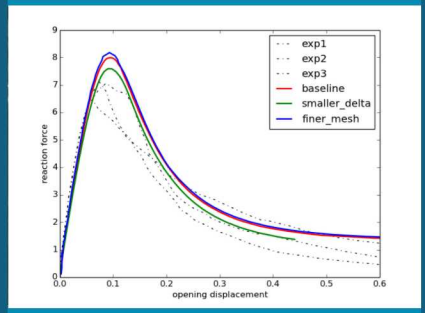
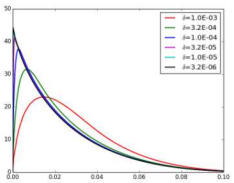
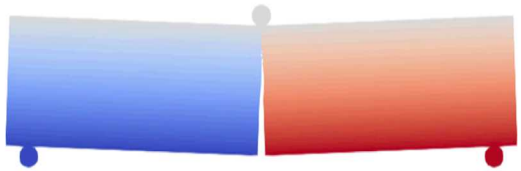
SAND2018-7844C

Variational Peridynamic Fracture

A "phase-field" peridynamic damage model







PRESENTED BY

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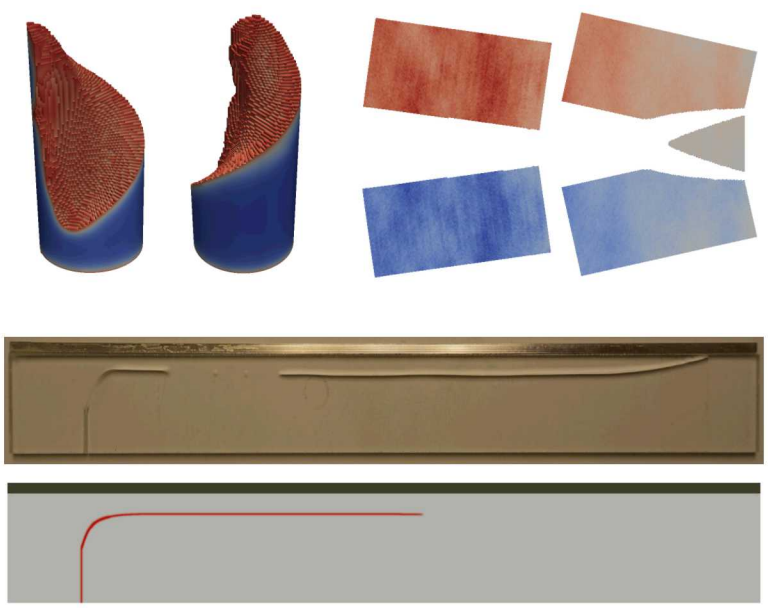
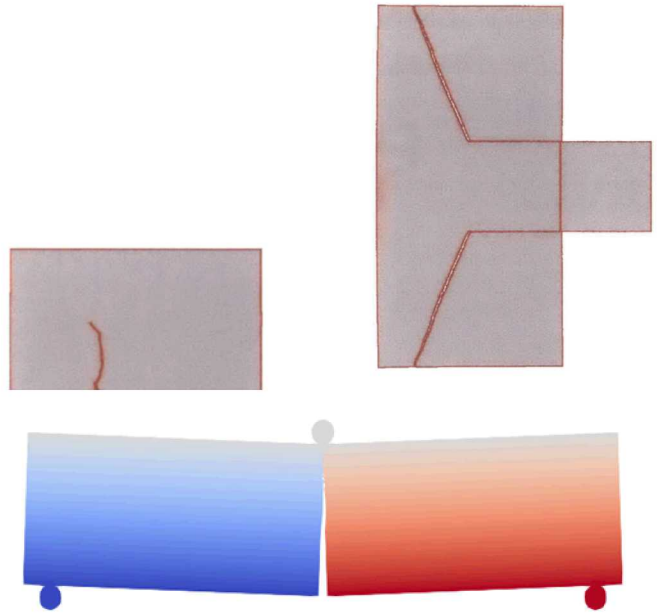
Overview

- Variational fracture and phase-field models
- Variational peridynamic fracture
- Quasi-brittle peridynamics
- Implications

What's the difference?



phase-field



peridynamics

Variational fracture mechanics

Energetic competition between bulk strain energy and surface creation

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

Approximate surface integral by a volume integral

Regularized potential energy:

