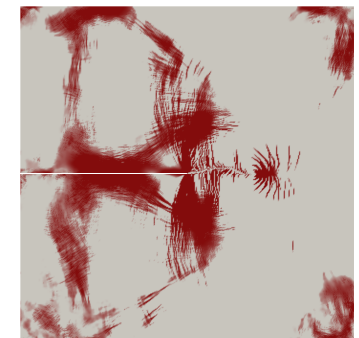
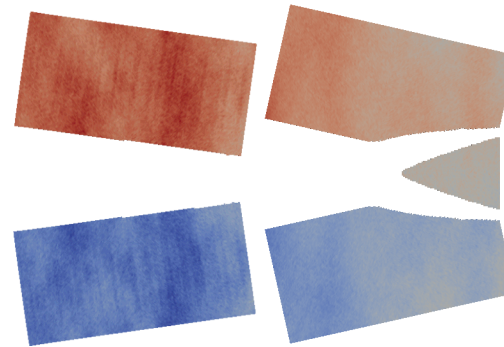
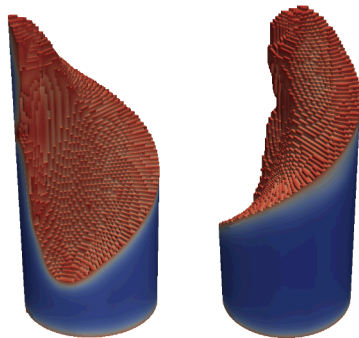


*Exceptional service in the national interest*

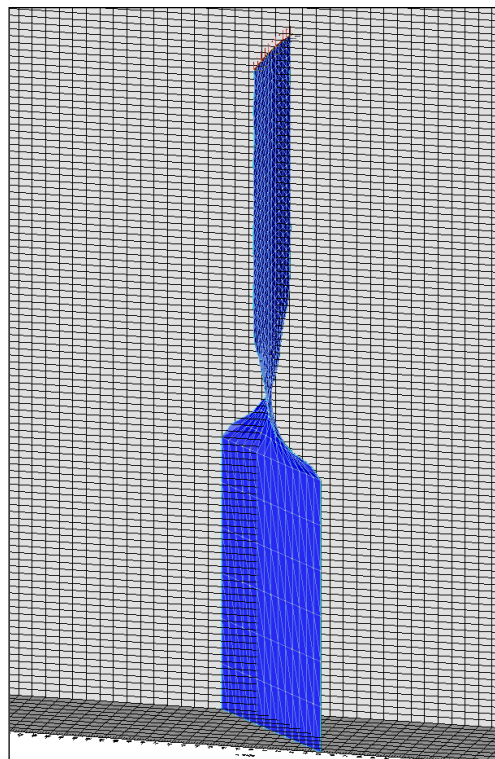


# Inverse methods for fracture based on a parabolic regularization of brittle cohesive laws

Michael Tupek

# Fracture Renaissance

- Several promising fracture methods have emerged in recent years



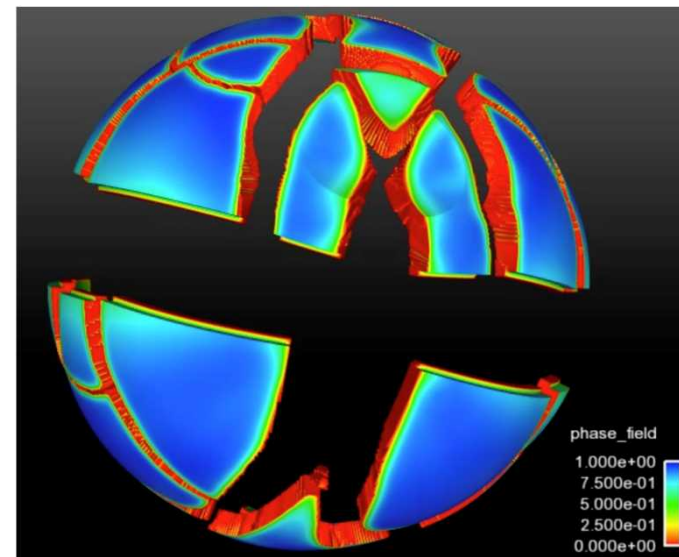
Duarte 2011

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

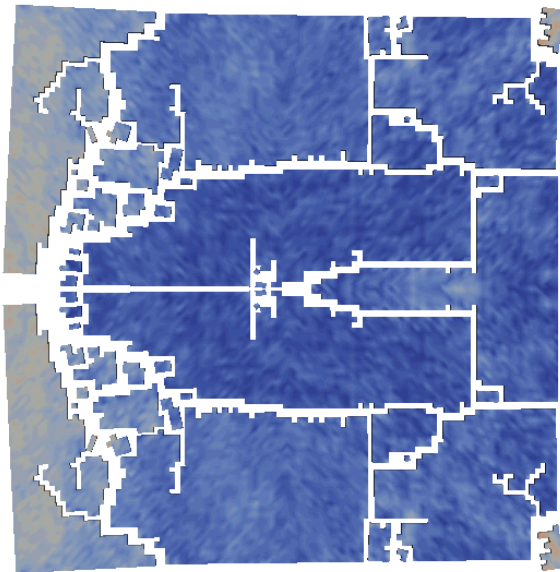
**inverse = predictions → decisions**

# Forward Problem: Phase Field Fracture

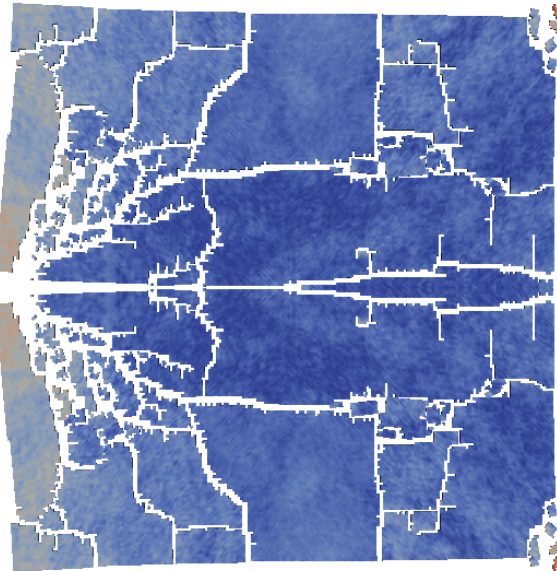
# Classical damage models: ill-posed

- 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

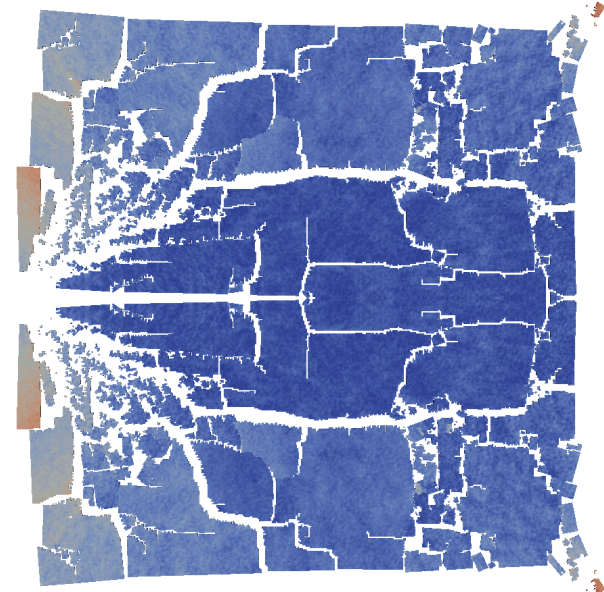
Max principal stress criterion with element death shows significant mesh dependence



Coarse mesh

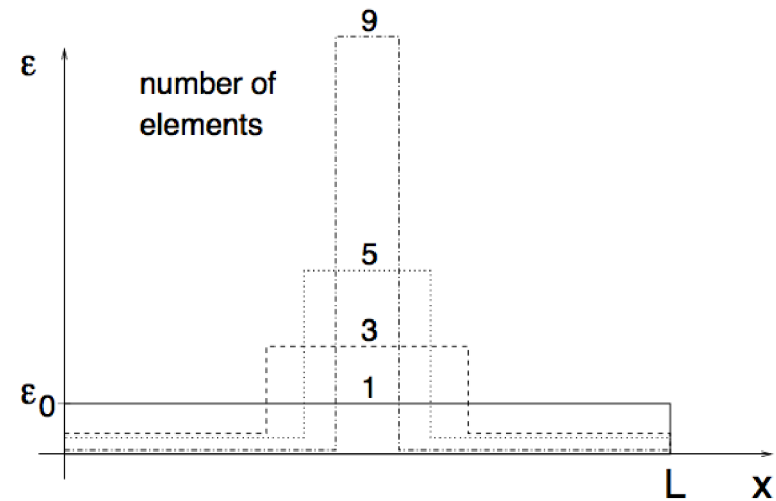
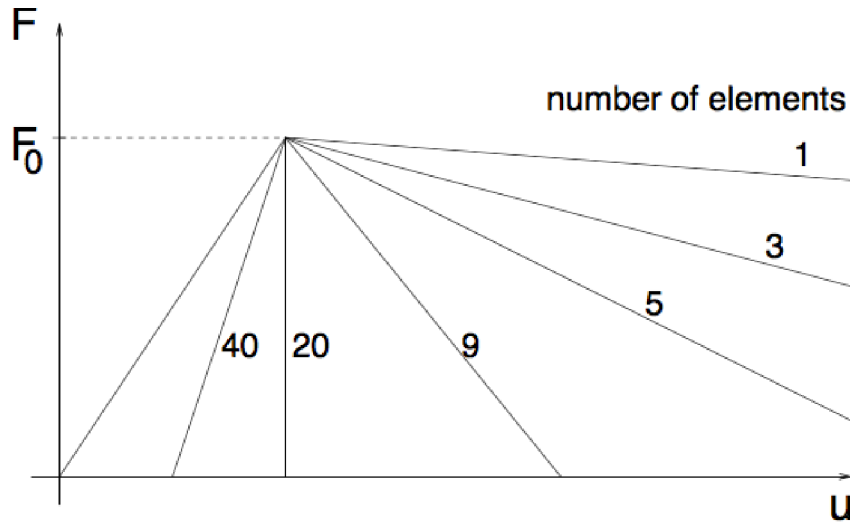
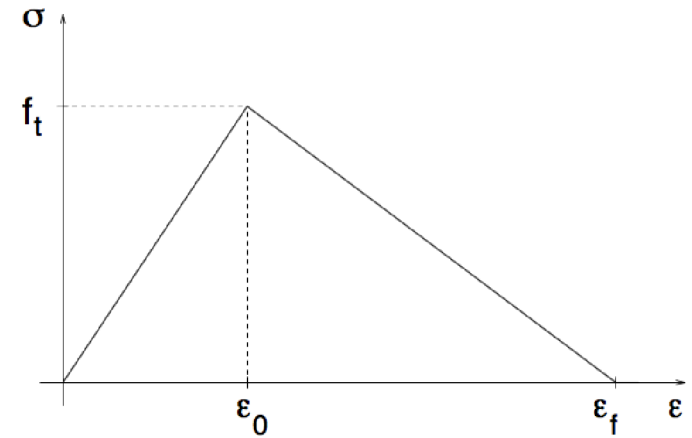
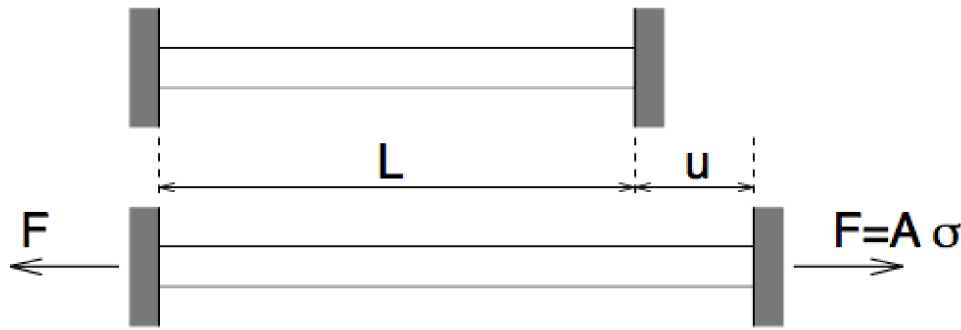


Medium mesh



Fine mesh

# Classical damage models: non-convergent



# Phase field fracture

Standard potential energy:

$$pot(u, \Gamma) = \int_{\Omega} e(r^s u) dv + \int_{\Gamma} G_c da$$

Approximate surface integral by a volume integral

Elliptically regularized potential energy:

$$I(u, d) = \int_{\Omega} (g(d) + e(r^s u) + \bar{e}(r^s u)) dv + \int_{\Omega} G_c \gamma_l d \varepsilon$$

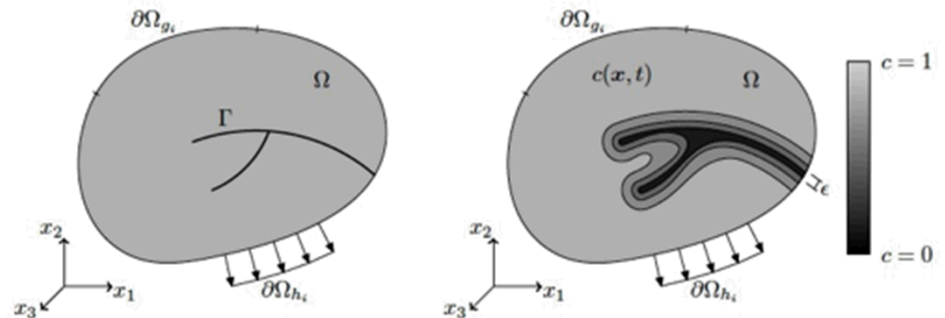


Common crack density:

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

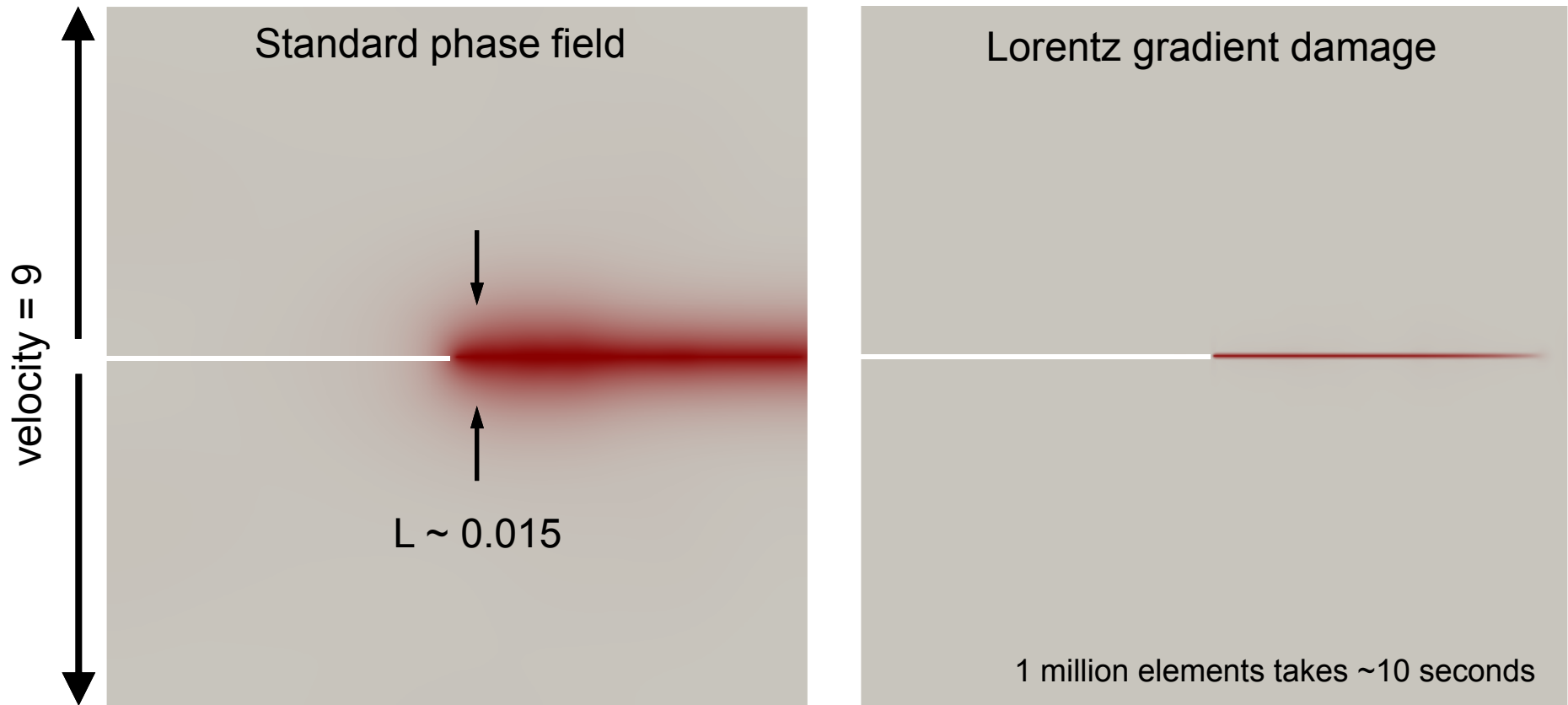
Stress degradation:

$$g = (1 - d)^2$$



# Limitations to standard phase field

- No threshold, some damage for any  $\varepsilon \neq 0$
- Regularization length scale tied directly to fracture properties  $\sigma_{\max} = \frac{9}{16} \sqrt{\frac{EG_c}{6L}}$



$$\sigma_{\max} = 250e6 \quad G_c = 100e3 \quad E = 200e9$$

# Cohesive gradient damage model

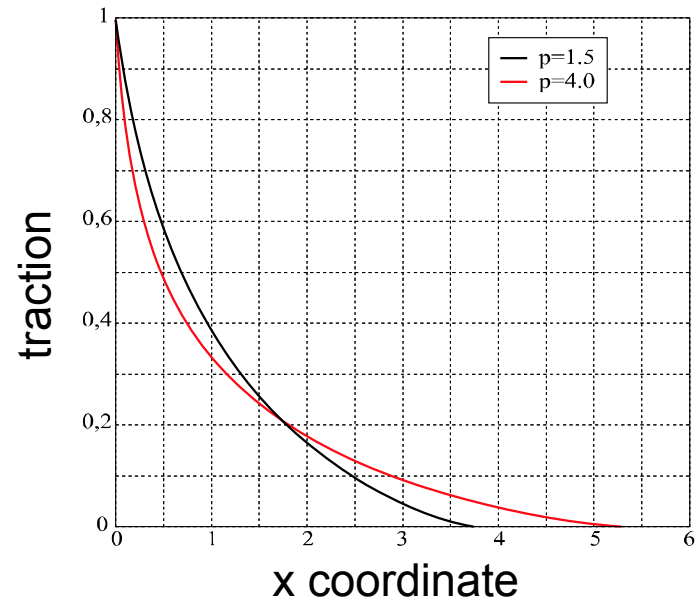
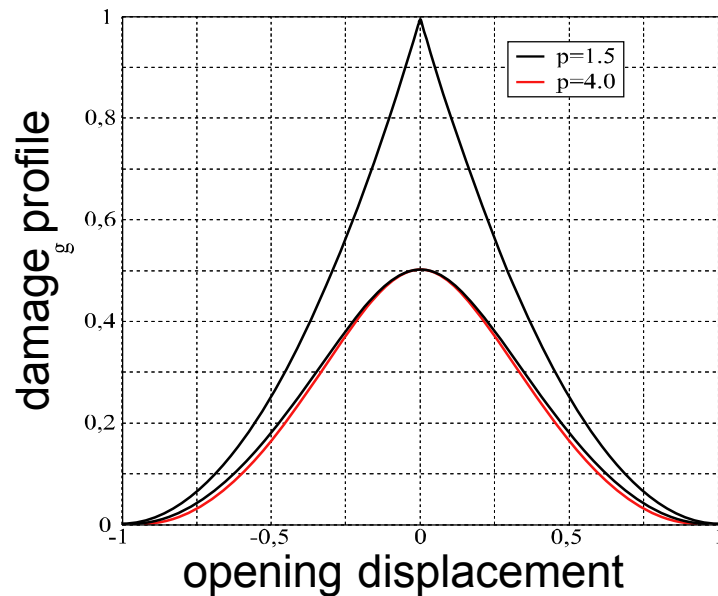
- Regularized gradient damage model by Lorentz, et al. 2011
- Shown to converge to cohesive zone model as  $L \rightarrow 0$

