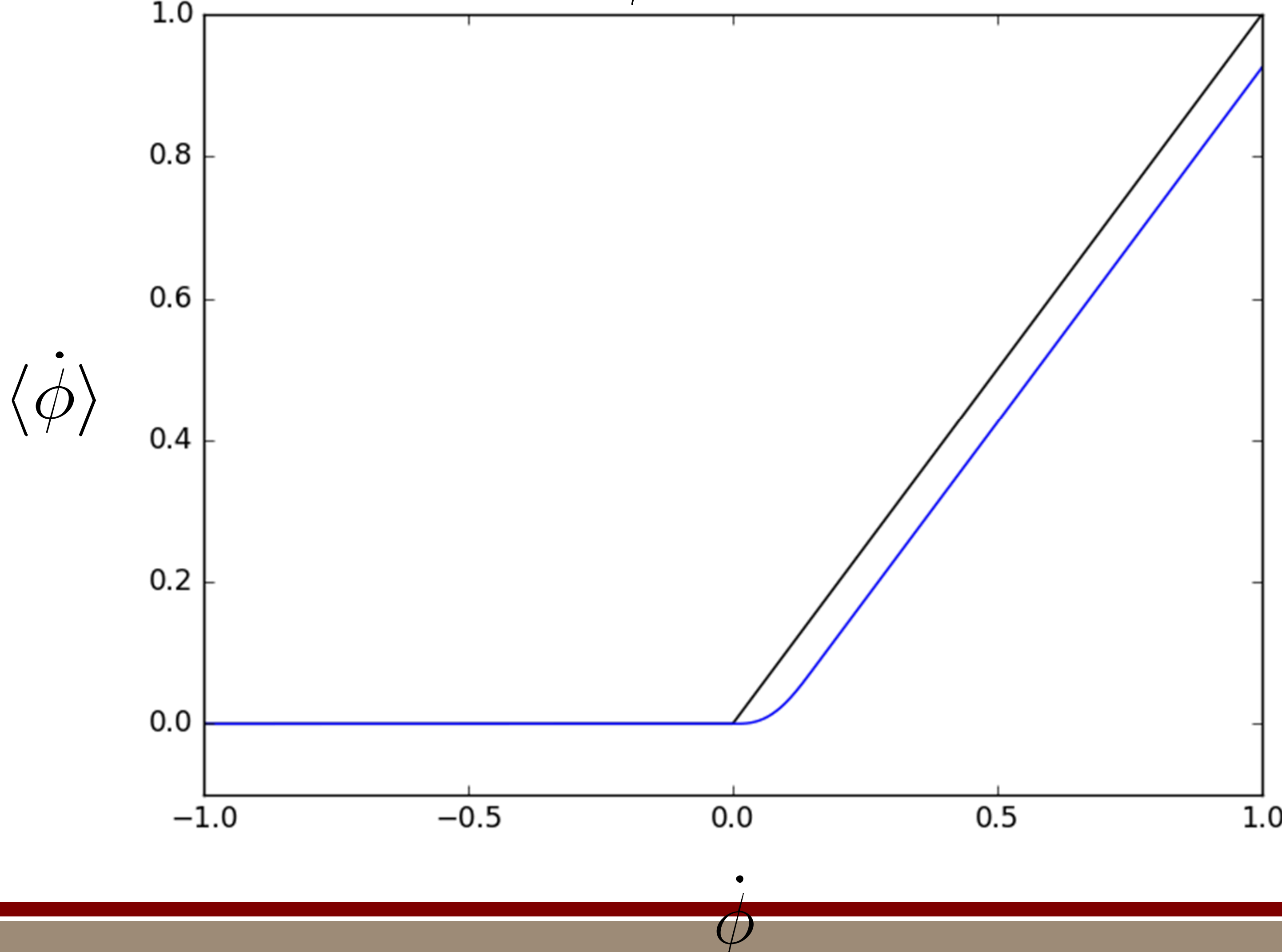


# Smoothed quantity of interest



# Differentiable approximation to

$$\dot{\phi} \geq 0$$



# 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

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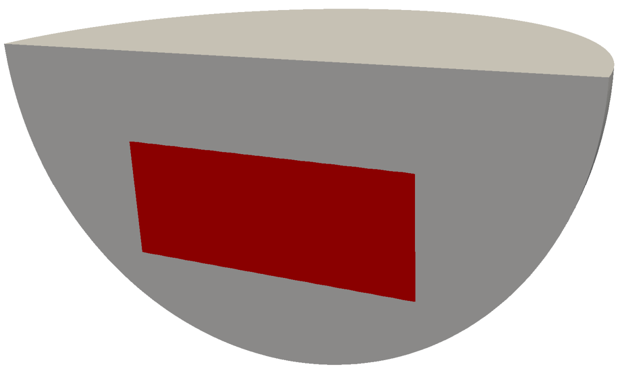
- Minimize discrepancy between observed displacements and simulated displacements by varying phase (volume fraction) element by element
- Sandia's ROL library used to perform the optimization



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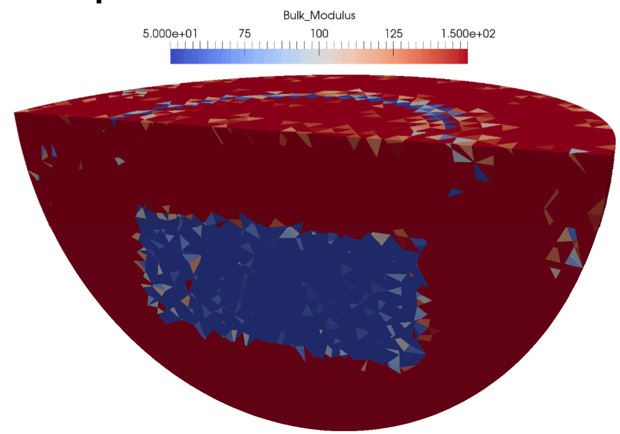
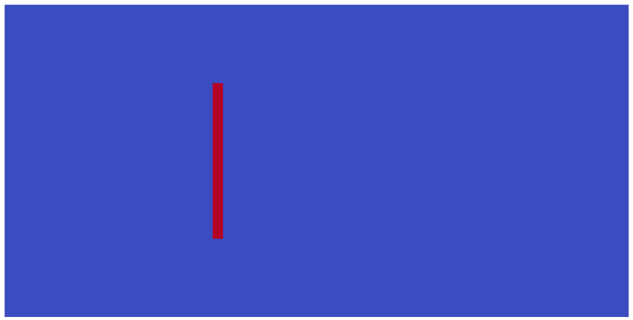
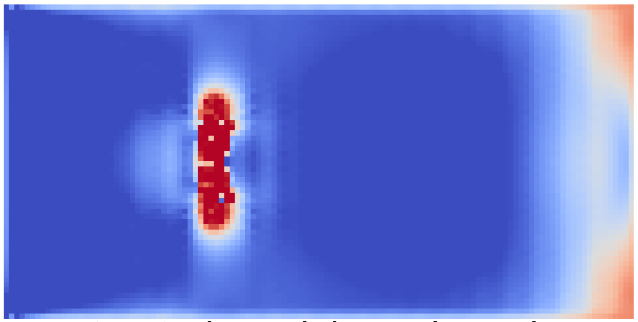