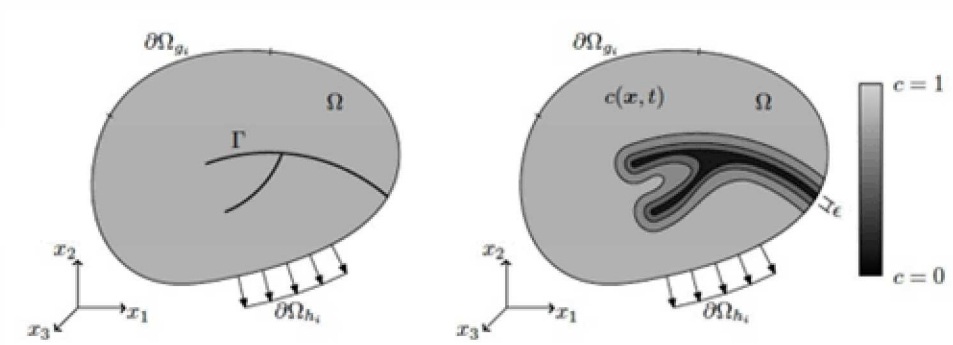
$$\Pi_l(u, d) = \int_{\Omega} \psi_e(\varepsilon^s(u))\, dv + \int_{\Omega} G_c \gamma_l\, dv$$

Crack density:

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

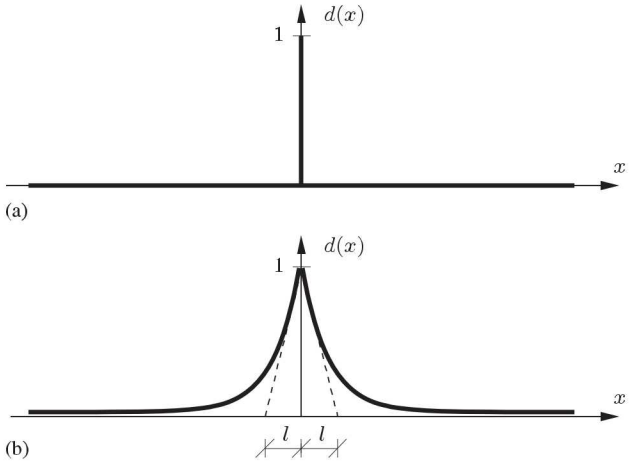
Stress degradation:

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



**The variational approach to fracture*, Bourdin, Francfort, Marigo, 2008

Surface regularization intuition

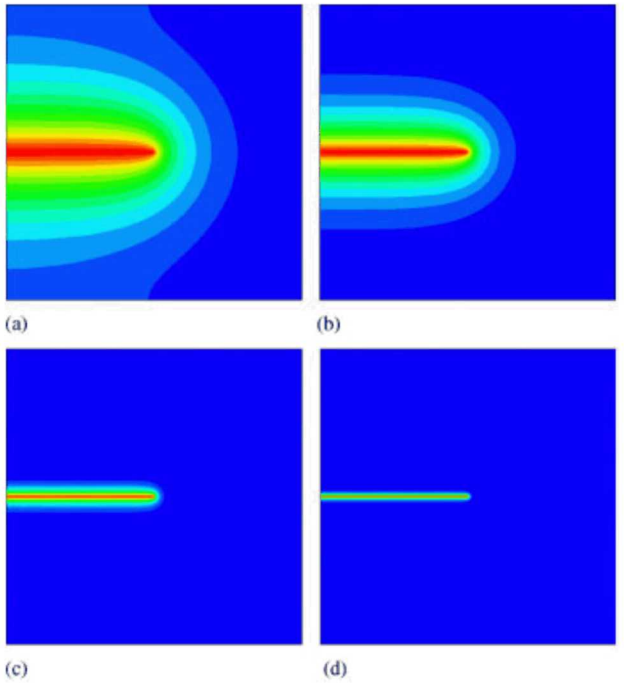


$$d(x) = \mathrm{e}^{-|x|/l}$$

$$d(x) - l^2 d''(x) = 0 \quad \text{in } \mathscr{B}$$

$$I(d) = \frac{1}{2}\int_{\mathscr{B}} \{d^2 + l^2 d'^2\}\,\mathrm{d}V$$

$$I(d = \mathrm{e}^{-|x|/l}) = l\Gamma$$



Regularized crack geometry with different length scales

Miehe, 2010

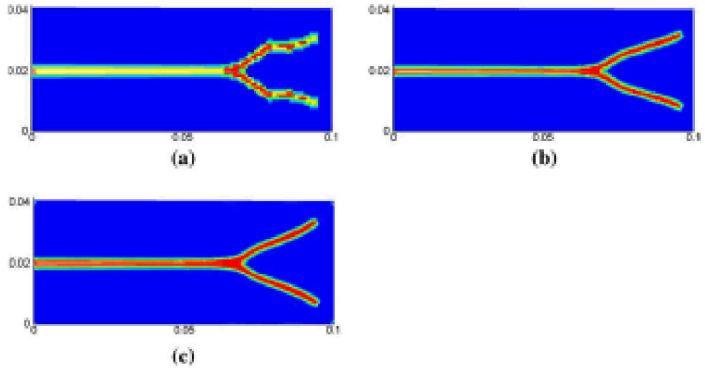
Crack "surface area": $\Gamma_l(d) := \dfrac{1}{2l}\displaystyle\int_{\mathscr{B}} \{d^2 + l^2 d'^2\}\,\mathrm{d}V$

Peridynamic overview

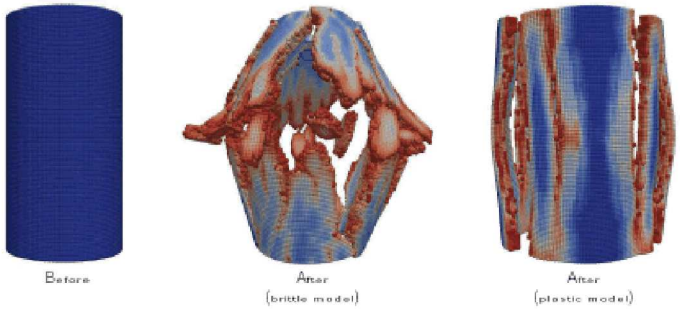
Integral formulation: $\rho \ddot{u}(x,t) = \int_H f(u(x',t) - u(x,t), x' - x)\, dV_{x'} + b(x,t)$

"In peridynamics, cracks are part of the solution, not part of the problem"
- F. Bobaru

Convergence for 2D crack branching:
(Ha, Bobaru 2010)

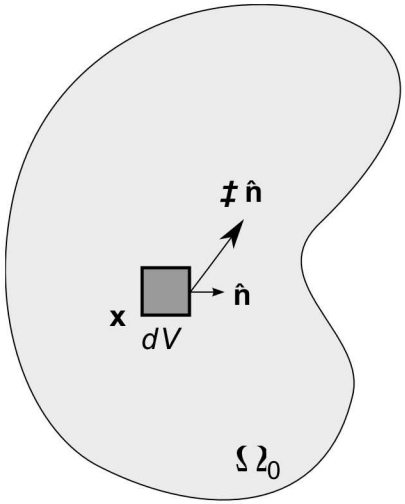


Brittle and Ductile Failure in 3D:
(Parks 2012)

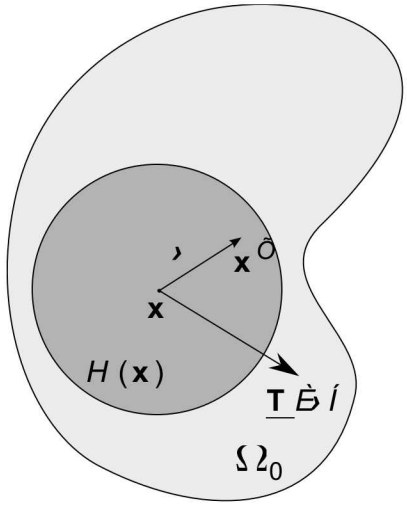


Peridynamic overview

- Integral formulation of continuum mechanics originally proposed by Stewart Silling in 2000.
- Stress is replaced with long-range forces, $\underline{\mathbf{T}}\langle \mathbf{x}, t \rangle$.
- Bond $\xi := \mathbf{x}' - \mathbf{x}$.



Classical control volume, normal $\hat{\mathbf{n}}$ and traction vector $\mathbf{t}\hat{\mathbf{n}}$.



Peridynamic bond ξ and bond-force $\underline{\mathbf{T}}\langle \mathbf{x}, t \rangle$.