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

$$g'(\phi) \psi_e^+ + k = c \nabla^2 \phi \quad \text{Phase field equation}$$

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

Derivable from a phase potential



# Parameters of damage model

Depends on cohesive fracture parameters:

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

Note: the fracture energy,  $G_c$ , is ignored in most damage models

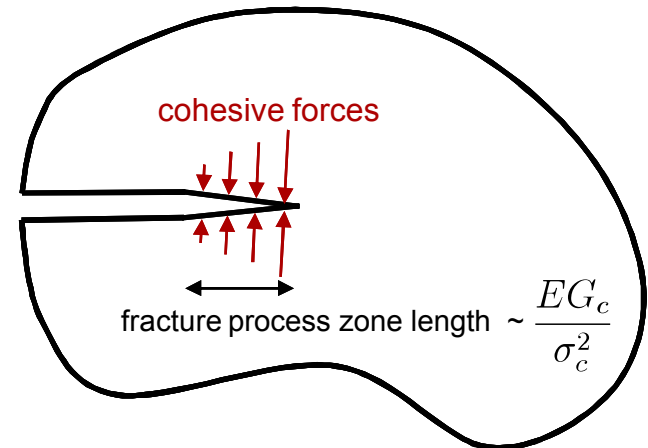
Physically justified constraints on the parameters ensures

- Regularization length scale 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)

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

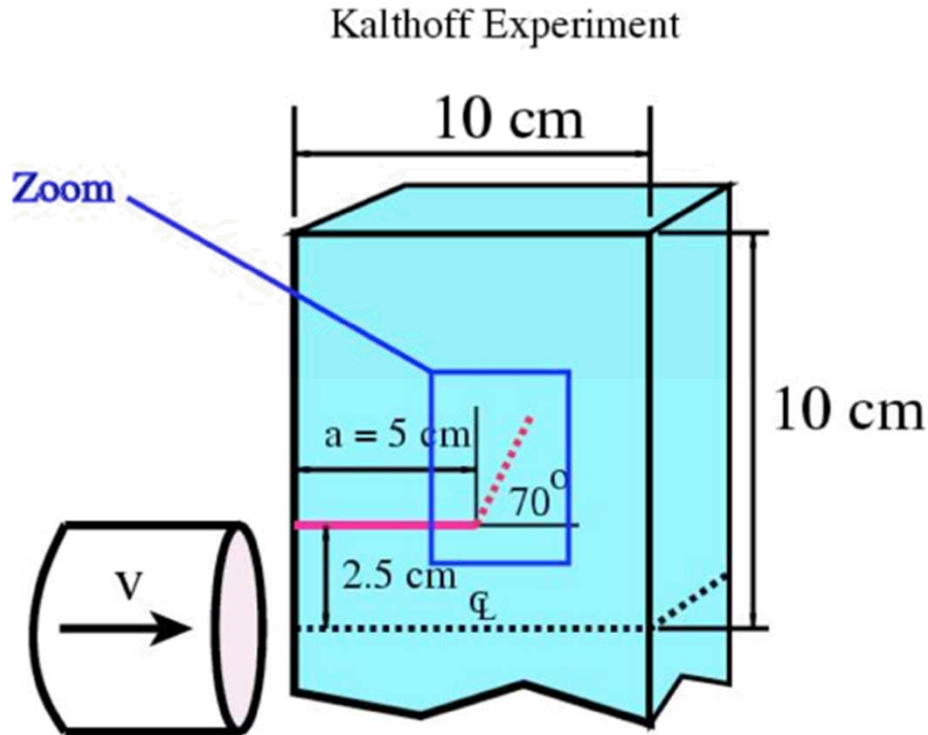
- Integrate parabolic equation explicitly!

- Hyperbolic timestep constraint:  $\Delta t \leq \frac{1}{s} \Delta x$

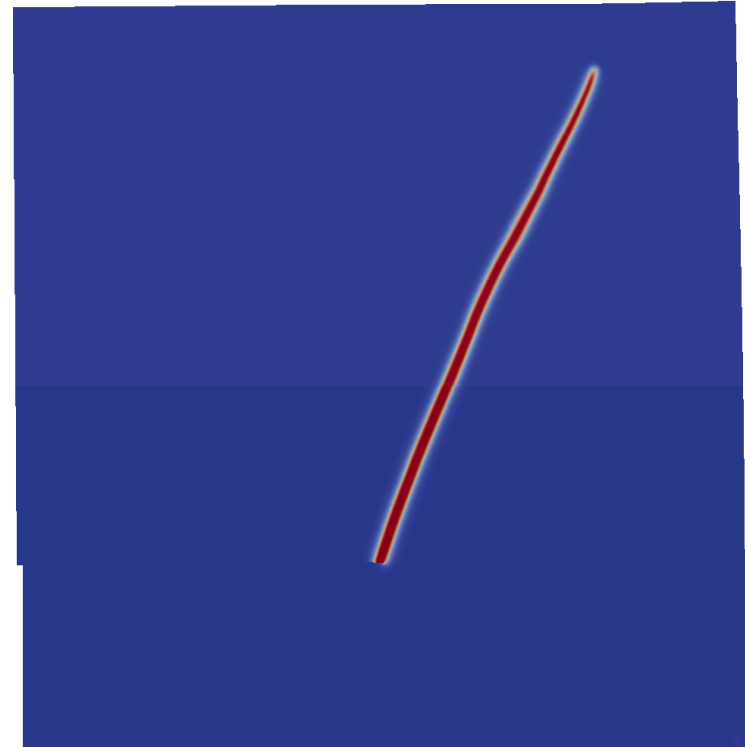
- Parabolic timestep constraint:  $\Delta t \leq \frac{\eta}{c} (\Delta x)^2$

- Can use hyperbolic timestep if:  $\eta \geq \frac{c}{s \Delta x} = \frac{3}{8} \frac{G_c}{s} \frac{L}{\Delta x}$

# Kalthoff validation



Damage contour

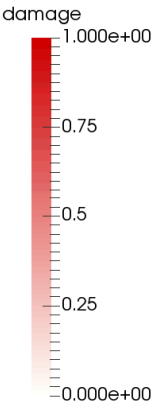
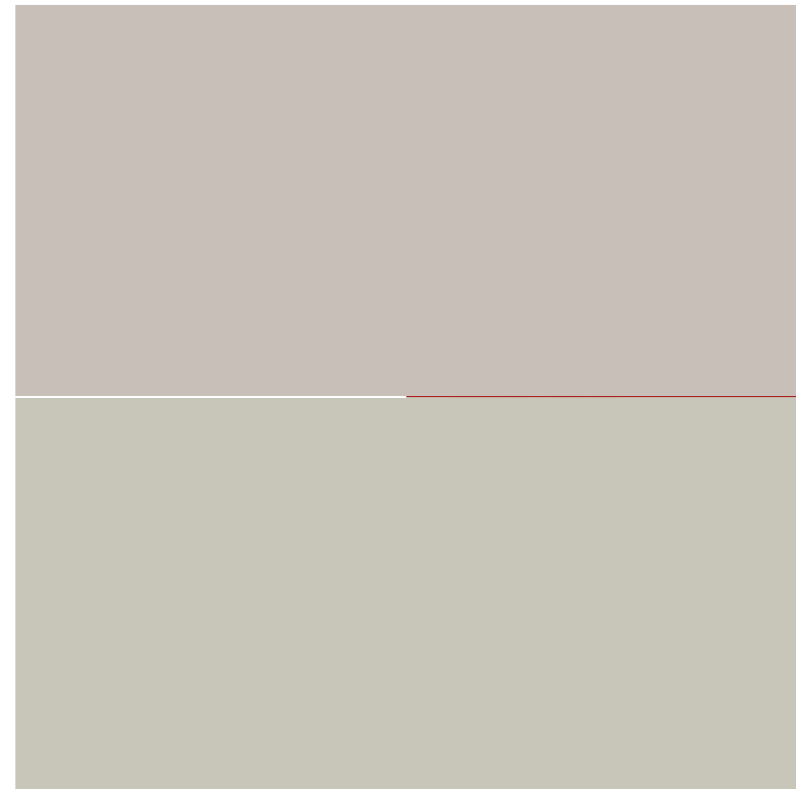
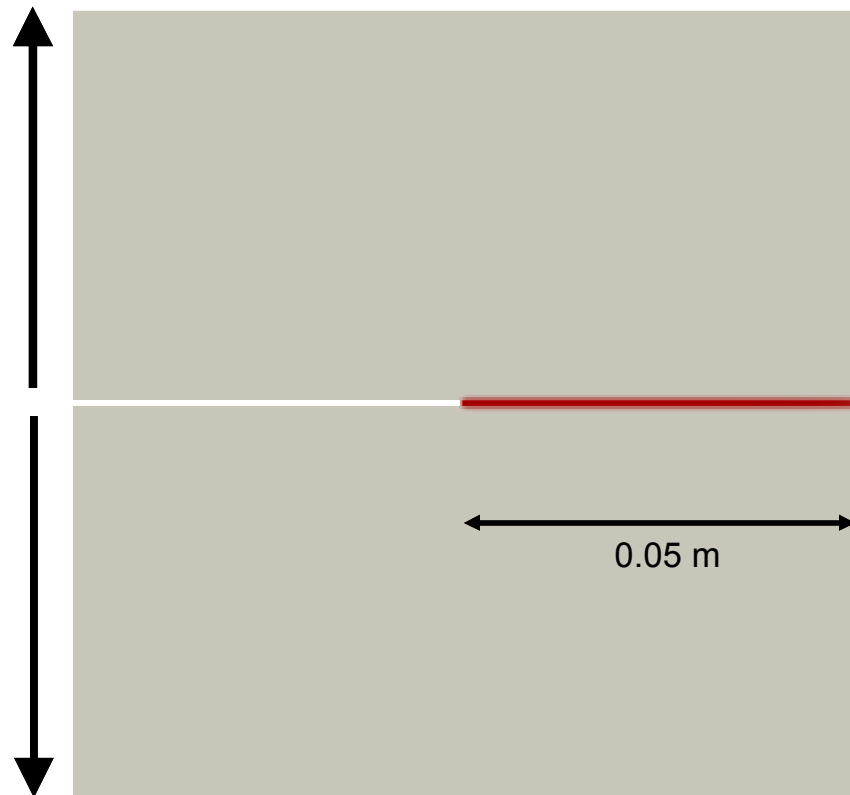


Achieves the expected crack propagation angle:  $\sim 70^\circ$

# Mode-I: Length scale refinement

Length-scale decreases with  $\Delta x$

$v = 25 \text{ m/s}$



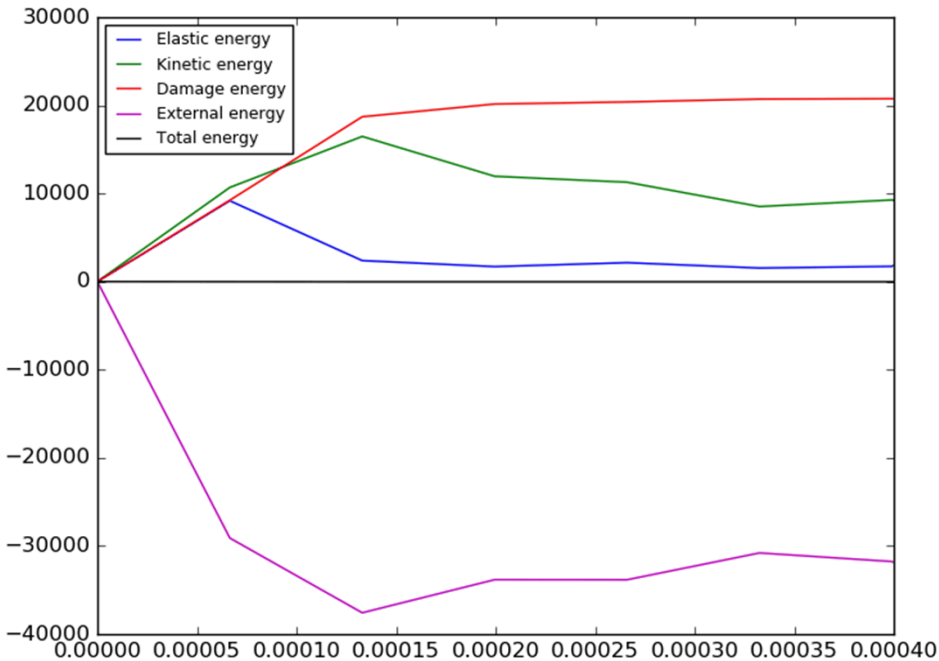
71.5 thousand elements

14.4 million elements

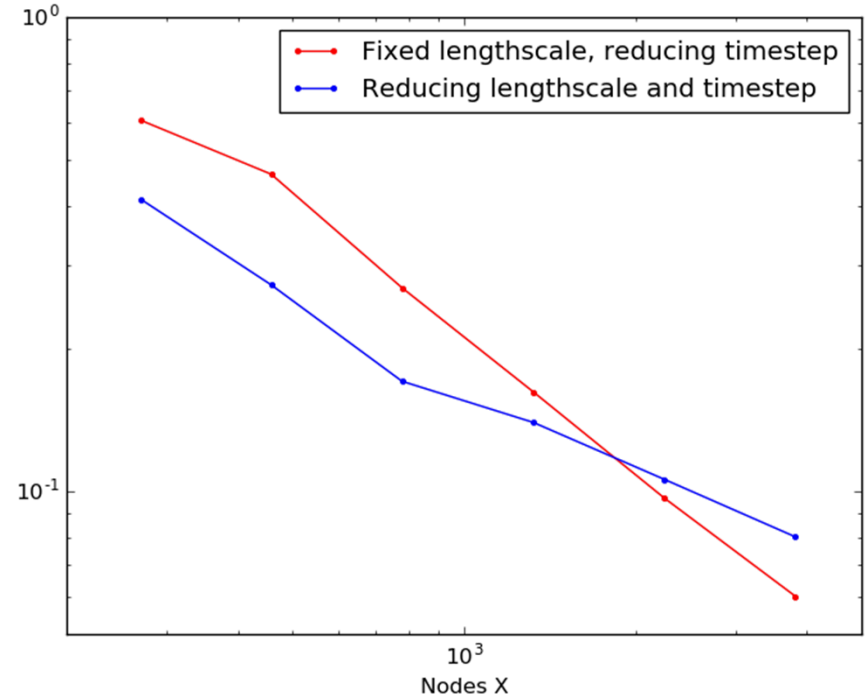
$G_c = 4\text{e}5$

# Accuracy

## Total numerical energy is preserved



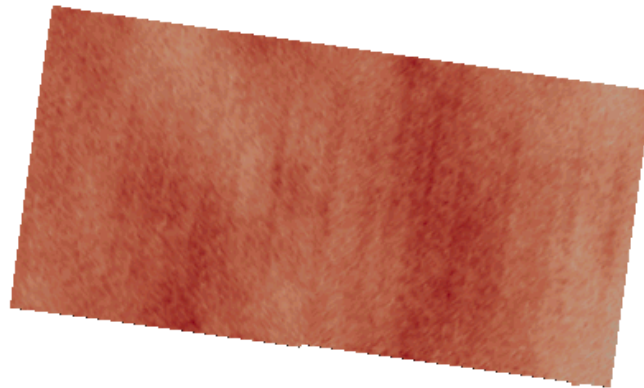
## Dissipated fracture energy error



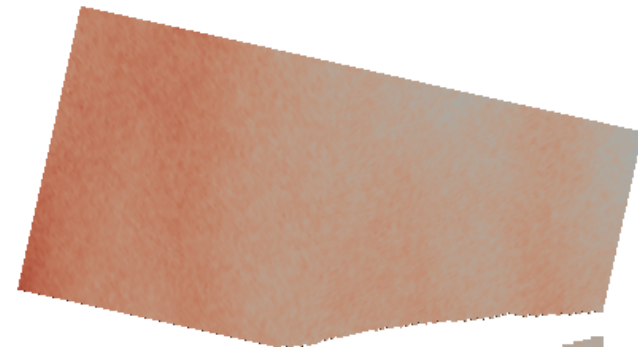
- Convergence rate of  $\sim 1$  for fixed length scale
- Convergence rate of  $\sim 0.5$  otherwise
- Dissipation due to viscous regularization is non-negligible

# Importance of fracture energy

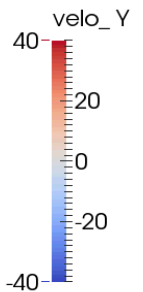
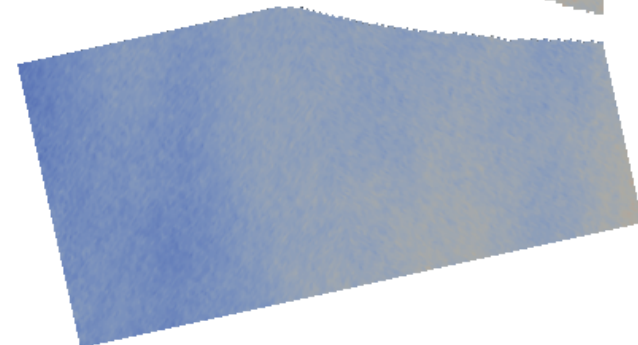
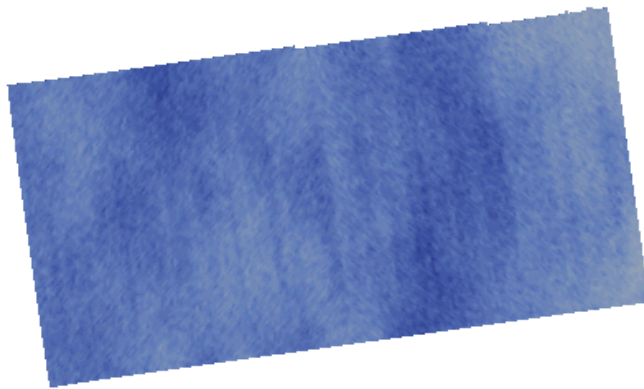
Mode-I crack transition to branching