Reconstructed material properties due to observed surface displacements in Sierra-SD



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.

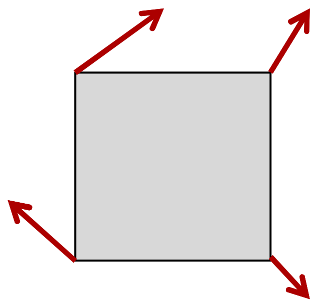
# Add up the savings

- Explicitly integrating damage: O(10X)
- Structured grid: O(2X)
- Linear kinematics: O(2X)
- 2D instead of 3D: O(2X)
- GPU instead of serial CPU: O(150X)
- Adjoint sensitivites: O(nElements / 10)

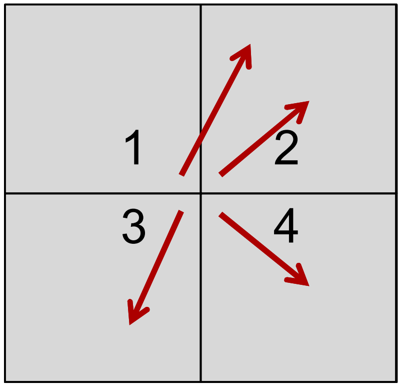
- For a 1,000,000 element simulation, these feature result in a saving of O(1e8)
- This takes us from the average human lifetime to a few minutes If one were doing mesh modifications (with the same number of elements), this factor would go up by a significant factor again