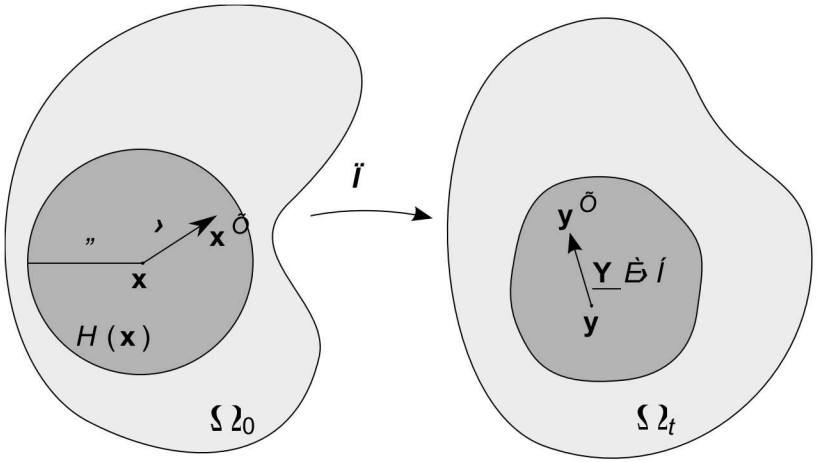
$$\rho\ddot{\mathbf{u}} = \dot{\mathbf{o}} \cdot \mathbf{t}$$

$$\rho\ddot{\mathbf{u}} = \int_{H} \underline{\mathbf{T}}\langle \mathbf{x}, t \rangle - \underline{\mathbf{T}}\langle \mathbf{x}', t \rangle \, d\xi$$

Peridynamic overview

The horizon at x is given

$$H(\mathbf{x}) = \{\xi \in \mathbb{R}^3 \mid (\xi + \mathbf{x}) \in \mathcal{B},\ |\xi| < \delta\}.$$



A vector-state $\underline{\mathbf{A}}[\mathbf{x}]$ at a point $\mathbf{x} \in \mathcal{B}$ is a function

$$\underline{\mathbf{A}}[\mathbf{x}]\langle\xi\rangle : H(\mathbf{x}) \to \mathbb{R}^3.$$

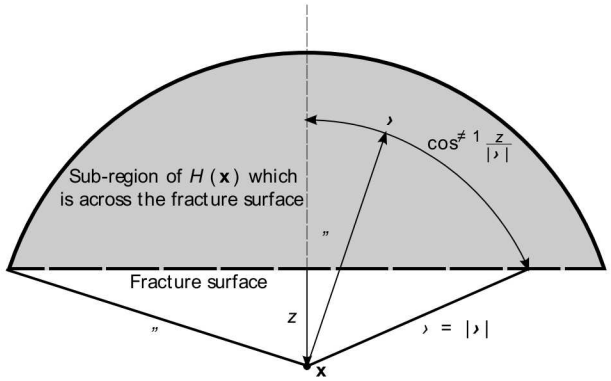
Deformation vector-state: $\boxed{\underline{\mathbf{Y}}[\mathbf{x}]\langle\xi\rangle = \mathbf{y}(\mathbf{x}+\xi) \neq \mathbf{y}(\mathbf{x})}$ $\forall \xi \in H(\mathbf{x})$.

Peridynamic overview

	Classical Continuum	Peridynamics
Deformation Measure	$\mathbf{F} = \nabla \mathbf{y}$	$\underline{\mathbf{Y}}$
Conjugate Force	$\mathbf{P}(\mathbf{F})$	$\underline{\mathbf{T}}(\underline{\mathbf{Y}})$
Angular Momentum	$\mathbf{P}\mathbf{F}^T = \mathbf{F}\mathbf{P}^T$	$\mathbf{0} = \int_H \underline{\mathbf{T}}\langle \mathbf{x}, \boldsymbol{\xi} \rangle \Diamond \underline{\mathbf{Y}}\langle \mathbf{x}, \boldsymbol{\xi} \rangle \, dV_{\boldsymbol{\xi}}$
Elasticity	$\mathbf{P} = \nabla \hat{W}(\mathbf{F})$	$\underline{\mathbf{T}} = \hat{\underline{W}}(\underline{\mathbf{Y}})$
Kinematics	$\det(\mathbf{F}) > 0$	$\underline{\mathbf{Y}}\langle \mathbf{x}, \boldsymbol{\xi} \rangle \neq \mathbf{0}$, for $\|\boldsymbol{\xi}\| \neq 0$