High  $G_c$

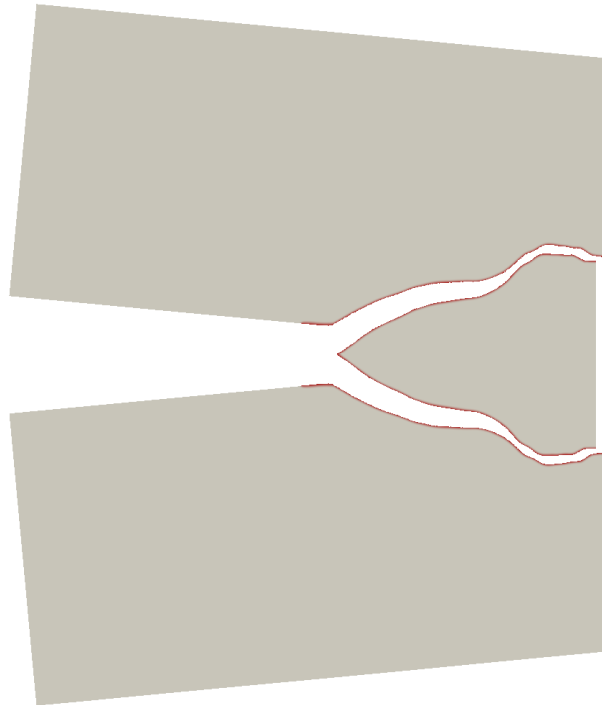


Low  $G_c$

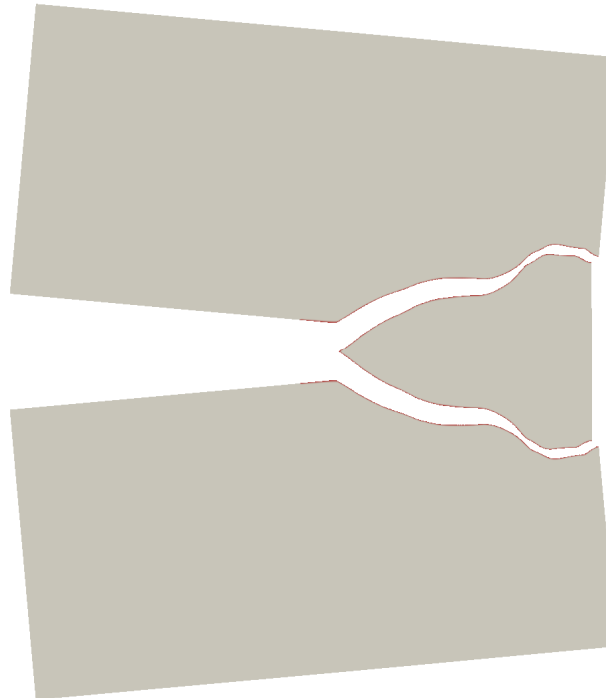


Branching is emergent, not prescriptive

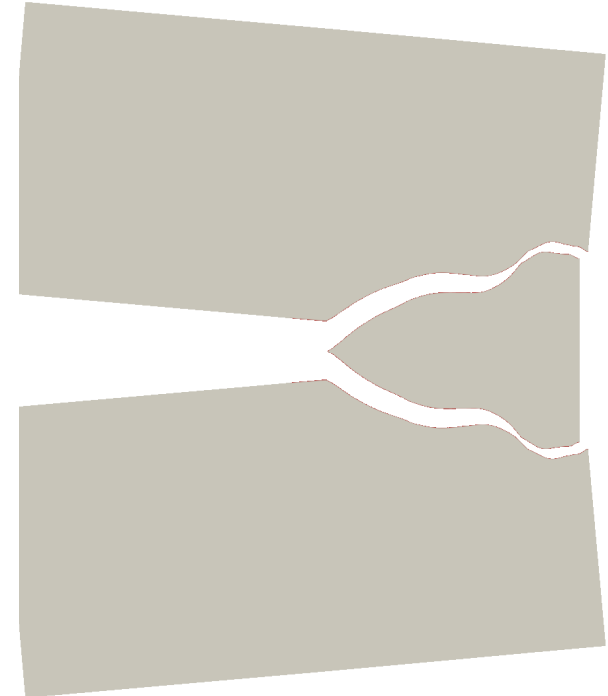
# Branching: mesh insensitivity



1.4 million elements



4.1 million elements



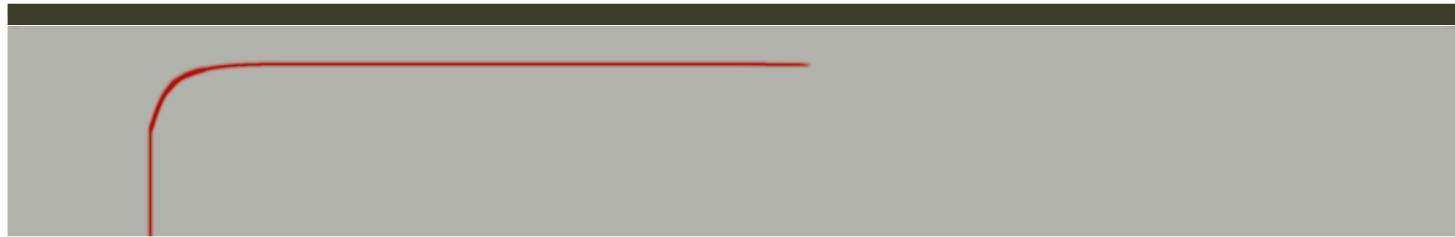
11.8 million elements

Runs in ~5 hours on 1 GPU

# Thermally loaded glass-metal interface



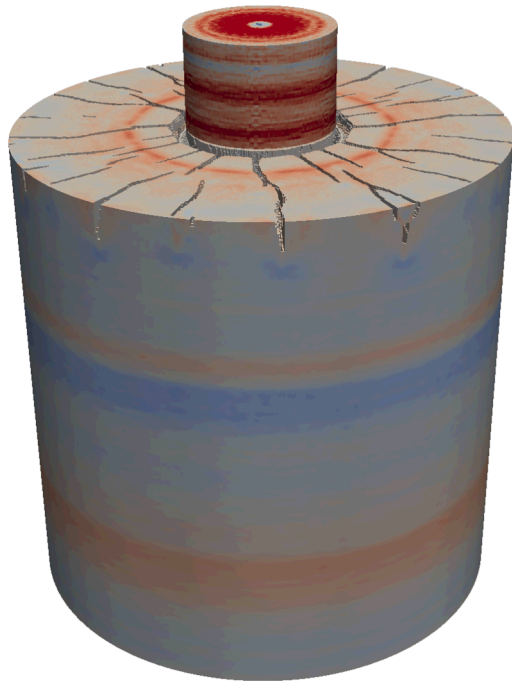
Experimentally observed crack path



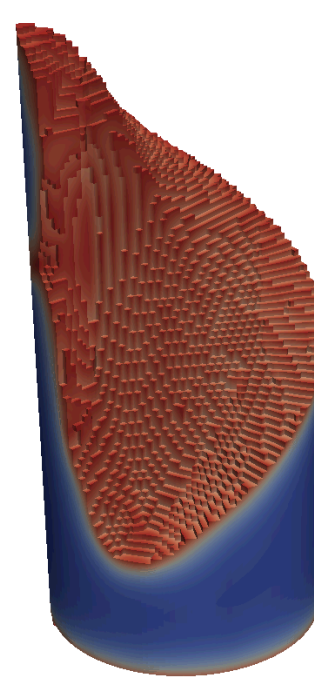
1.5 million element simulation runs in 6 hours on 1 GPU

- Loaded by temperature drop
- Metal on top contracts relative to glass below
- Initial vertical crack propagates upward
- Eventually turns to run parallel to the glass-metal interface

# Demonstrations in 3D



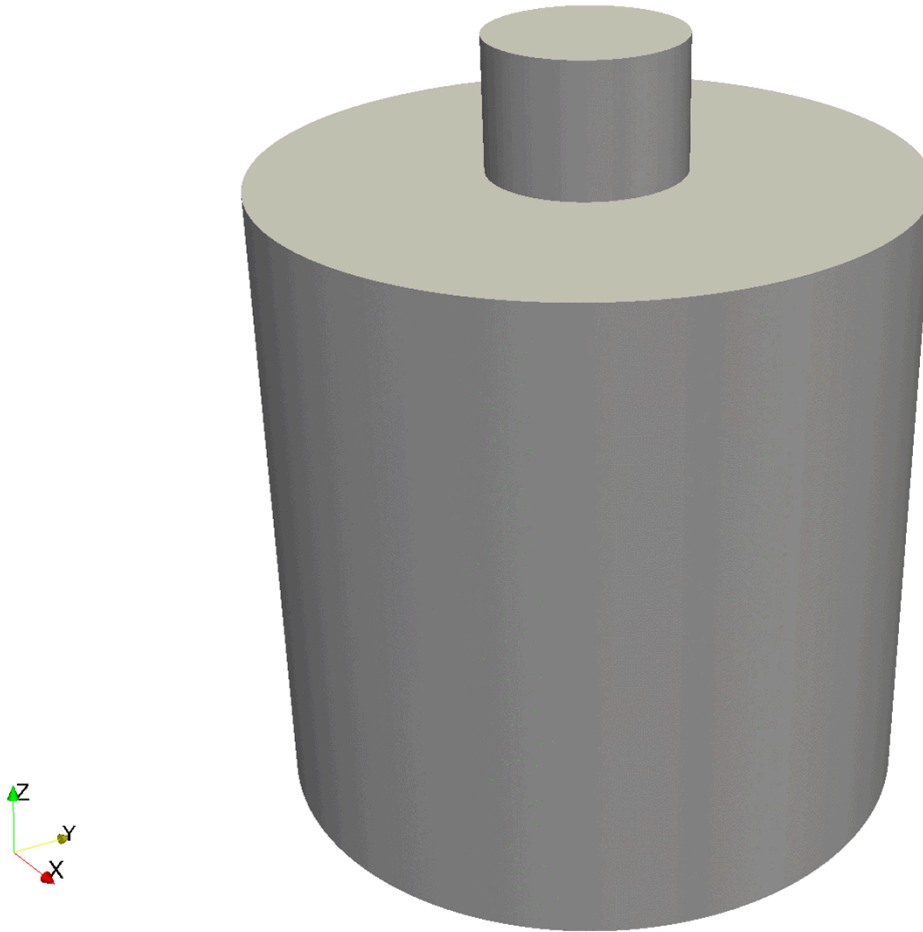
Ceramic impact



Brittle torsion fracture

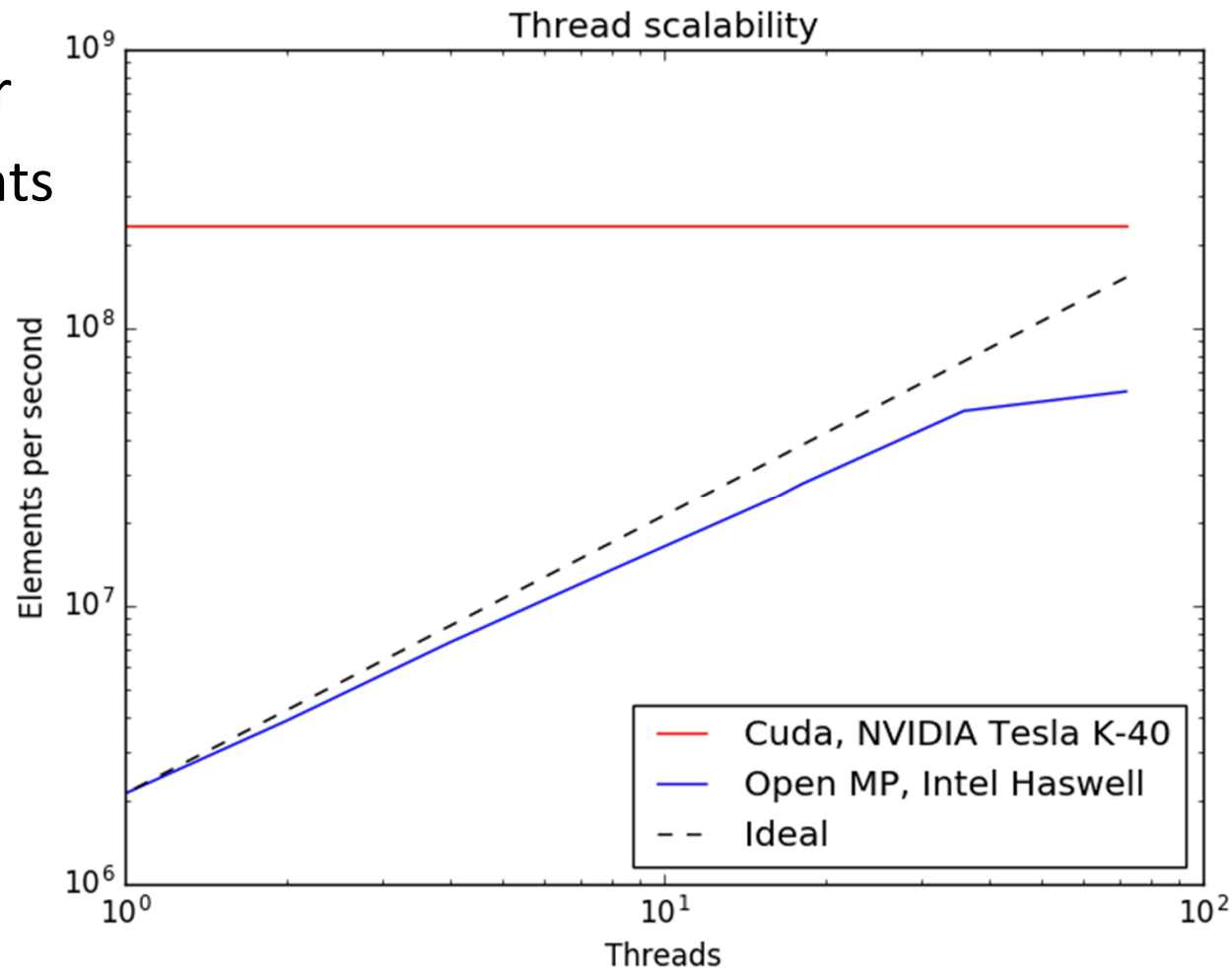
- Captures complex 3D crack patterns
- No explicit geometry representation
- Naturally predicts initiation, branching and coalescence

# 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



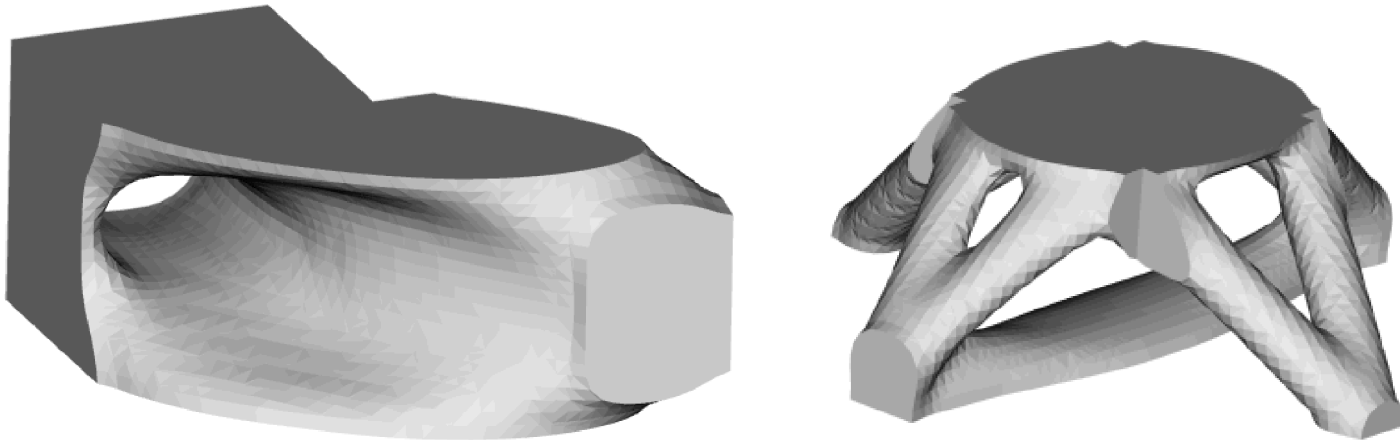
# Conclusions and future work

- Efficient gradient damage models can be constructed which are cohesive
- Method is massively thread scalable (and MPI scalable)
- Explicit time integration is possible  
(and more than 10 X faster than single linear phase solve)
- Ongoing work with John Dolbow to verify model in fragmentation scaling studies

# Inverse Problem

# Inverse methods:

- Quantities of interest are differentiable functions
- Large # decision variables
- Often, # of decision variables is proportional to mesh resolution
- Require inexpensive gradient evaluations



Example: Topology optimization using  
Sandia's Plato code

# Inverse methods

Solve multiple “forward” prediction simulations in order to

- Design
- Calibrate properties
- Match observations

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

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

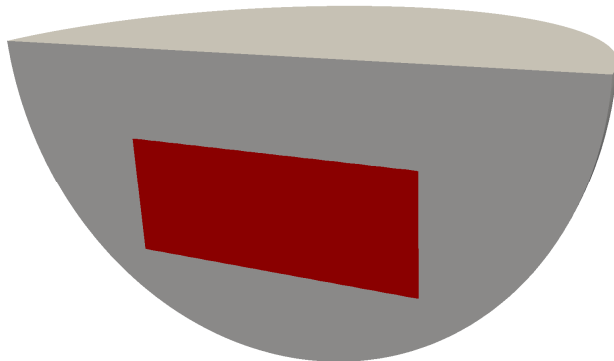


Quantity of interest depends on

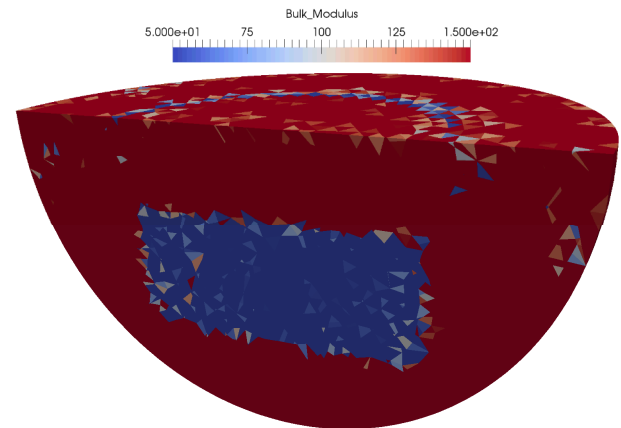
- physical solution  $\mathbf{u}$
- design parameters  $\theta$



Constrained by the physics



Initially unknown hidden tunnel subjected to surface excitation



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

# Fracture Inverse Problems

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

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# Review of the adjoint method

- Computing finite difference gradients requires many, many solves:  $O(\text{\#design parameter})$
- 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:  $\frac{dg(\mathbf{u}^N; \theta)}{d\theta}$

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

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

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# Adjoint of a recursion relation