# Determinacy in a threaded world

- Computing adjoint for explicit dynamics requires checkpointing and re-computing solutions
- This makes run-to-run determinacy necessary
- Use data duplication:



Loop over element:
store all element forces



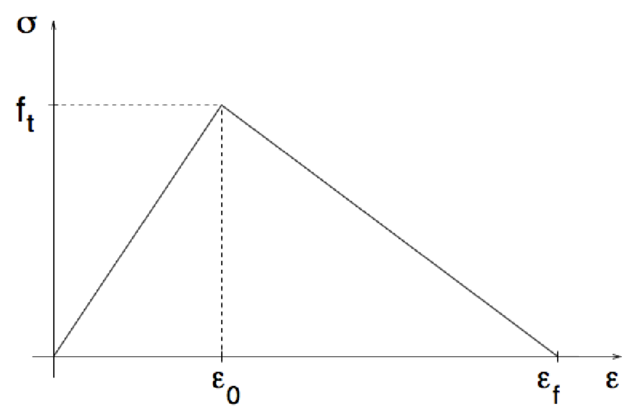

Loop over nodes:
sum forces in predetermined order

- Consider a purely local model of damage
- Stress-strain relationship

$$\sigma(x,t) = (1 - d(x,t))\mathbb{C}\,\epsilon(x,t)$$

- Strain-displacement

$$\epsilon(x,t) = \nabla^{s} u(x,t)$$



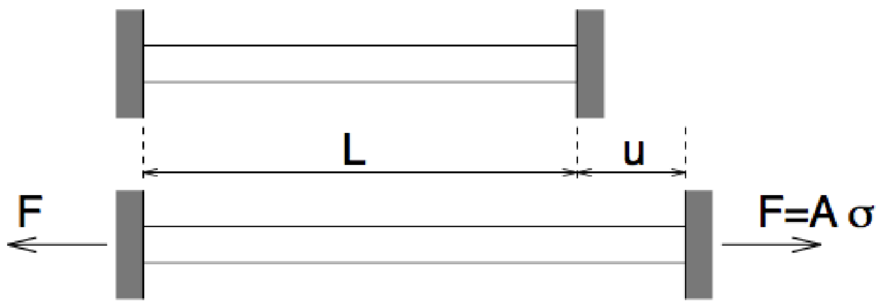

- Local state variable

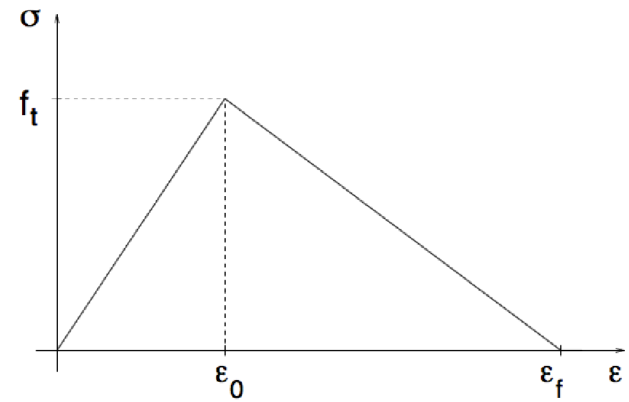
$$Y(x,t) = Y(\epsilon(x,t))$$

- Damage evolution

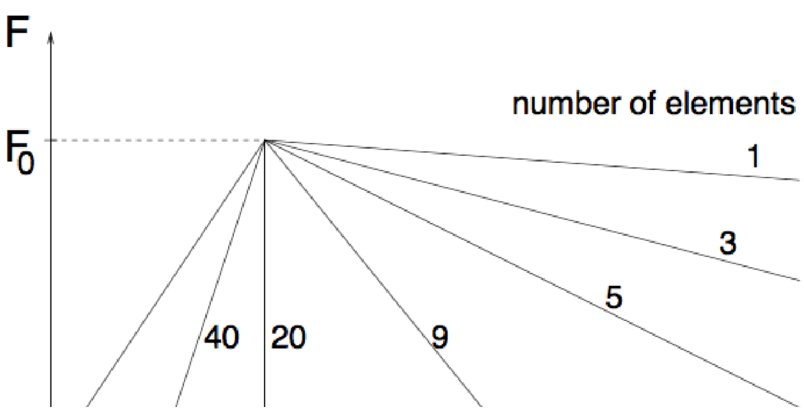
$$d(x,t) = D\left(\max_{\tau \le t} Y(x,\tau)\right) \qquad d(x,t) = \frac{Y_f}{Y_f - Y_0}\left(1 - \frac{Y_0}{Y}\right)$$