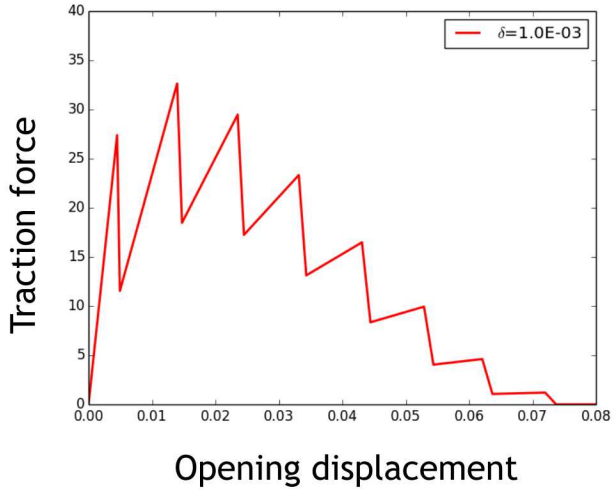
Peridynamic bond-breaking (critical stretch)

$$\int_0^{\delta}\int_{x_1}^{\delta}\int_{-\cos^{-1}(x_1/\xi)}^{\cos^{-1}(x_1/\xi)} w(\xi)\,\xi\,d\theta\,d\xi\,dz = \frac{G_c}{2}$$



Schematic for the domain of integration (modified from Silling 2005).

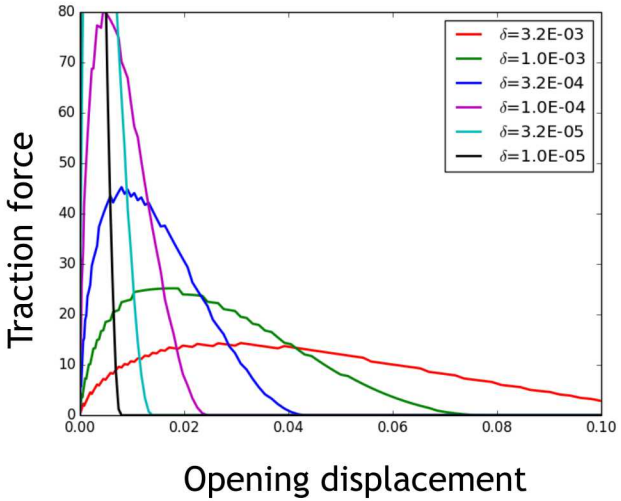
8 particles in horizon



Limitations

1. Discontinuous force-displacement response when discretized
2. Griffith fracture as $\delta \to 0$ (horizon/dispersion tied to process zone size)
3. Extension to state-based peridynamics not obvious
   - Foster 2011 energy based bond-failure criterion
   - Tupek 2014 instantaneous bond-energy failure criterion
   - Tupek 2013 pairwise damage criterion

Varying horizon size



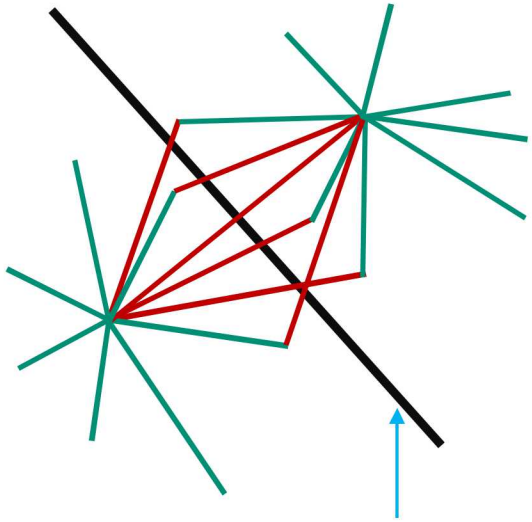
Nonlocal measure of crack surface area

Rethink as geometric *regularization* using damage "state" $\underline{\mathrm{d}}\langle\boldsymbol{\xi}\rangle$

$$\mathcal{A}_\alpha(\underline{\mathrm{d}}) = \int_\Omega \int_{\mathcal{H}(\mathbf{x})} \tilde{\alpha}(\boldsymbol{\xi})\, \underline{\mathrm{d}}\langle\boldsymbol{\xi}\rangle \, d\boldsymbol{\xi}\, d\mathbf{x}$$

where

$$\int_0^\delta \int_{x_1}^\delta \int_{-\cos^{-1}(x_1/\xi)}^{\cos^{-1}(x_1/\xi)} \tilde{\alpha}(\xi)\, \xi \, d\theta \, d\xi \, dx_1 = {}^1\!/_2$$



crack surface area Γ

Then solution

$$\underline{\mathrm{d}}^\star = \arg\left\{ \inf_{\underline{\mathrm{d}} \in \mathcal{W}} \mathcal{A}(\underline{\mathrm{d}}) \right\}$$