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

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

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

Strang's Interpretation:

$$\mathbf{v}_{N \times 1} = (\mathbf{A}_{N \times N} \mathbf{B}_{N \times N}) \mathbf{u}_{N \times 1}$$

vs

$$\mathbf{v}_{N \times 1} = \mathbf{A}_{N \times N} (\mathbf{B}_{N \times N} \mathbf{u}_{N \times 1})$$

# Example with explicit Newmark

Explicit Newmark time integration

$$\mathbf{u}^{n+1} = \mathbf{u}^n + \Delta t \mathbf{v}^n + \frac{\Delta t^2}{2} \mathbf{a}^n$$

$$\mathbf{v}^{n+1/2} = \mathbf{v}^n + \frac{\Delta t}{2} \mathbf{a}^n$$

$$\mathbf{a}^{n+1} = \boldsymbol{\pi}^{n+1}(\mathbf{u}^{n+1})$$

$$\mathbf{v}^{n+1} = \mathbf{v}^{n+1/2} + \frac{\Delta t}{2} \mathbf{a}^{n+1}$$

Explicit adjoint

$$\hat{\mathbf{a}}^{n+1/2} = \hat{\mathbf{a}}^{n+1} + \frac{\Delta t}{2} \hat{\mathbf{v}}^{n+1}$$

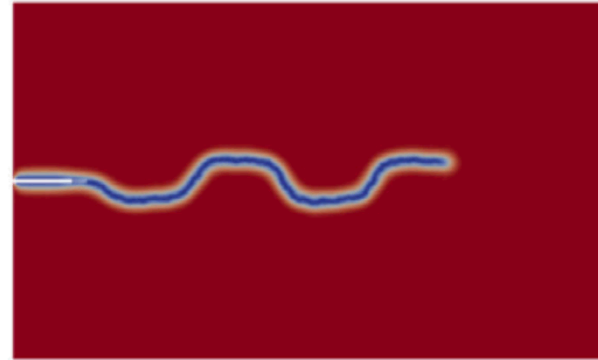
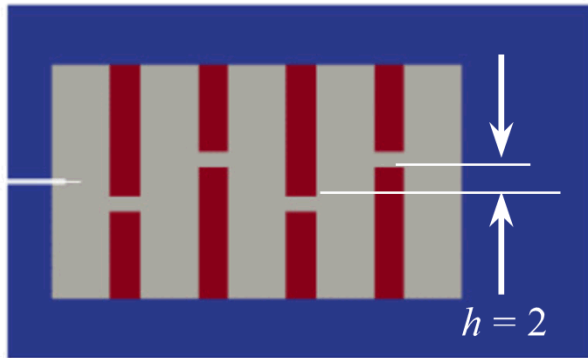
$$\hat{\mathbf{u}}^n = \hat{\mathbf{u}}^{n+1} + \hat{\mathbf{a}}^{n+1/2} \cdot \boldsymbol{\pi}_{,\mathbf{u}}^{n+1}$$

$$\hat{\mathbf{v}}^n = \hat{\mathbf{v}}^{n+1} + \Delta t \hat{\mathbf{u}}^n$$

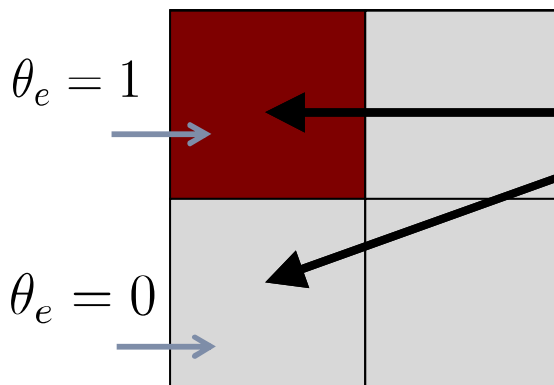
$$\hat{\mathbf{a}}^n = \frac{\Delta t}{2} \hat{\mathbf{v}}^n$$

# Heterogeneous material design

- Hossain, Hsueh, Bourdin, Bhattacharya 2014 show heterogeneous materials can be tougher than its constituents!



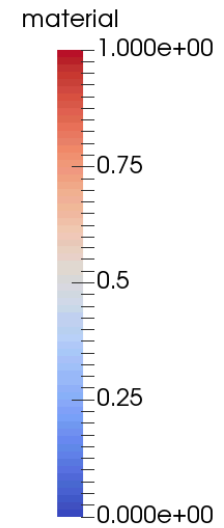
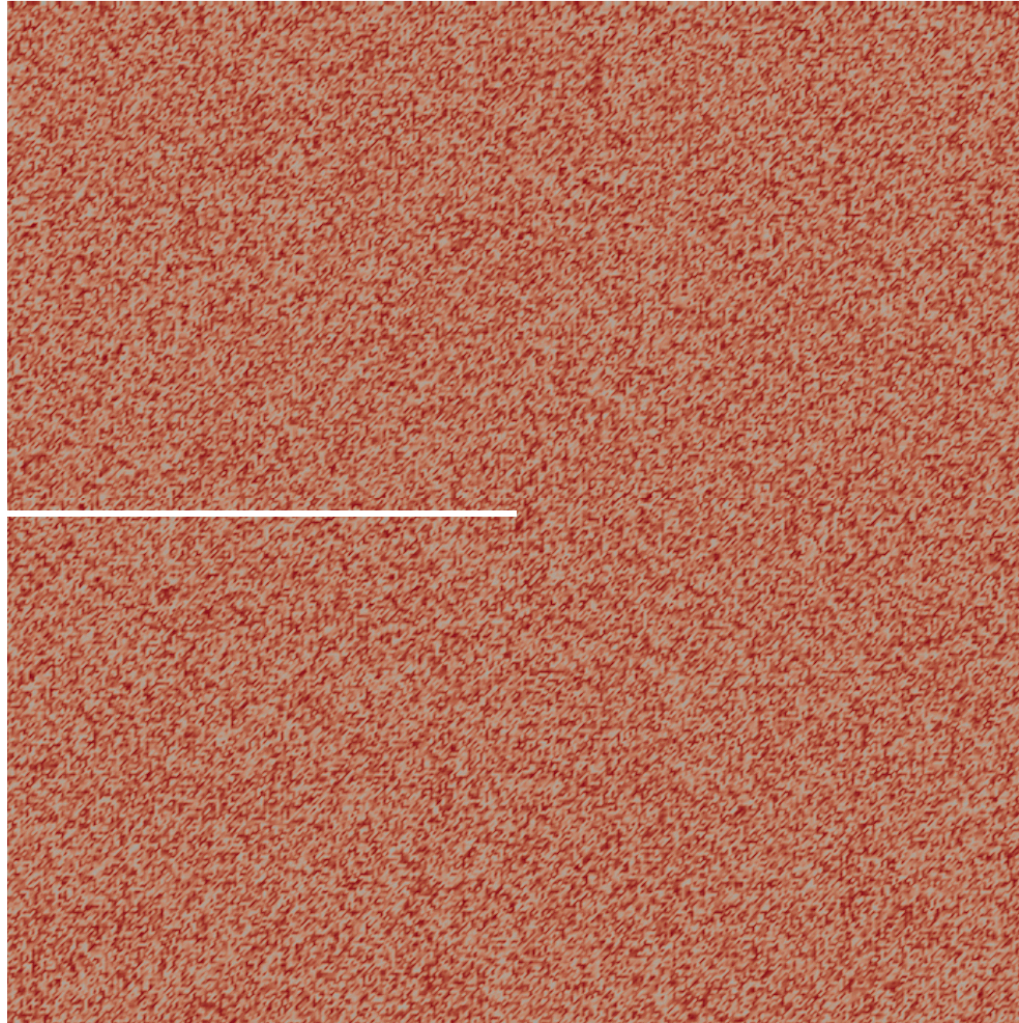
- Use adjoint framework and Sandia's *Rapid Optimization Library* to automatically design tougher material



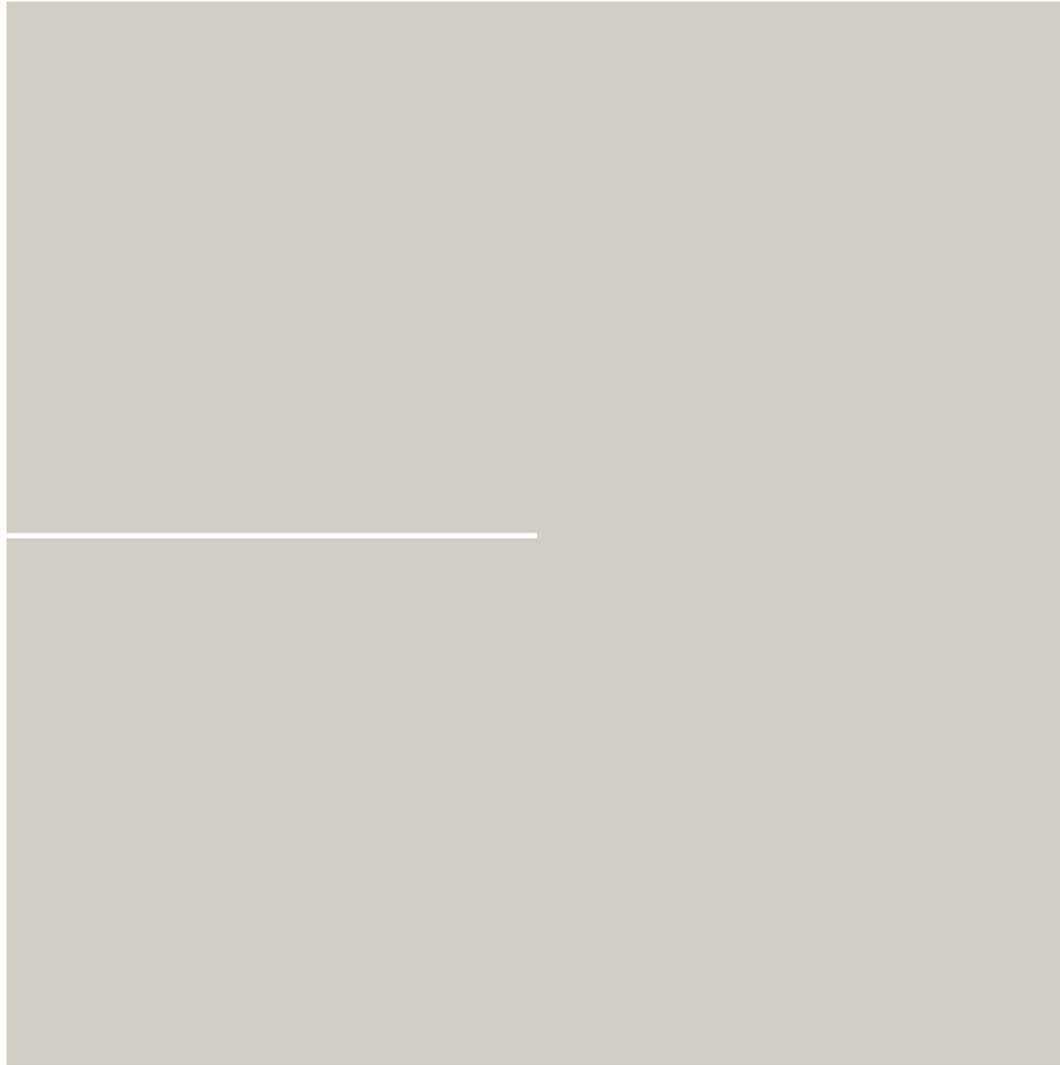
Each element chooses to be compliant or **stiff**:  $\theta_e \in [0, 1]$