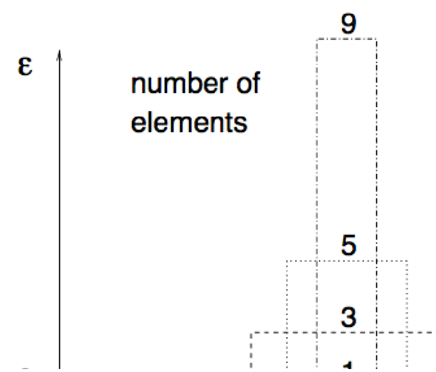
- Consider a 1D bar in tension (quasi-statics)




- Discretized with finite elements (from Jirasek, 2002):



- Basic idea: replace Y with a non-local version:

$$d(x,t) = D\left(\max_{\tau \le t} \tilde{Y}(x,\tau)\right)$$

- Integral-type models (Pijaudier-Cabot and Bazant, 1987) employ a non-local state variable, e.g.

$$\tilde{Y}(x,t) = \int_{V_x} \alpha(x,z)\, Y(z,t)\, dz$$

- Gradient-type models (de Borst et. al, 1995)

$$\tilde{Y}(x,t) - c\Delta \tilde{Y}(x,t) = Y(x,t) \quad \text{in } \Omega \qquad n \cdot \nabla \tilde{Y} = 0 \quad \text{on } \partial\Omega$$

- These two approaches are closely related (Huerta and Pijaudier-Cabot,

- Introduced by Rodriguez-Ferran et al. (2005)
- Stress-strain and strain-displacement:

$$\sigma(x,t) = (1 - d(x,t))C\epsilon(x,t) \qquad \epsilon(x,t) = \nabla^s u(x,t)$$

- Non-local displacement:

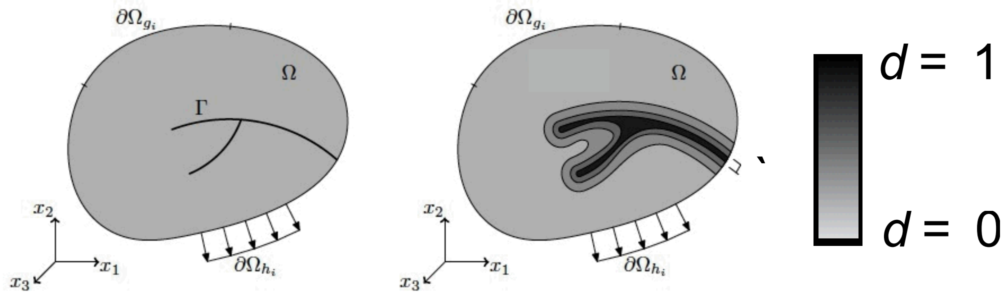
$$\tilde{u}(x,t) - c\Delta\tilde{u}(x,t) = u(x,t) \quad \text{in } \Omega \qquad \tilde{u} = u \quad \text{on } \partial\Omega$$

- Non-local strains and state variable:

$$\epsilon_{NL}(x,t) = \nabla^s\tilde{u}(x,t) \qquad Y_{NL}(x,t) = Y(\epsilon_{NL}(x,t))$$

- Damage evolution:

$$d(x,t)) = D\left(\max_{\tau \leq t} Y_{NL}(x,\tau)\right)$$

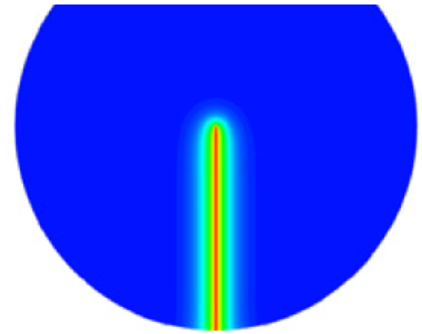



- Motivated differently from gradient damage
- Basic idea: replace the sharp discontinuity by a small, but finite zone with sharp gradients in a mathematically consistent manner with a crack-density functional

$$\Gamma \;\square\; \Gamma_l(d) = \quad \gamma_l(d, r\;\; d)\, dV$$

- Fracture energy (for brittle materials):

$$G_c\, dA \;\square\; \quad G_c\, \gamma_l\, dV$$



- Common crack-density functional:

$$\gamma_l = \frac{1}{2l} d^2 + \frac{l}{2} |\nabla d|^2$$

- Coincides with forms obtained in gamma-convergent regularizations of free-discontinuity problems (Ambrosio and Tortorelli, 1990).