satisfies

$$\mathcal{A}_\alpha(\underline{\mathrm{d}}^\star) = \Gamma$$

$$\mathcal{W} = \left\{ \underline{\mathrm{d}} \;\middle|\; \begin{array}{l} 0 \le \underline{\mathrm{d}}\langle\boldsymbol{\xi}\rangle \le 1,\ \forall\, \boldsymbol{\xi} \in \mathcal{H}(\mathbf{x}),\ \forall\, \mathbf{x} \in \Omega, \\ \underline{\mathrm{d}}\langle\boldsymbol{\xi}\rangle = 1 \text{ for bonds cut by surface} \end{array} \right\}$$

Variational peridynamic fracture (general statement)

$$\{\mathbf{y}^\star, \underline{\mathrm{d}}^\star\} = \arg\left\{ \inf_{\underline{\mathrm{d}}\in\mathcal{D},\ \mathbf{y}(\mathbf{x})=\hat{\mathbf{y}} \text{ for } \mathbf{x}\in\Omega_E} \mathcal{L}(\mathbf{y}, \underline{\mathrm{d}}) \right\},$$

$$\mathcal{L}(\mathbf{y}, \underline{\mathrm{d}}) = \int_\Omega \psi(\underline{\mathrm{Y}}, \underline{\mathrm{d}})\, dV + G_c \mathcal{A}_\alpha(\underline{\mathrm{d}}),$$

$$\mathcal{D} = \left\{ \underline{\mathrm{d}} \,\middle|\, 0 \le \underline{\mathrm{d}}_{[\mathbf{x}]}\langle\boldsymbol{\xi}\rangle \le 1,\ \forall\, \boldsymbol{\xi} \in \mathcal{H}(\mathbf{x}),\ \forall\, \mathbf{x} \in \Omega. \right\}$$

Dynamics:

$$\mathcal{S}(\mathbf{y}, \dot{\mathbf{y}}, \underline{\mathrm{d}}) := \int_{t_1}^{t_2} \left[\mathcal{L}(\mathbf{y}, \underline{\mathrm{d}}) - \int_\Omega \frac{\rho}{2} \dot{\mathbf{y}}^2\, d\mathbf{V} \right] dt$$

$$\rho \ddot{\mathbf{y}}_{[\mathbf{x}]}(t) = -\partial_{\mathbf{y}} \mathcal{L}(\mathbf{y}(t), \underline{\mathrm{d}}(t))$$

$$\underline{\mathrm{d}}(t) = \arg \inf_{\underline{\mathrm{d}}(t)\in\mathcal{D}} \mathcal{L}(\mathbf{y}(t), \underline{\mathrm{d}}(t))$$

Specialization to bond-based

Bond-based peridynamic strain energy

$$\psi(\underline{\mathrm{Y}}) = \frac{\kappa}{2}\int_{\mathcal{H}} \tilde{\omega}(\xi)\,\underline{\varepsilon}^2\langle\boldsymbol{\xi}\rangle\,d\xi$$

$$\int_{\mathcal{H}} \tilde{\omega}(\xi)\,d\xi = 1$$

$$\underline{\varepsilon}\langle\boldsymbol{\xi}\rangle = \frac{|\mathbf{y}'-\mathbf{y}| - |\mathbf{x}'-\mathbf{x}|}{|\mathbf{x}'-\mathbf{x}|}$$

Variational bond-based peridynamic fracture

$$\psi(\underline{\varepsilon},\underline{\mathrm{d}}) = \frac{\kappa}{2}\int_{\mathcal{H}} \tilde{\omega}(\xi)\,\underline{\varepsilon}^2\langle\boldsymbol{\xi}\rangle\,\hat{g}(\underline{\mathrm{d}}\langle\boldsymbol{\xi}\rangle)\,d\boldsymbol{\xi} + G_c\int_{\mathcal{H}} \tilde{\alpha}(\xi)\hat{h}(\underline{\mathrm{d}}\langle\boldsymbol{\xi}\rangle)\,d\boldsymbol{\xi}$$