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

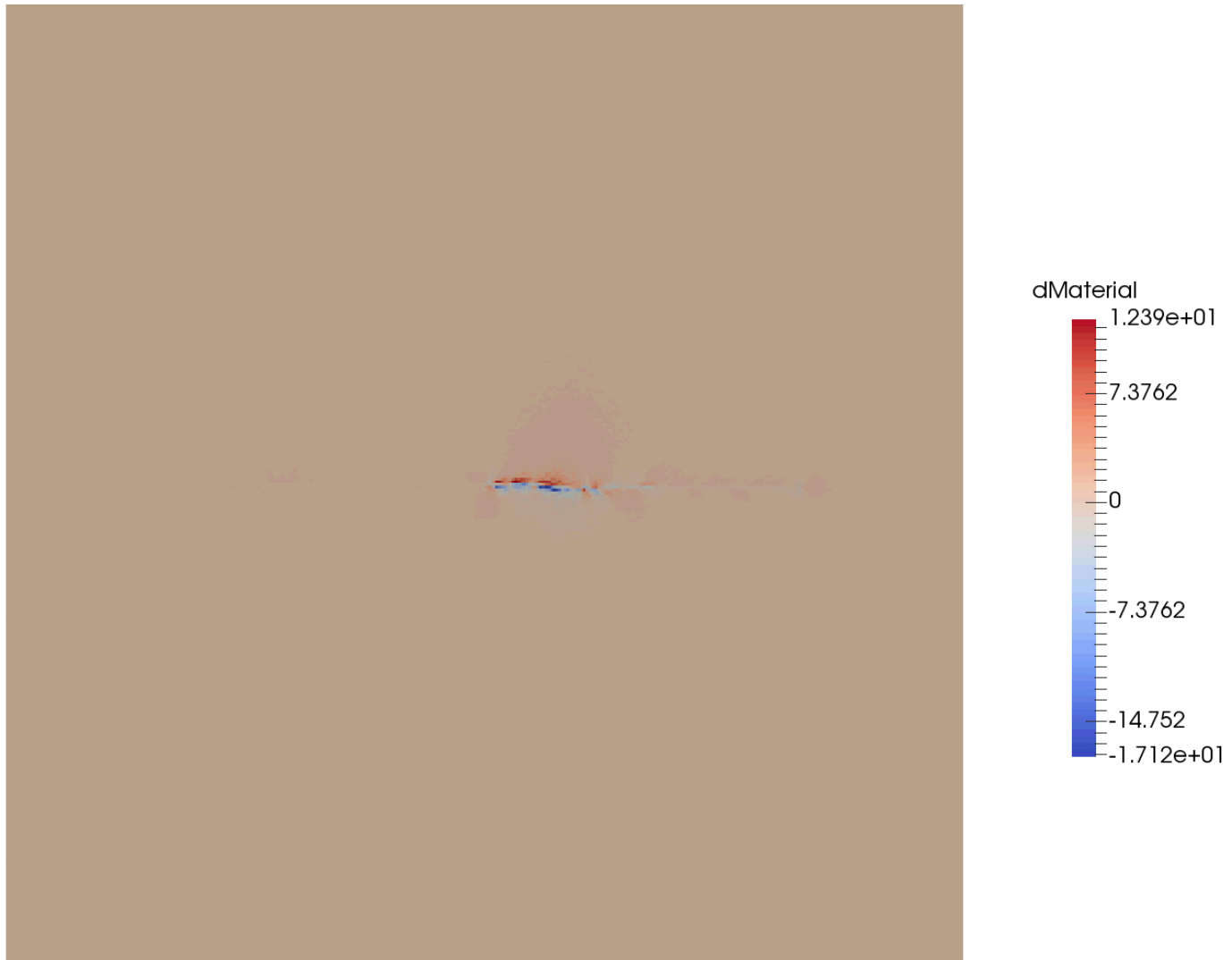
# Initial material property guess



# Damage evolution

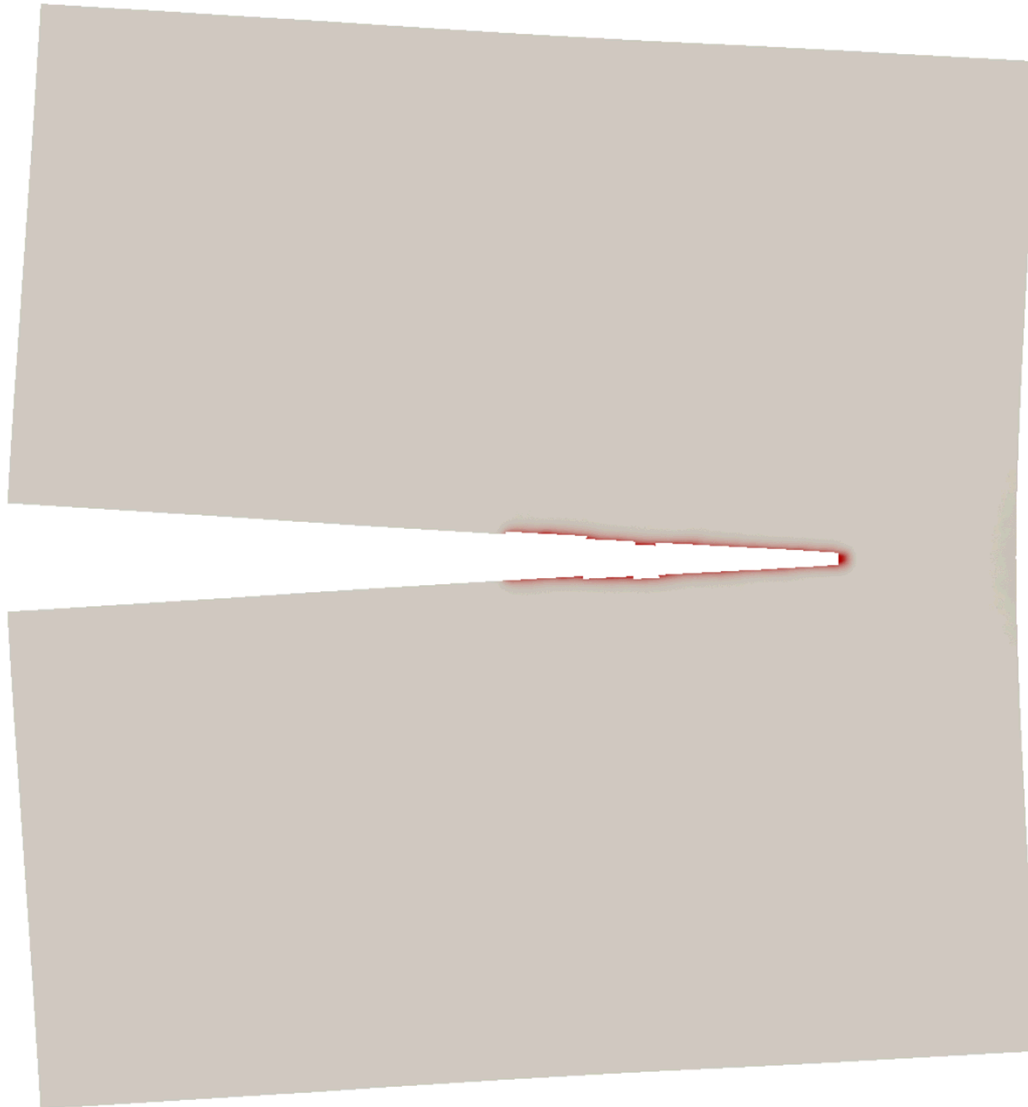


# Adjoint sensitivity to initial props

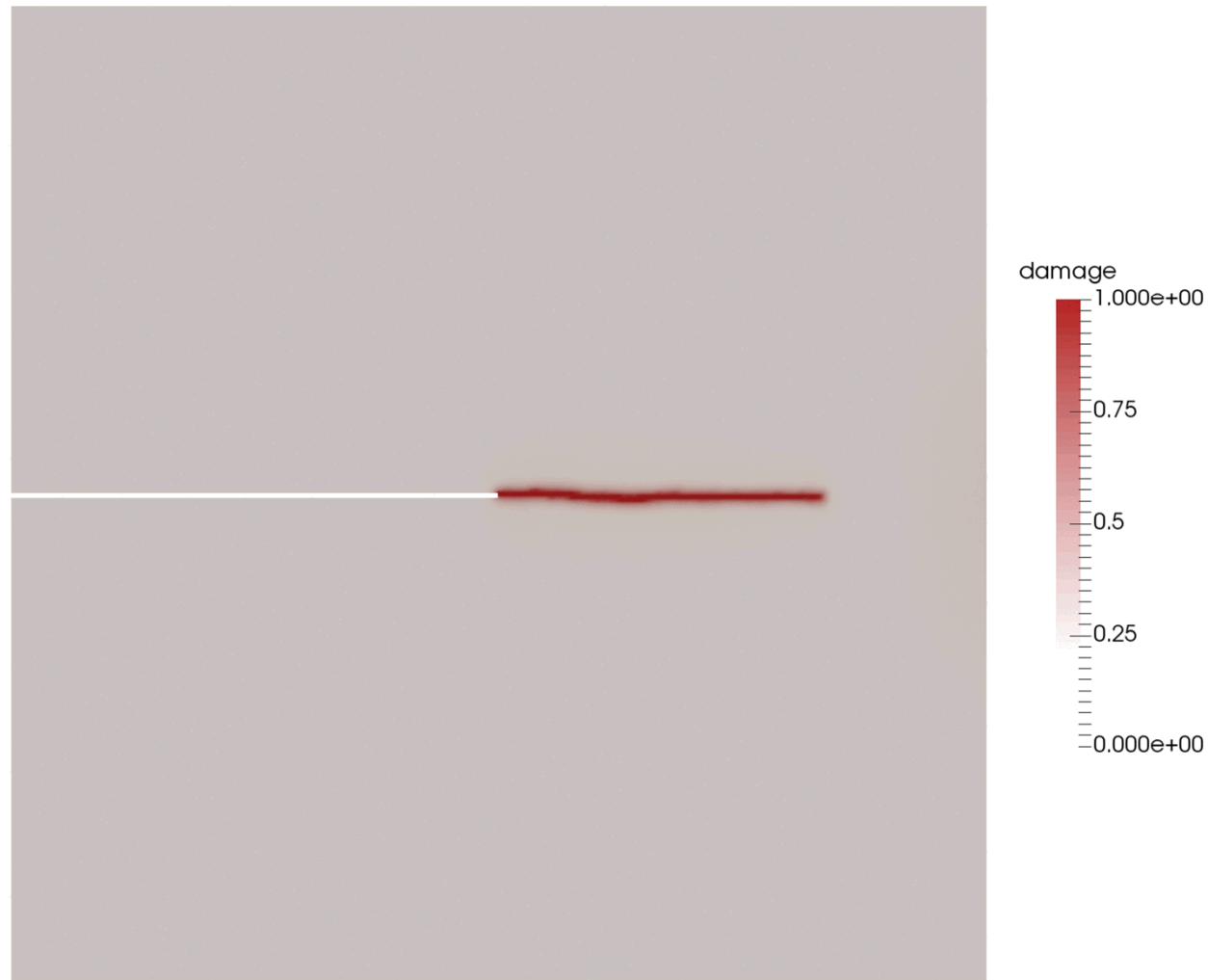


~6 times the cost of a forward simulation

# Minimize crack propagaion

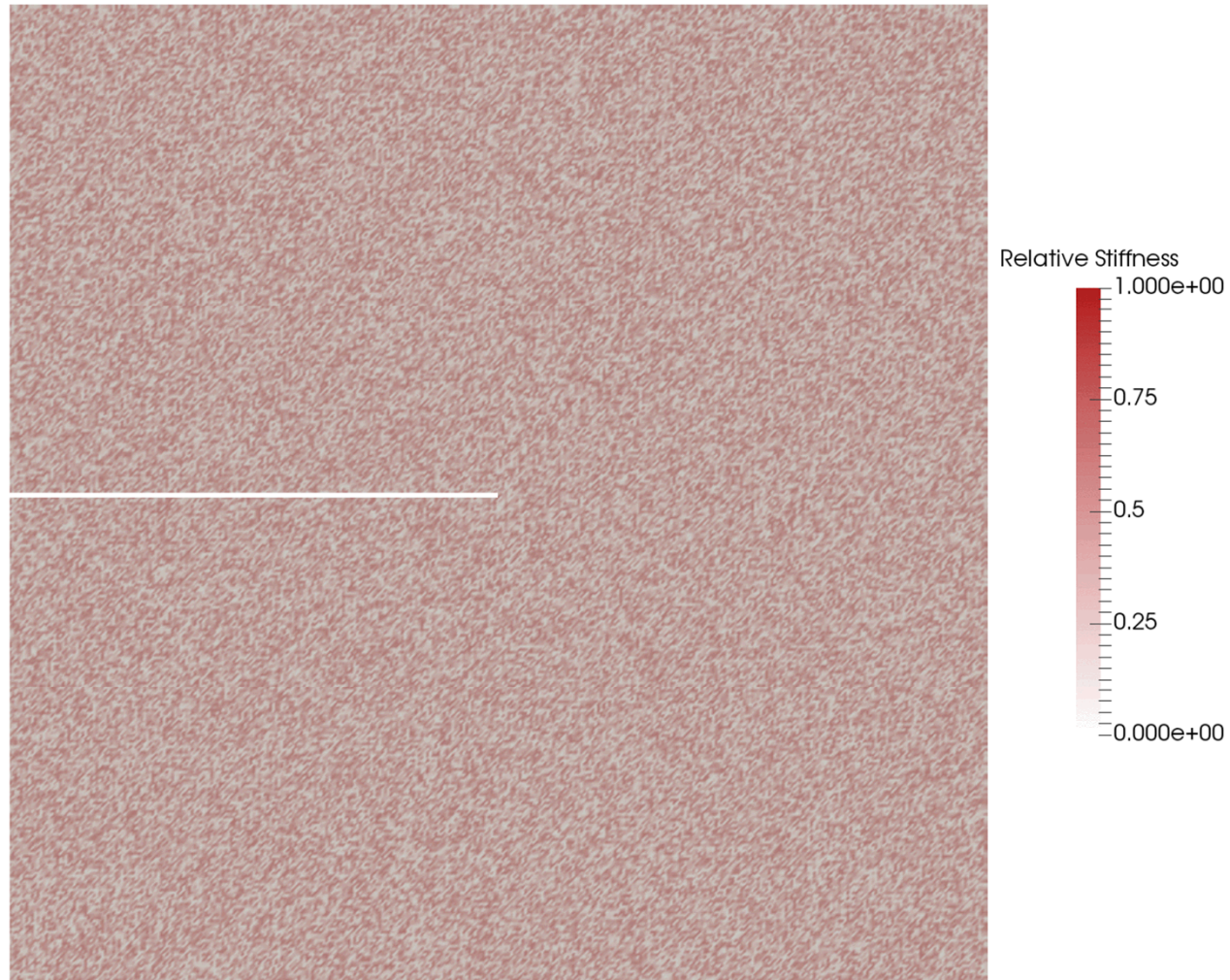


# Minimize crack propagation



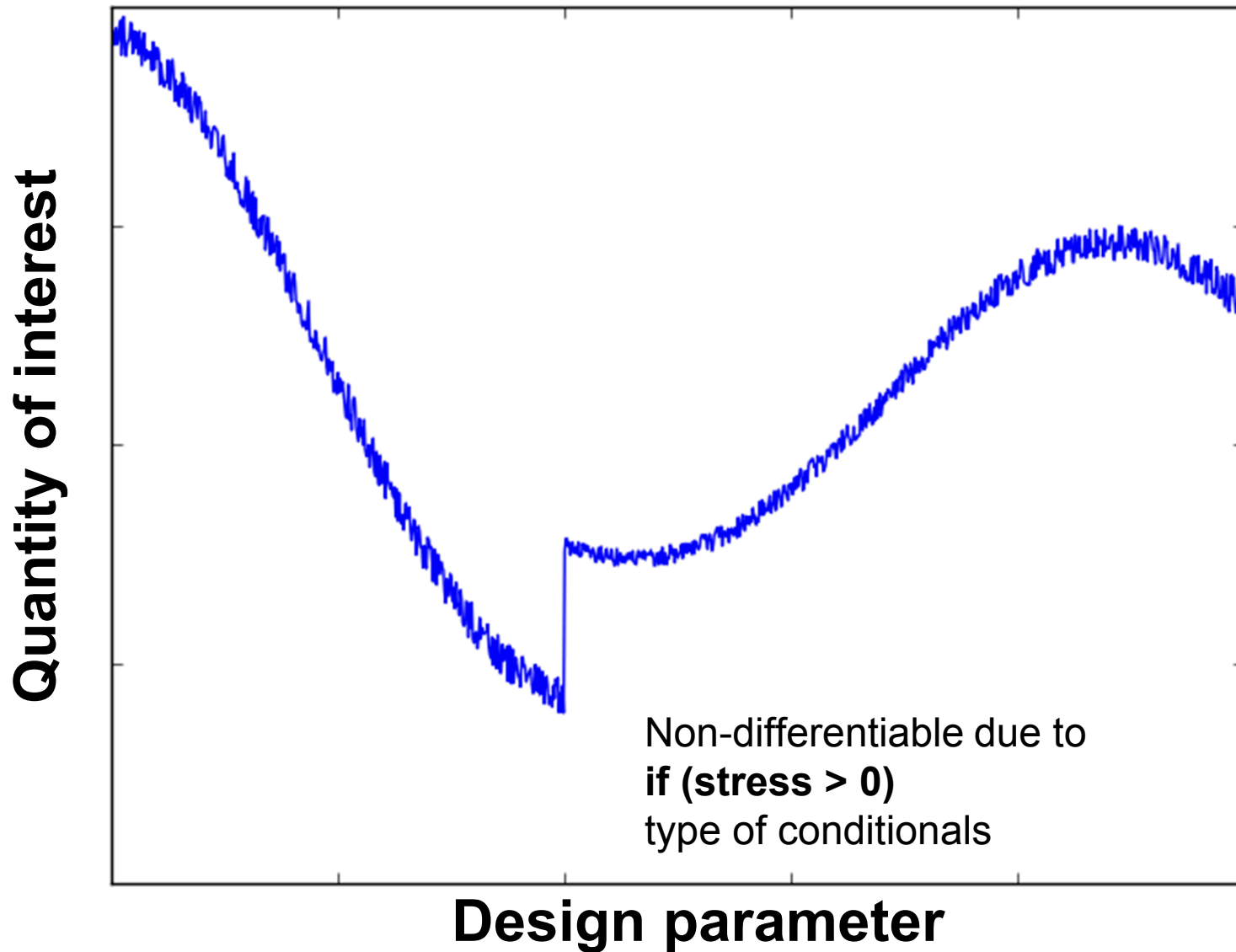
Un-deformed configuration

# Find locally optimal design

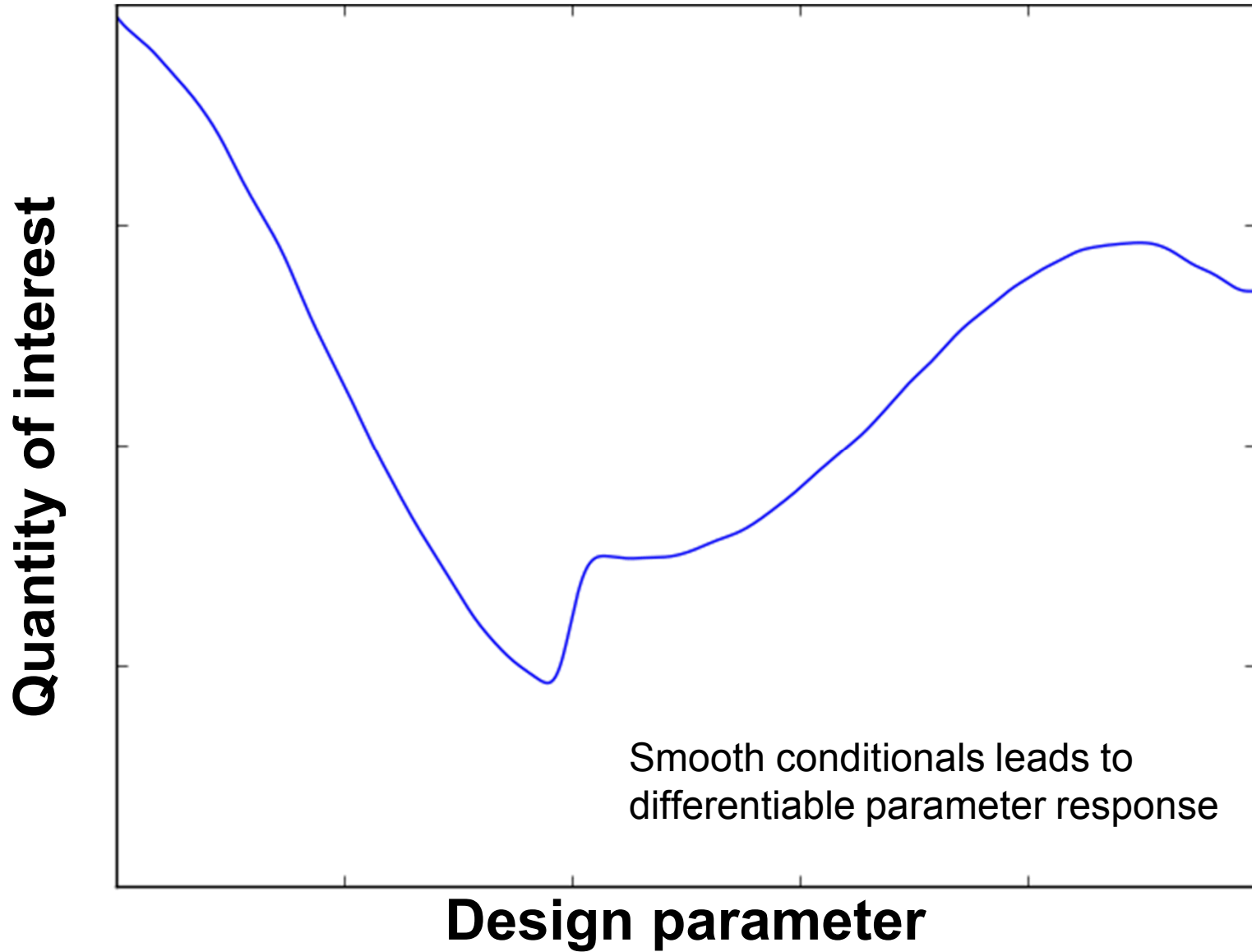


121801 design parameter gradients

# Non-smooth quantity of interest

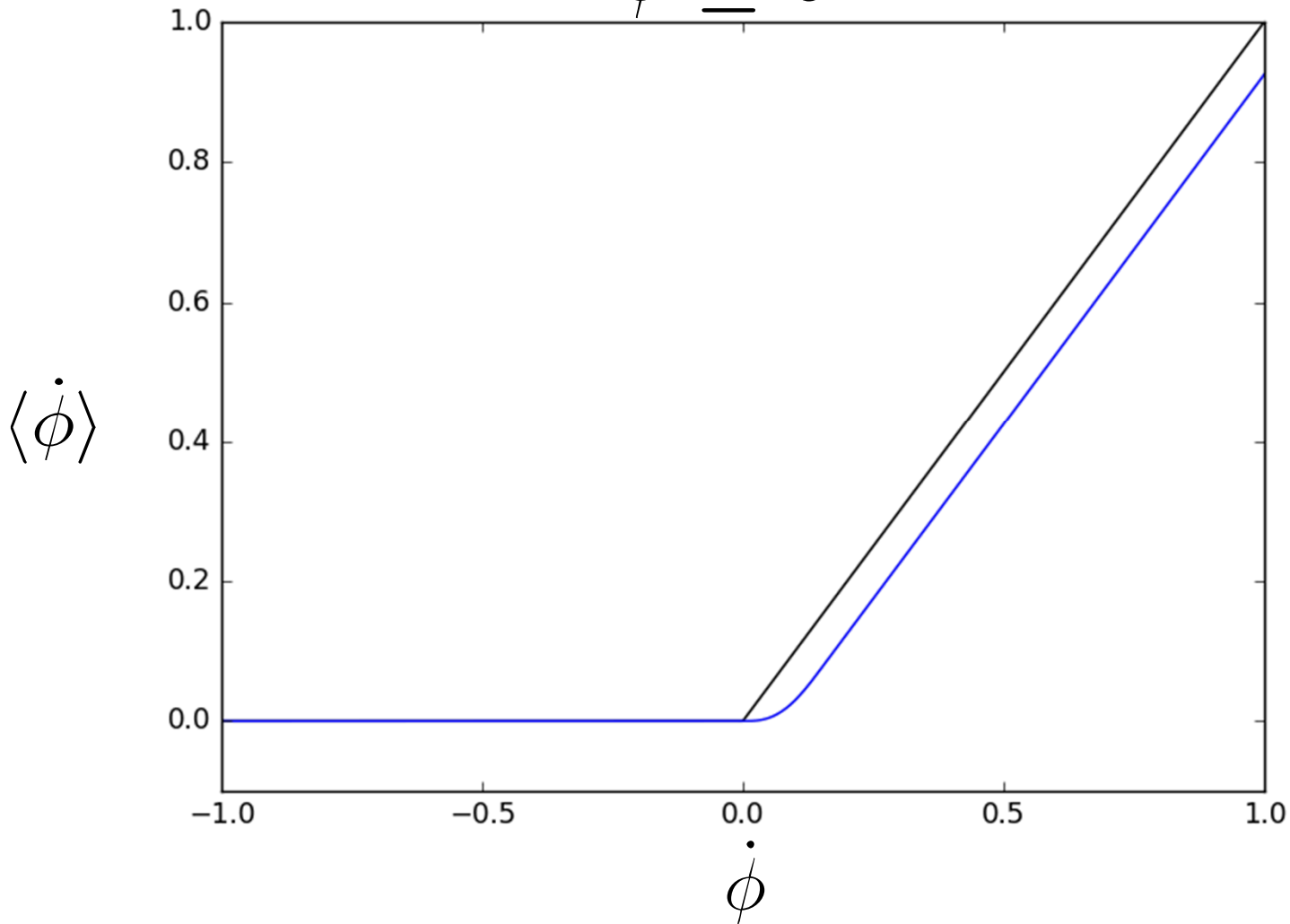


# Smoothed quantity of interest



# Differentiable approximation to

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



# Library for efficient computation of parameter sensitivities

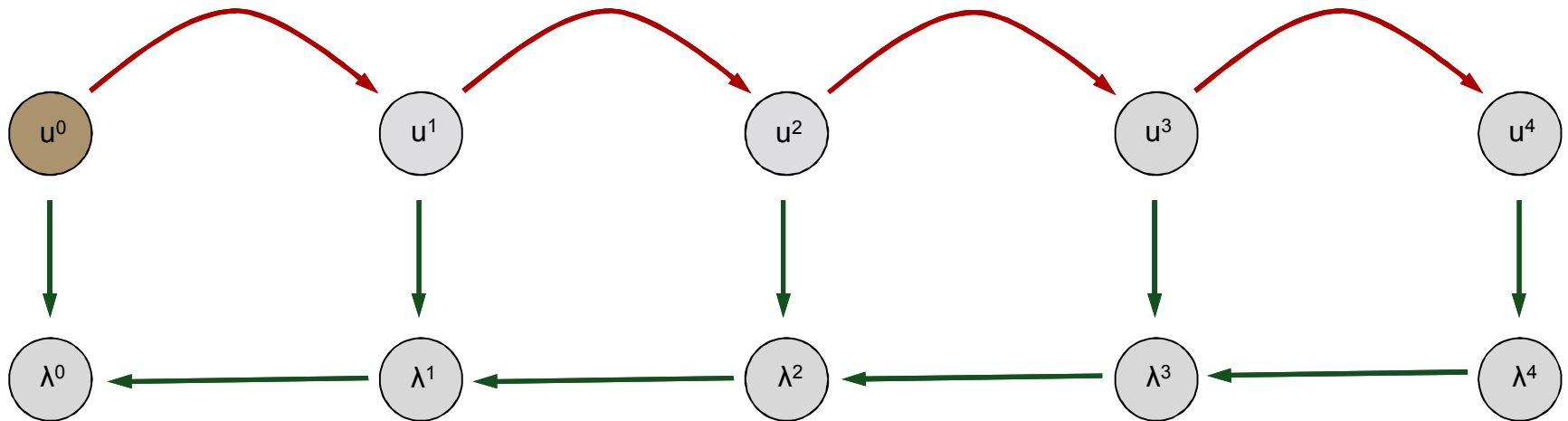
- Developed C++ library: simplifies the implementation and testing of *adjoint* sensitivities for explicit dynamic simulations
- Users define
  - State:  $\mathbf{u}$  (e.g. displacements)
  - Design parameters:  $\boldsymbol{\theta}$  (e.g. initial material properties, BCs, etc.)