- Minimization principle of diffusive crack topology

$$d(\mathrm{x}) = \arg \left\{ \inf_{d \in W} \Gamma_l(d) \right\} \qquad W = \{ d \,|\, d(\mathrm{x}) = 1 \text{ at } \mathrm{x} \in \Gamma \}$$

- Gives rise to Euler-Lagrange equation:

$$d - l^2 \Delta d = 0 \quad \text{in } \Omega \qquad \nabla d \cdot \mathrm{n} = 0 \quad \text{on } \partial\Omega$$

- Standard total potential energy (elastostatics)

$$\Pi_{pot}(\mathbf{u},\Gamma) = \int_{\Omega} \psi_e(\nabla^s \mathbf{u})\, dv + \int_{\Gamma} G_c\, da$$

- Phase field regularization

$$\Pi_l(\mathbf{u}, d) = \int_{\Omega} \left( g(d)\, \psi_e^+(\nabla^s \mathbf{u}) + \psi_e^-(\nabla^s \mathbf{u}) \right) dv + \int_{\Omega} G_c \gamma_l\, da$$

- Degradation function requirements

$$\begin{cases} g : [0,1] \to [0,1] \\ g'(d) < 0 \quad d \in [0,1] \\ g'(1) = 0 \end{cases} \qquad g = (1-d)^2$$

- Stress-strain response

$$\sigma(x,t) = (1 - d(x,t))\,C\,\varepsilon(x,t)$$

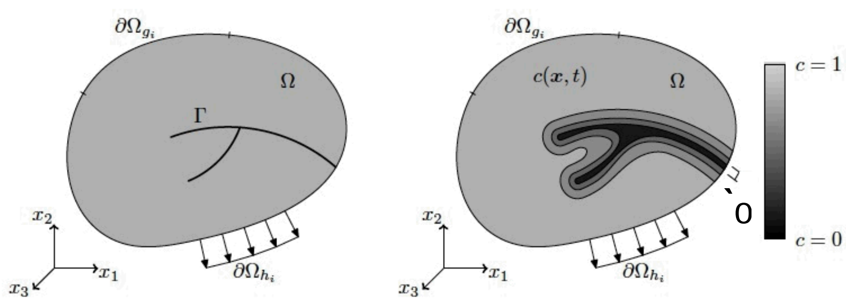
$$\sigma(x,t) = [(1 - d(x,t))^2 + k]\,C\,\varepsilon^{+}(x,t) + C\,\varepsilon^{-}(x,t)$$

- Non-local equations

$$\tilde{Y}(x,t) - c\Delta\tilde{Y}(x,t) = Y(x,t) \quad \text{in } \Omega$$

$$d\left(\frac{2lH(\varepsilon_e^{+})}{G_c} + 1\right) - l^2 \Delta d = \frac{2lH(\varepsilon_e^{+})}{G_c}$$

- Total potential energy




$$\Psi_{pot}(\mathbf{u},\Gamma) = \int_\Omega \psi_e(\nabla^s \mathbf{u})\, dv + \int_\Gamma G_c\, da$$

- Approximate the fracture energy with a crack density functional (Miehe et al. 2010)

$$\int_\Gamma G_c\, da \approx \int_\Omega G_c \Gamma_{c,\ell}\, dv \qquad \Gamma_{c,\ell} = \frac{1}{4\ell_0}\left[(c-1)^2 + 4\ell_0|\nabla c|^2\right]$$

- Implementation based on Borden et al. (2012)