Simplifies to bond-wise minimization problem

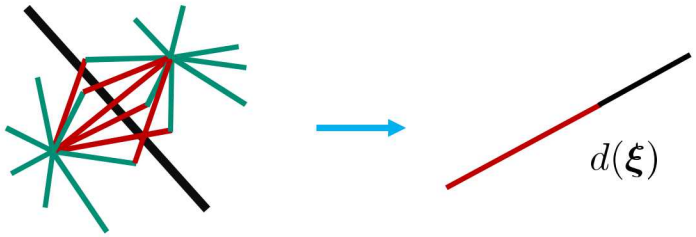
$$d^\star = \arg\min_{d|0\le d\le 1}\left\{\bar{\psi}\hat{g}(d) + \eta(\xi)\hat{h}(d)\right\}$$

$$\bar{\psi} := \tfrac{\kappa}{2}\underline{\varepsilon}^2\langle\boldsymbol{\xi}\rangle$$

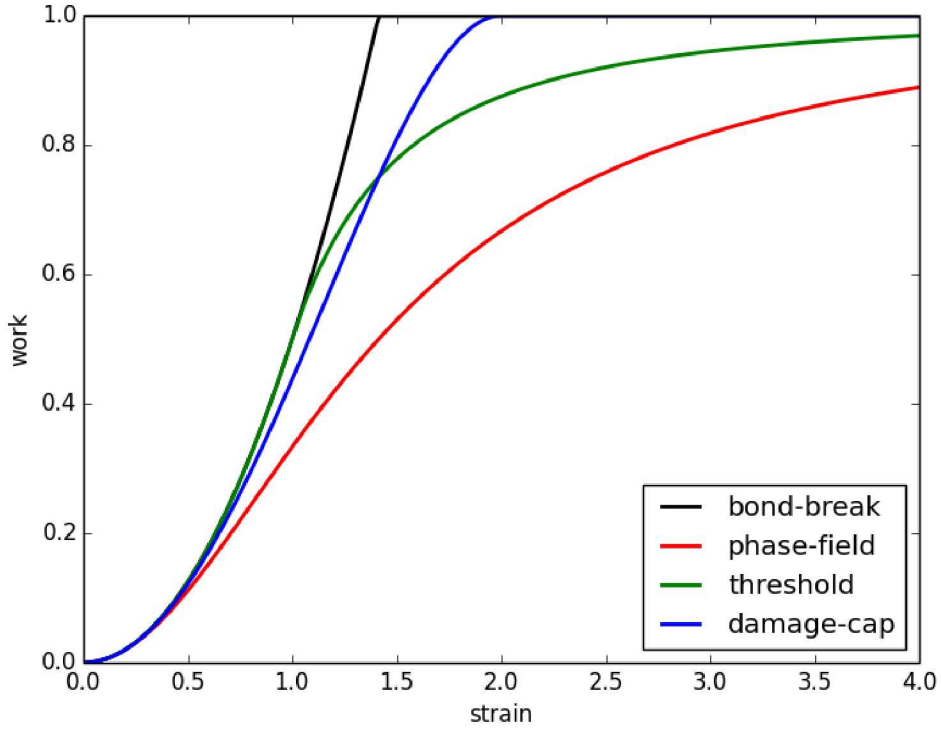
$$\eta(\xi) := G_c\tfrac{\tilde{\alpha}(\xi)}{\tilde{\omega}(\xi)}$$

$$\hat{\omega}(\xi) = \frac{1}{\delta}\left(1-\frac{\xi}{\delta}\right)$$

$$\hat{\alpha}(\xi) = \frac{3}{\delta^2}\left(1-\frac{\xi}{\delta}\right)$$



Degradation and surface potential options



bond-break (critical stretch)

$$g_1(d) = 1 - d,\ h_1(d) = d$$

phase-field

$$g_2(d) = (1 - d)^2,\ h_2(d) = d^2$$

threshold

$$g_2(d) = (1 - d)^2,\ h_1(d) = d$$

damage-cap

$$g_1(d) = (1 - d),\ h_2(d) = d^2$$

- Effectively a pair-wise potential
- Satisfy Lipton's conditions for convex-concave potentials?