- Operators:

$\mathbf{u}^{n+1} = \mathbf{f}(\mathbf{u}^n, \boldsymbol{\theta})$	$\frac{\partial \mathbf{f}(\mathbf{u}^n, \boldsymbol{\theta}) \cdot \boldsymbol{\mu}}{\partial \mathbf{u}^n}$	$\frac{\partial \mathbf{f}(\mathbf{u}^n, \boldsymbol{\theta}) \cdot \boldsymbol{\mu}}{\partial \boldsymbol{\theta}}$
q.o.i. = $g(\mathbf{u}^N, \boldsymbol{\theta})$	$\frac{\partial g(\mathbf{u}^N, \boldsymbol{\theta})}{\partial \mathbf{u}^N}$	$\frac{\partial g(\mathbf{u}^N, \boldsymbol{\theta})}{\partial \boldsymbol{\theta}}$

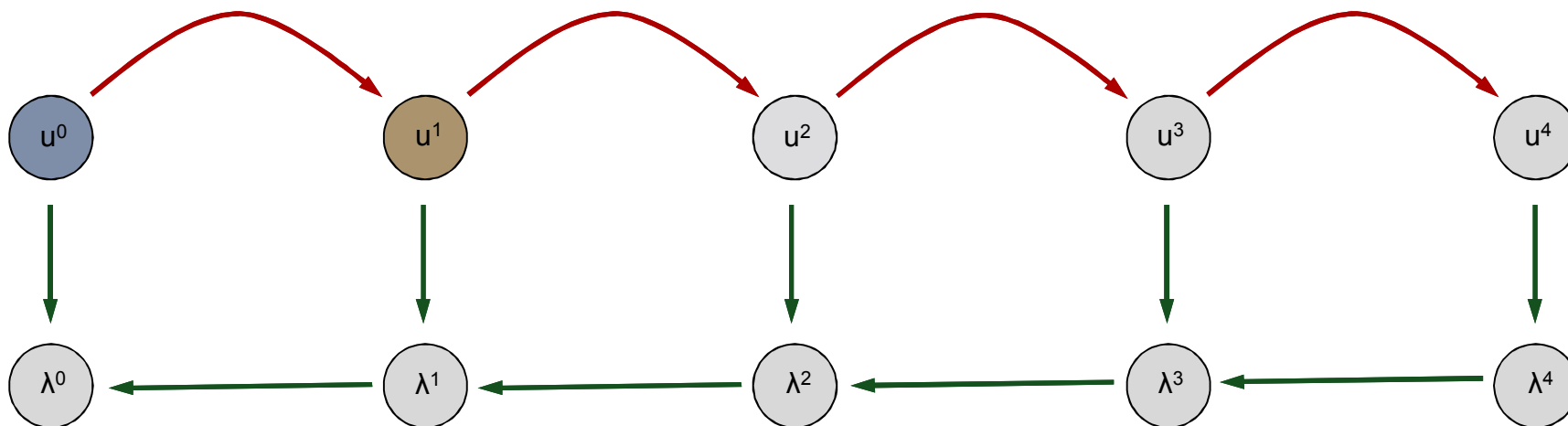
- Library automatically computes  $\frac{dg(\mathbf{u}^N, \boldsymbol{\theta})}{d\boldsymbol{\theta}}$
- 1,000 – 1,000,000+ parameter sensitivities take time of ~10 forward solves

# Checkpointing for backward integration



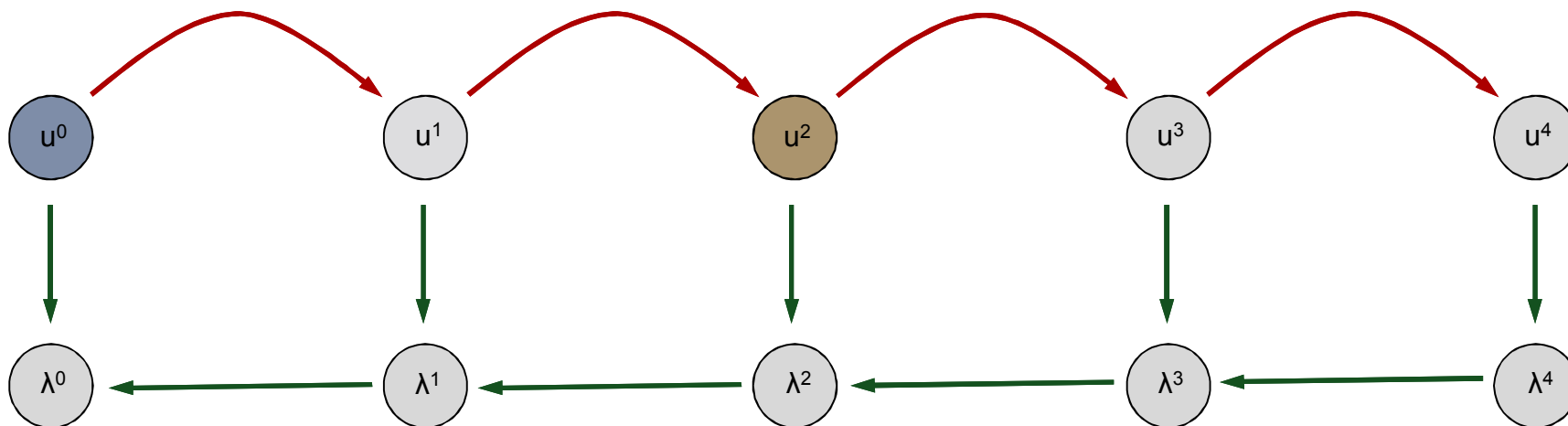
Using *Minimal Repetition Checkpointing Algorithm* by Q. Wang, et al.

# Checkpointing for backward integration



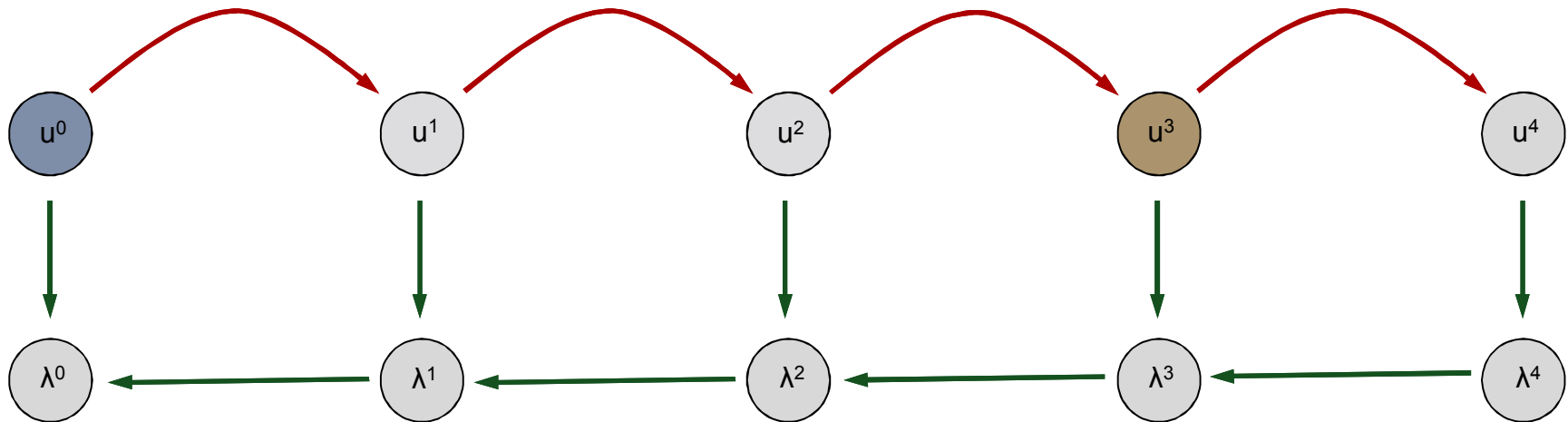
Using *Minimal Repetition Checkpointing Algorithm* by Q. Wang, et al.

# Checkpointing for backward integration



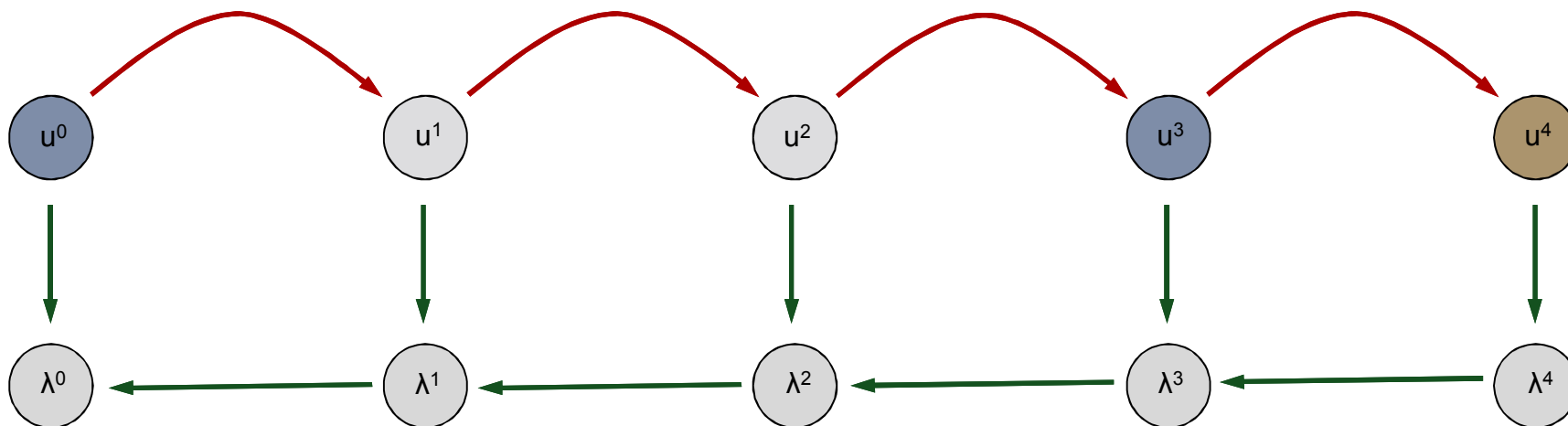
Using *Minimal Repetition Checkpointing Algorithm* by Q. Wang, et al.

# Checkpointing for backward integration



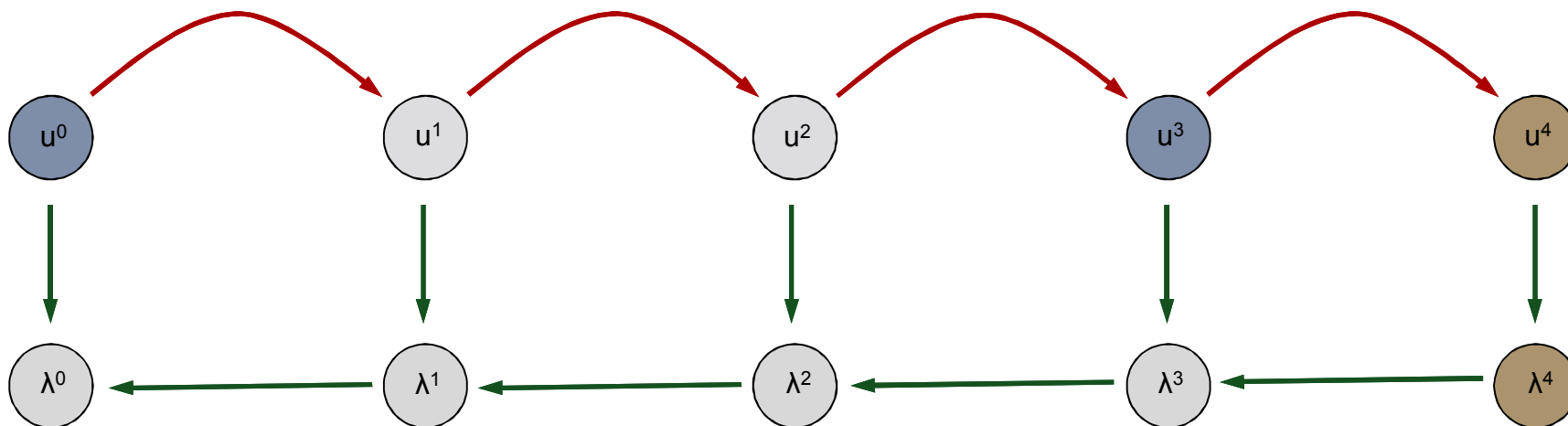
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# Checkpointing for backward integration



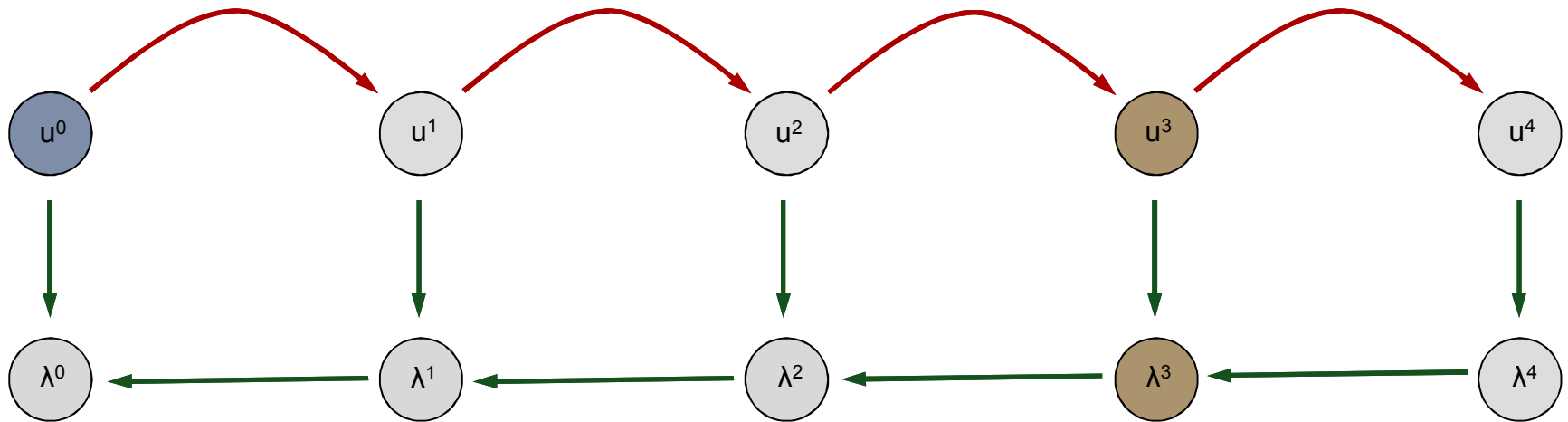
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# Checkpointing for backward integration



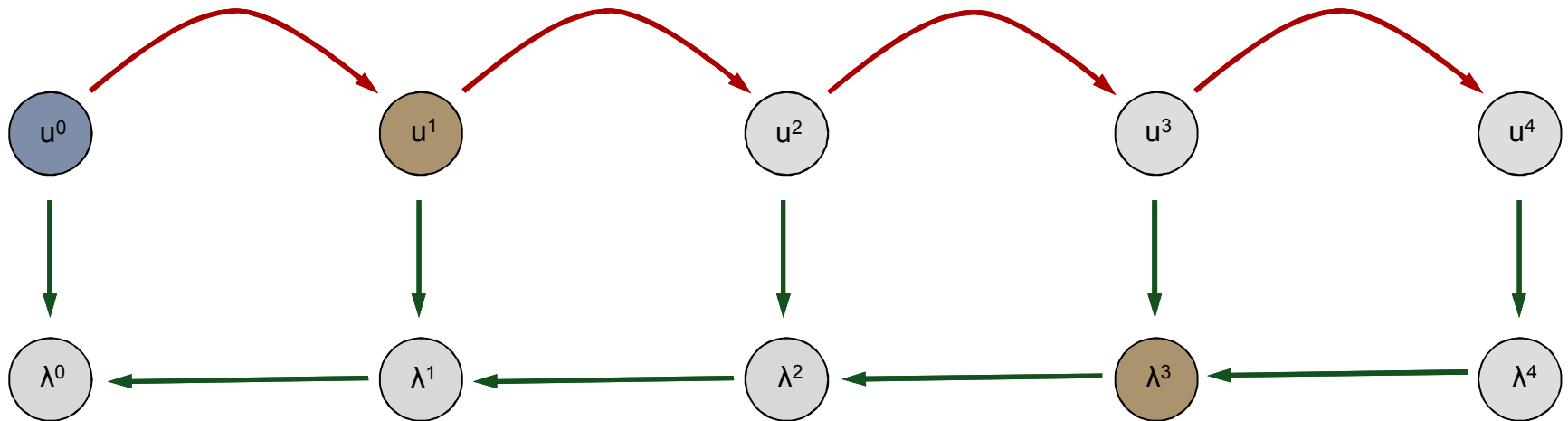
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# Checkpointing for backward integration



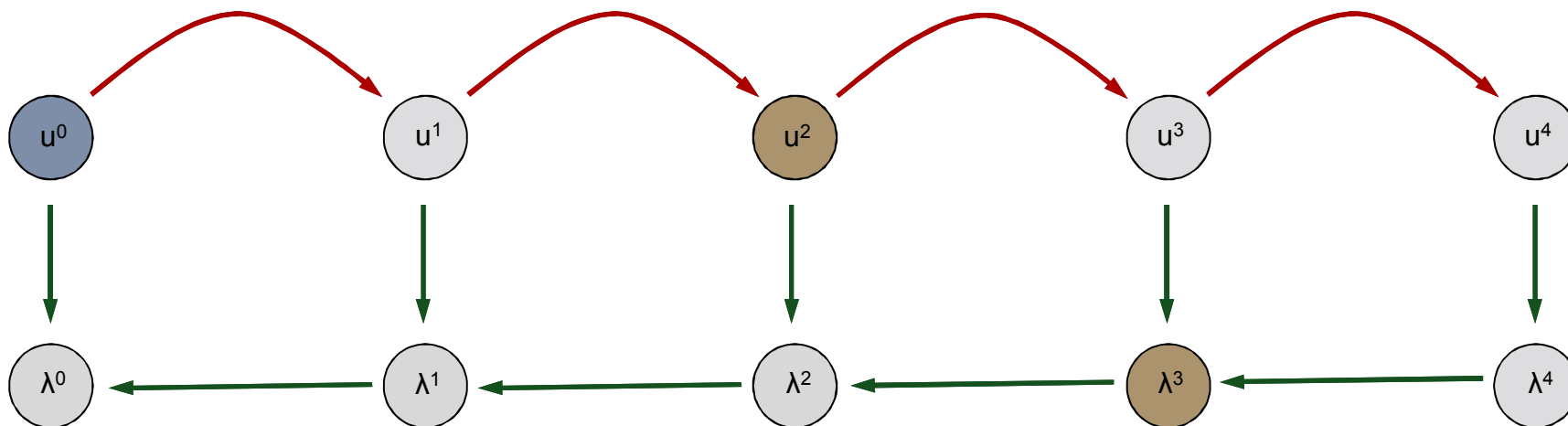
Using *Minimal Repetition Checkpointing Algorithm* by Q. Wang, et al.