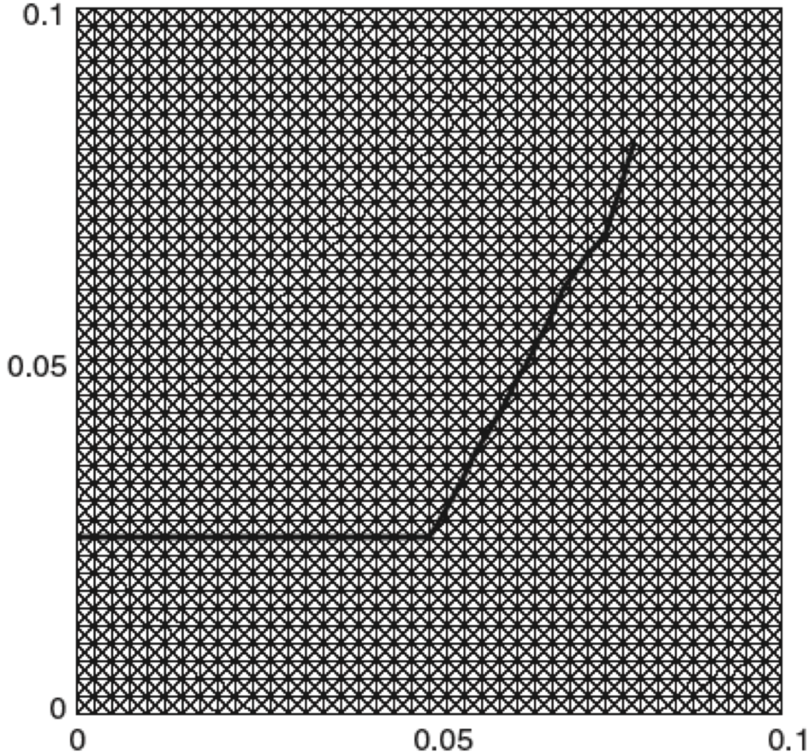
$$c = 1 - d$$

- Strong form for dynamics:

$$\frac{\partial \sigma_{ij}}{\partial x_j} = \rho \ddot{u}_i \quad \text{on } \Omega \times ]0, T[$$

$$\left[ \frac{4\ell_0 (1 - k) \psi_e^+}{G_c} + 1 \right] c - 4\ell_0^2 \frac{\partial^2 c}{\partial x_i^2} = 1 \quad \text{on } \Omega \times ]0, T[$$

$$\sigma_{ij} = [(1 - k)c^2 + k] \frac{\partial \psi_e^+}{\partial \varepsilon_{ij}} + \frac{\partial \psi_e^-}{\partial \varepsilon_{ij}}$$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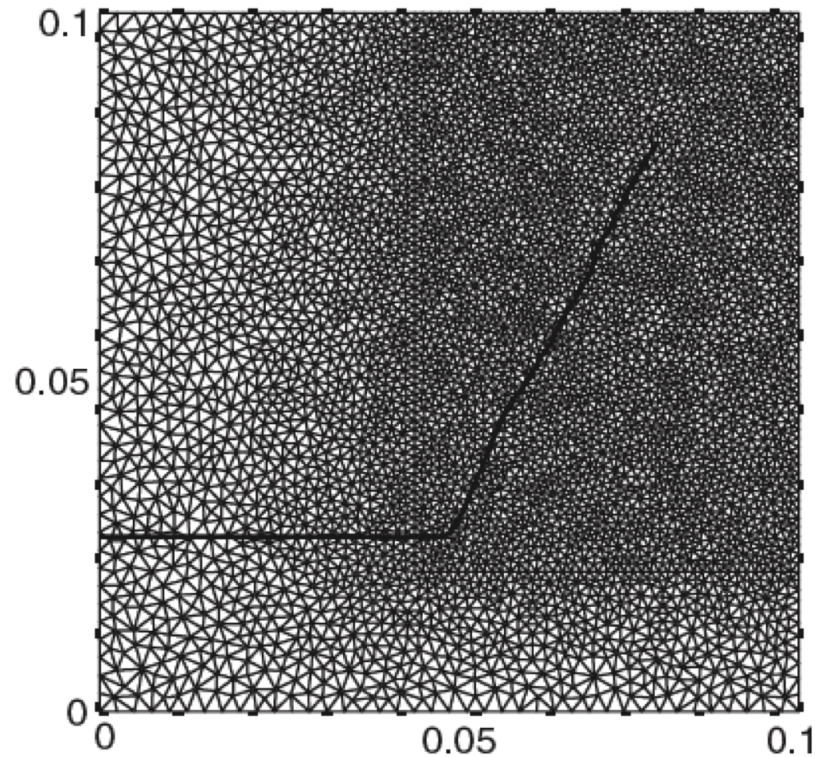
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