# Checkpointing for backward integration



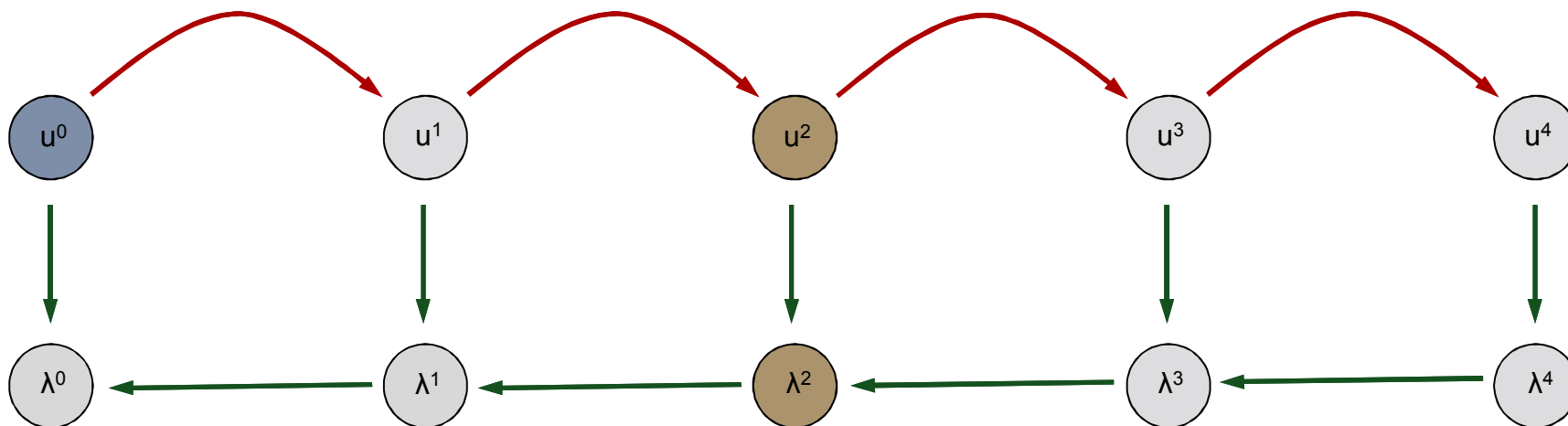
Using *Minimal Repetition Checkpointing Algorithm* by Q. Wang, et al.

# Checkpointing for backward integration



Using *Minimal Repetition Checkpointing Algorithm* by Q. Wang, et al.

# Checkpointing for backward integration



Using *Minimal Repetition Checkpointing Algorithm* by Q. Wang, et al.

# Library for efficient computation of parameter sensitivities

- Developed C++ library: simplifies the implementation and testing of *adjoint* sensitivities for explicit dynamic simulations
- Users define
  - State:  $\mathbf{u}$  (e.g. displacements)
  - Design parameters:  $\boldsymbol{\theta}$  (e.g. initial material properties, BCs, etc.)

- Operators:

$\mathbf{u}^{n+1} = \mathbf{f}(\mathbf{u}^n, \boldsymbol{\theta})$	$\frac{\partial \mathbf{f}(\mathbf{u}^n, \boldsymbol{\theta}) \cdot \boldsymbol{\mu}}{\partial \mathbf{u}^n}$	$\frac{\partial \mathbf{f}(\mathbf{u}^n, \boldsymbol{\theta}) \cdot \boldsymbol{\mu}}{\partial \boldsymbol{\theta}}$
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- Library automatically computes  $\frac{dg(\mathbf{u}^N, \boldsymbol{\theta})}{d\boldsymbol{\theta}}$
- 1,000 – 1,000,000+ parameter sensitivities take time of ~10 forward solves

# Adding up the savings

- Explicitly integrating damage:  $> 10 \times$
- Structured grid, linear kinematics:  $> 20 \times$
- GPU vs. CPU:  $> 100 \times$
- Adjoint sensitivities:  $> (\#Elements / 10) \times$
  
- For 100,000 element simulation:  $> 2e8$  times speedup
- From average human lifetime to  $\sim 10$  seconds

# Conclusions

- Adjoint method is too important to be ignored
  - Non-trivial to implement and maintain
  - Requires differentiability
  
- Thread scalability is too important to be ignored
  - Data movement kills performance
  - May need to rethink the algorithms we use
  - Hardware trends are likely to continue
  
- Next steps:
  - Adjoint method for dynamic contact, plasticity, etc.
  - Improve usability and robustness of inverse framework

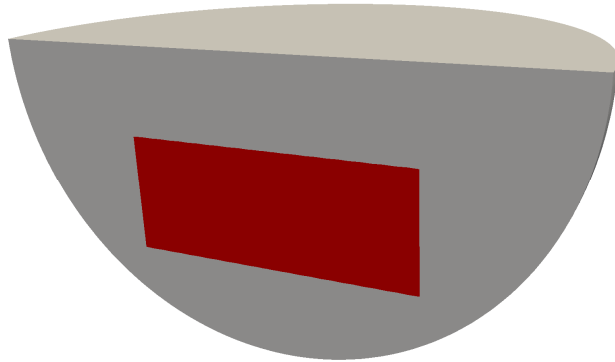
# Thanks

- Solid Mechanics Team
- John Dolbow
- Tim Walsh
- Kyle Starkey
- ROL team
- Kokkos team
- Sierra DevOps

# Extra slides

# Phase-field inversion examples

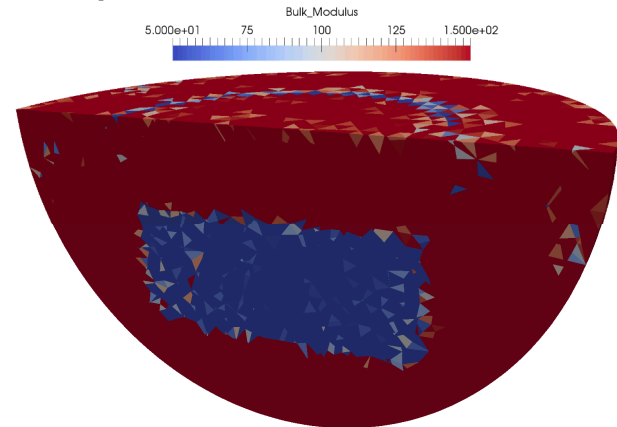
- Minimize discrepancy between observed displacements and simulated displacements by varying phase (volume fraction) element by element
- Sandia's ROL library used to perform the optimization



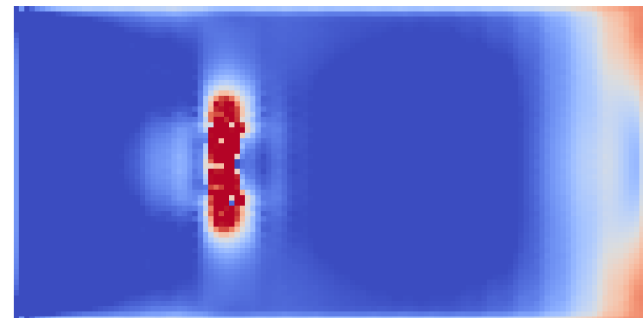
Initially unknown hidden tunnel subjected to surface excitation



Initial crack/damage in specimen



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



Reconstructed crack based on observed displacements due to acoustic excitation

# High fracture energy release rate

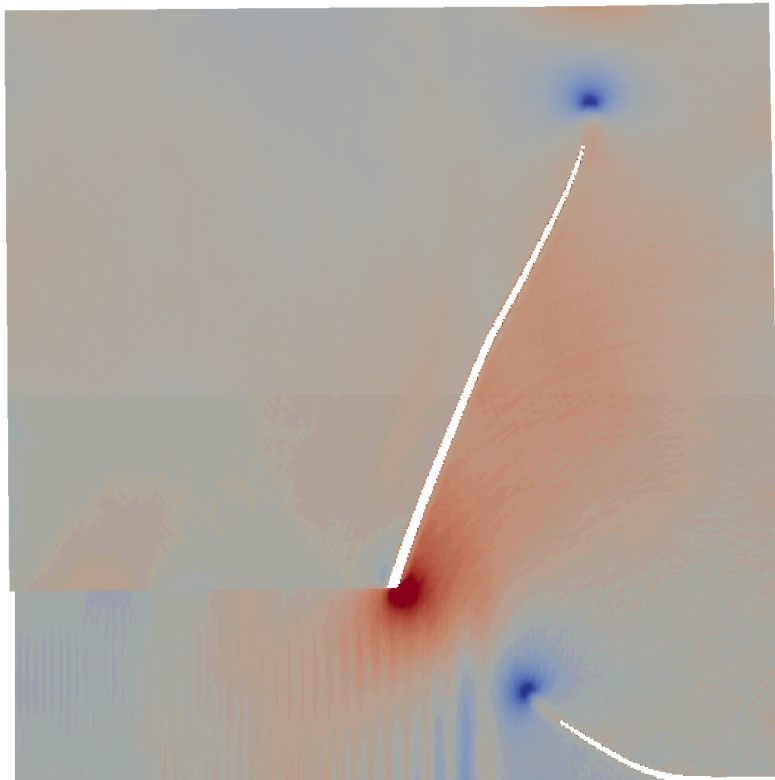


# Low fracture energy release rate

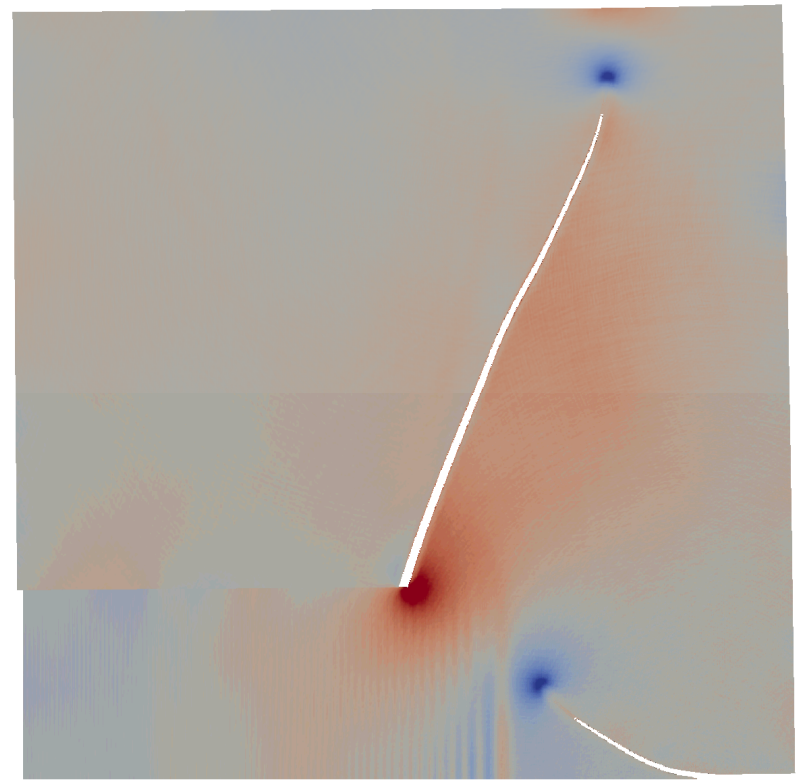


# Mesh insensitivity

Pressure contours for dynamic crack propagation

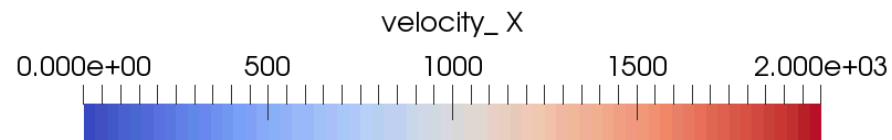
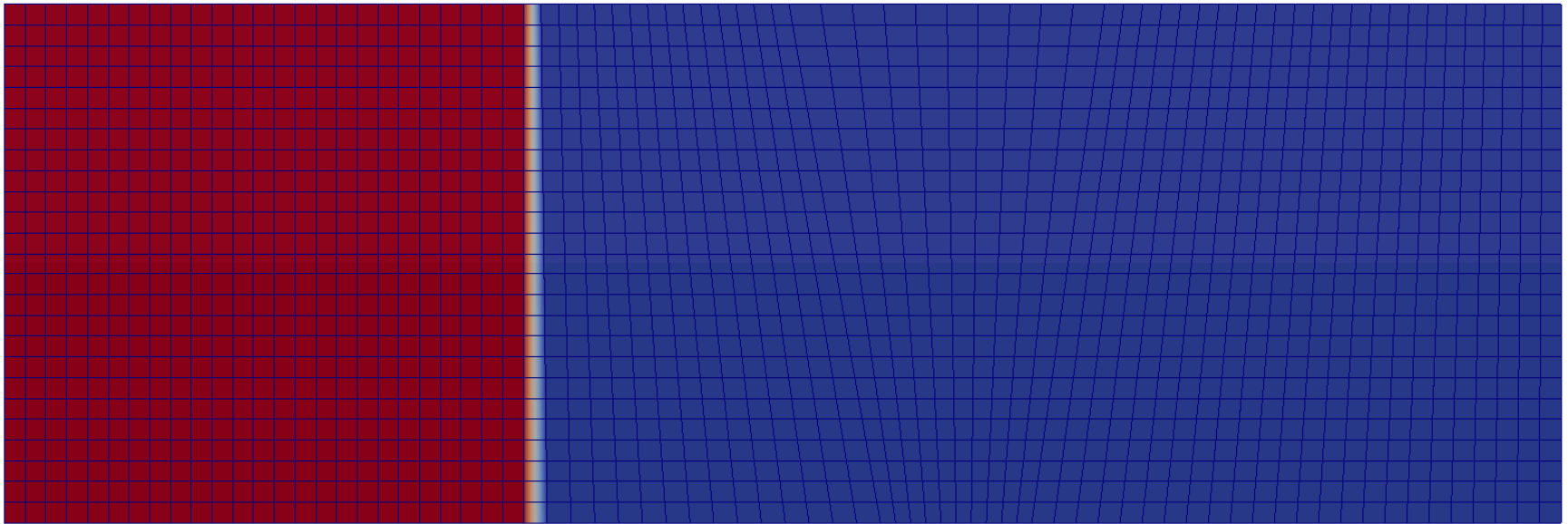


Medium mesh: 250k elements

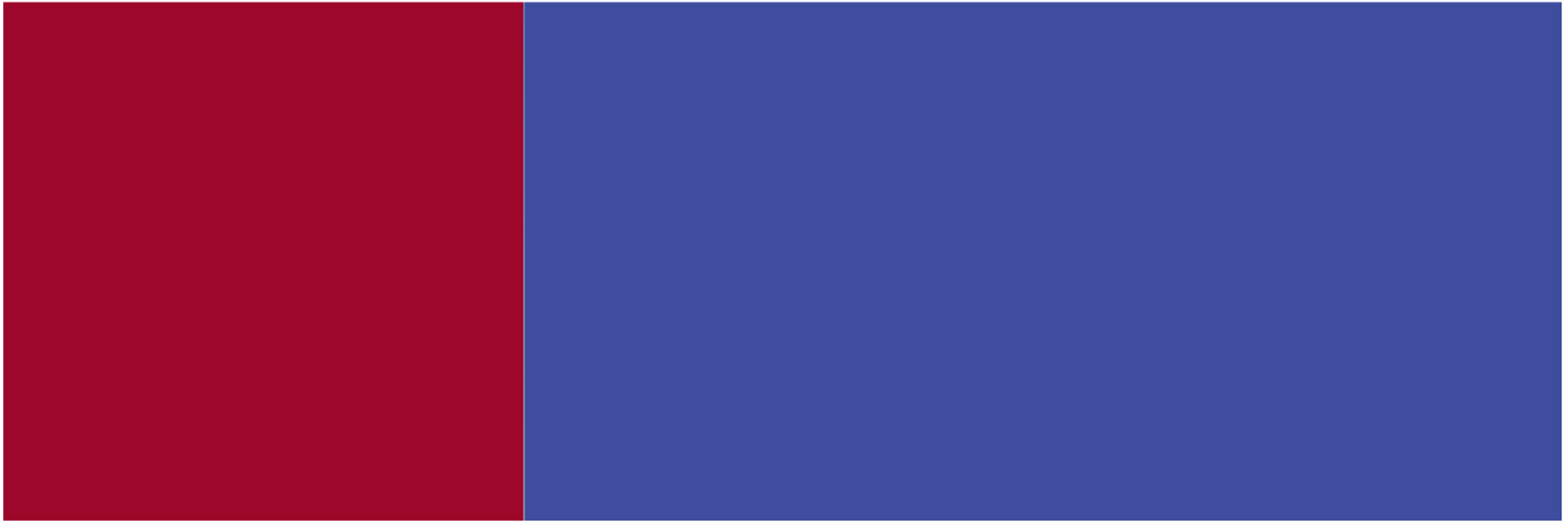


Fine mesh: 1,000k elements

# Spall example: Initial velocity

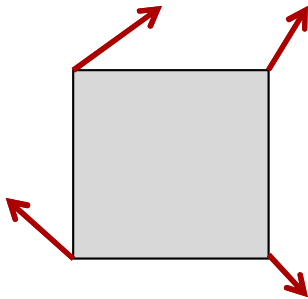


# Spall example:

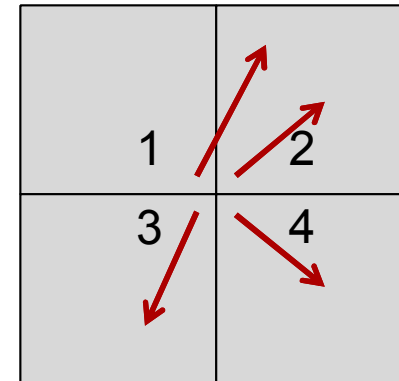


# Determinacy in a threaded world

- 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

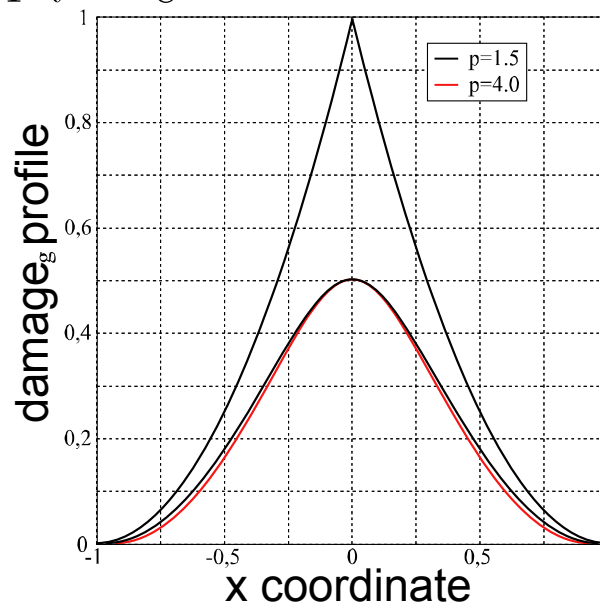
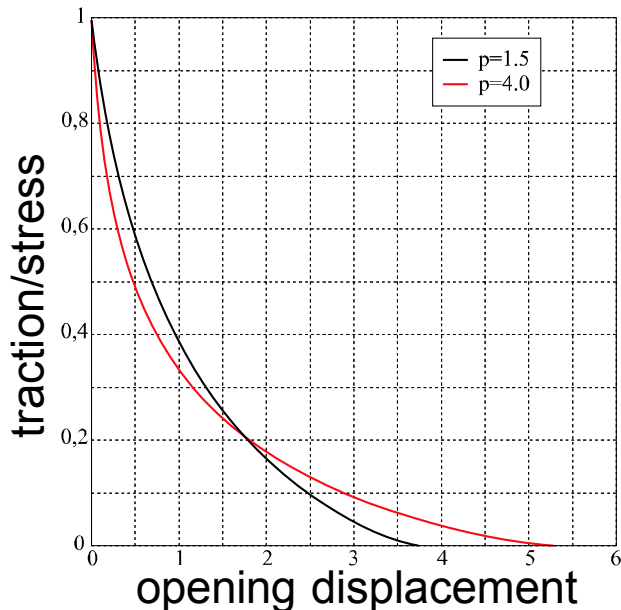
# Reintroducing the Lorentz model

- 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.

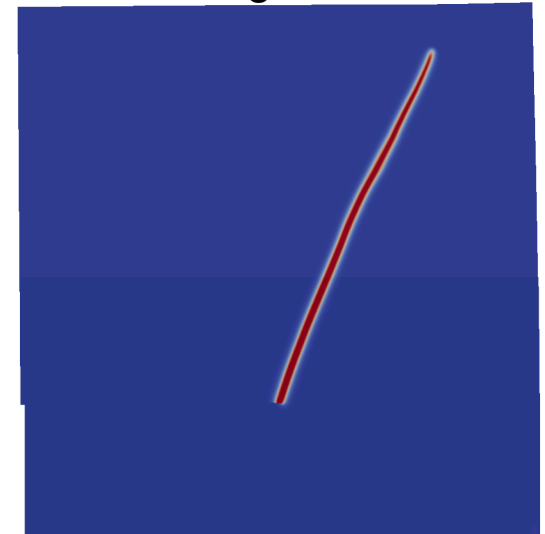
# Improved forward modeling of crack propagation in brittle materials

- 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

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



Damage contour



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:  $\sim 70^\circ$

# 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

$$\begin{aligned} & \min_{\boldsymbol{\theta}} g(\mathbf{u}, \boldsymbol{\theta}) \\ & \text{s.t. } \mathcal{L}(\mathbf{u}, \boldsymbol{\theta}) = \mathbf{0} \end{aligned}$$

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

# 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.

■ Consider a purely local model of damage

■ Stress-strain relationship

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

■ Strain-displacement

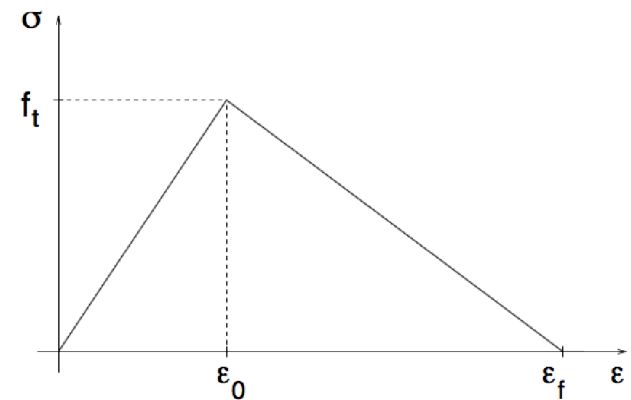
$$\epsilon(x, t) = r^s u(x, t)$$

■ Local state variable

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

■ Damage evolution

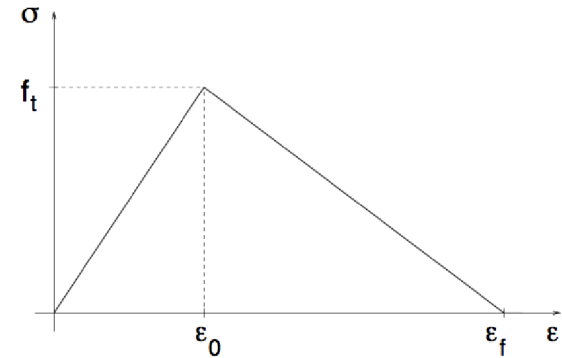
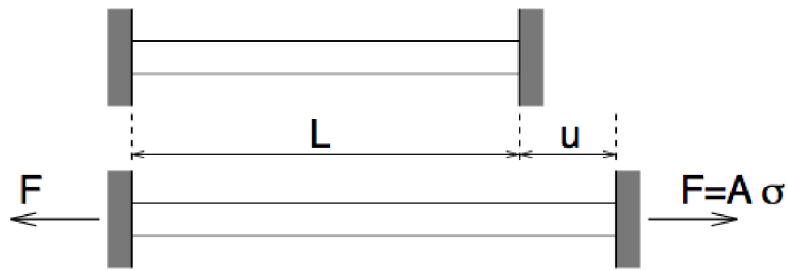
$$d(x, t) = D \max_{\xi \leq t} Y(x, \xi)$$



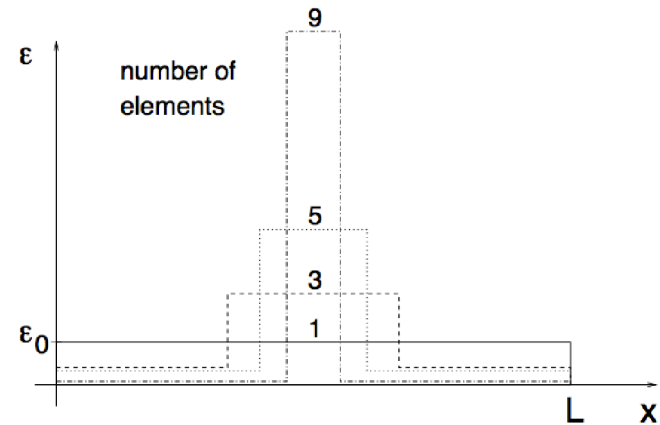
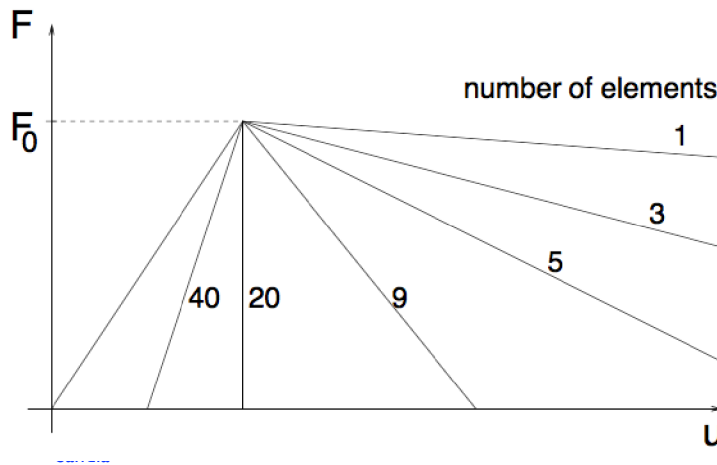
$$d(x, t) = \frac{Y_f}{Y_f - Y_0} \left( 1 - \frac{Y_0}{Y} \right)$$

## Fundamental Linearity (cont.)

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



Discretized with finite elements (from [Jirasek, 2002](#)):



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

$$d(x, t) = D \max_{\boxed{x} \leq t} \tilde{Y}(x, \boxed{x})$$

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

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

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

$$\tilde{Y}(x, t) - c\Delta \tilde{Y}(x, t) = Y(x, t) \quad \text{in } \boxed{x} \quad \text{nr } \tilde{Y} = 0 \quad \text{on } \partial \boxed{x}$$

- These two approaches are closely related (Huerta and Pijaudier-Cabot, 1998)

■ Introduced by **Rodriguez-Ferran et al. (2005)**

■ Stress-strain and strain-displacement:

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

■ Non-local displacement:

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

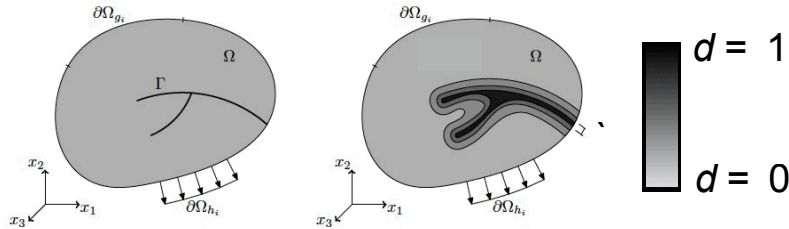
■ Non-local strains and state variable:

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

■ Damage evolution:

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

# Phase-Field Methods for Fracture



■ 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

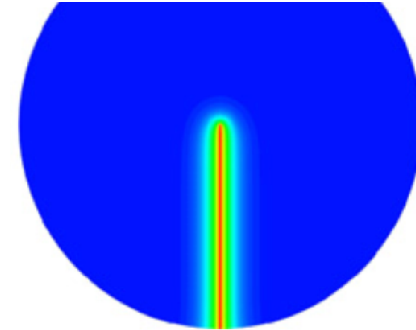
$$\Gamma \square \Gamma_I(d) = \int_{\Gamma} \gamma_I(d, r, d) dV$$

■ Fracture energy (for brittle materials):

$$G_c dA \square \int_{\Gamma} G_c \gamma_I dV$$

- Common crack-density functional:

$$y_l = \frac{1}{2l} d^2 + \frac{l}{2} |r \cdot d|^2$$



- Coincides with forms obtained in gamma-convergent regularizations of free-discontinuity problems (**Ambrosio and Tortorelli, 1990**).
- Minimization principle of diffusive crack topology

$$d(x) = \arg \left\{ \inf_{d \in W} \Gamma_l(d) \right\} \quad W = \{d \mid d(x) = 1 \text{ at } x \in \Gamma\}$$

- Gives rise to Euler-Lagrange equation:

$$d - l^2 \Delta d = 0 \quad \text{in } \mathbb{R}^2 \quad r \cdot d \cdot n = 0 \quad \text{on } \partial \mathbb{R}^2$$

Standard total potential energy (elastostatics)

$$pot(u, \Gamma) = \int_{\Omega} e(r^s u) dv + \int_{\Gamma} G_c da$$

Phase field regularization

$$I(u, d) = \int_{\Omega} (g(d) e^+(r^s u) + e^-(r^s u)) dv + \int_{\Gamma} G_c \gamma_I da$$

Degradation function requirements

$$\begin{aligned} & g : [0, 1] \rightarrow [0, 1] \\ & g^0(d) < 0 \quad d \in [0, 1] \\ & g^0(1) = 0 \end{aligned} \quad g = (1 - d)^2$$

## ■ Stress-strain response

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

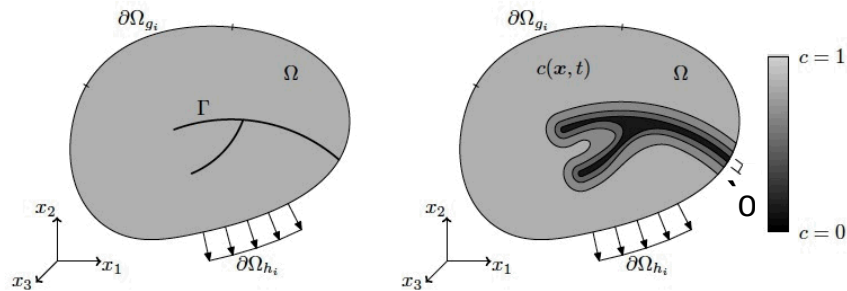
$$\sigma(x, t) = [(1 - d(x, t))^2 + k]C \epsilon^+(x, t) + C \bar{\epsilon}(x, t)$$

## ■ Non-local equations

$$\tilde{Y}(x, t) - c\Delta \tilde{Y}(x, t) = Y(x, t) \quad \text{in } \mathbb{R}^n$$

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

■ Total potential energy



$$pot(u, \Gamma) = \int_{\Omega} e(r^s u) dv + \int_{\Gamma} G_c da$$

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

$$\int_{\Gamma} G_c da \approx \int_{\Omega} G_c \Gamma_{c,n} dv \quad \Gamma_{c,n} = \frac{1}{4l_0} \left[ (c-1)^2 + 4l_0 |r_c|^2 \right]$$

- Implementation based on **Borden et al. (2012)**

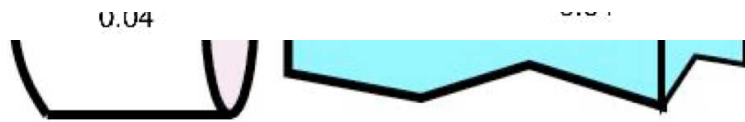
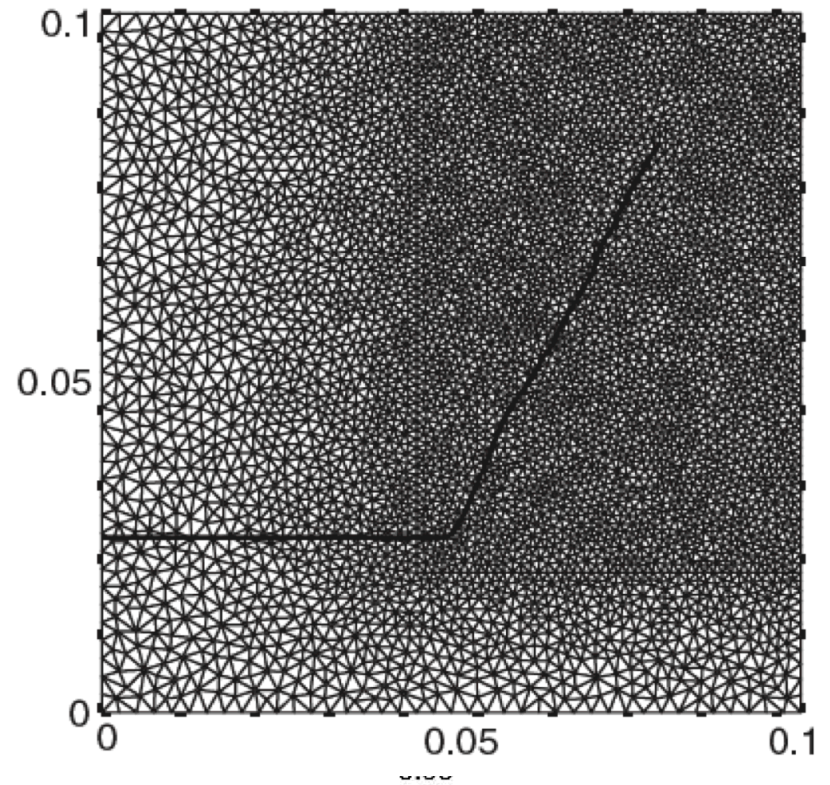
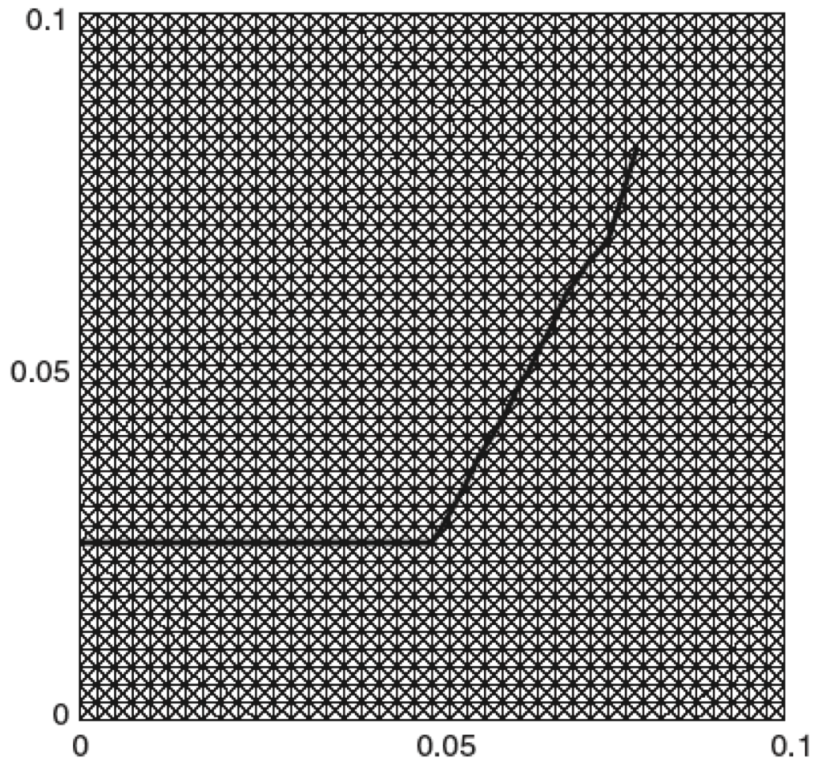
$$c = 1 - d$$

- Strong form for dynamics:

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

$$\frac{\partial}{\partial t} \left[ \frac{\rho_0 (1 - k) \dot{e}^+}{G_c} + 1 \right] c - \rho_0 \frac{\partial^2 c}{\partial x_i^2} = 1 \quad \text{on } \Omega \times ]0, T[$$

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



# Kalthoff Problem