Lipton, 2014

Degradation functions:

$$g_1(d) = 1 - d$$

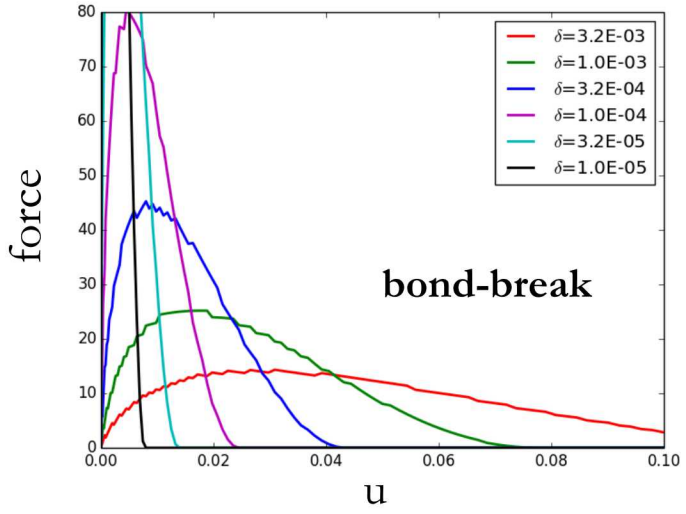
$$g_2(d) = (1 - d)^2$$

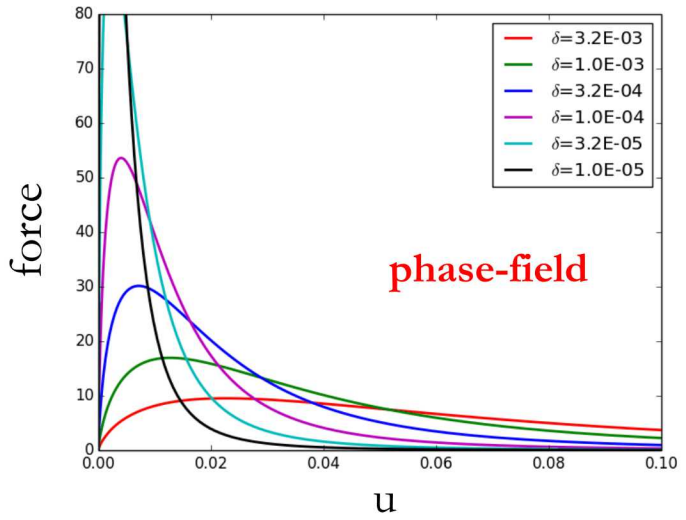
Damage potentials:

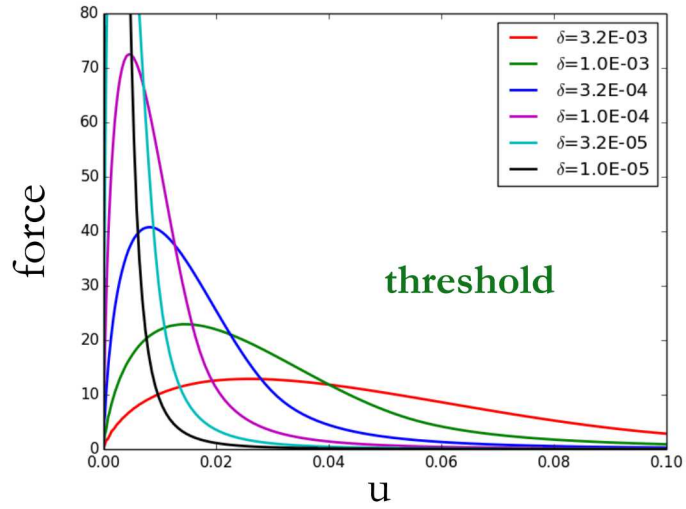
$$h_1(d) = d$$

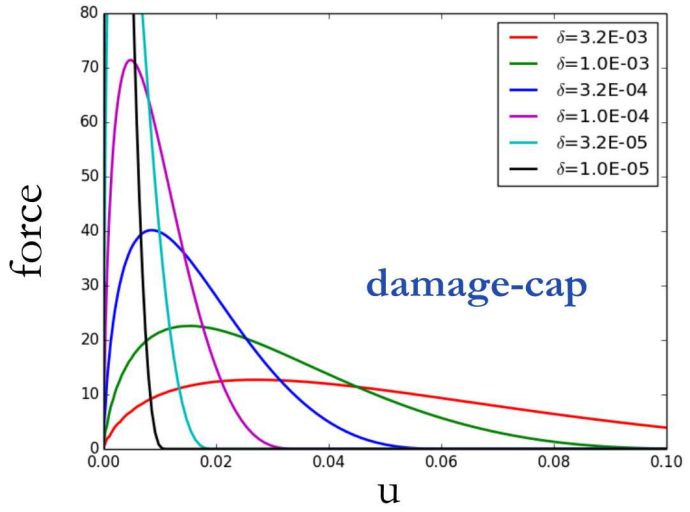
$$h_2(d) = d^2$$

Effective traction-separation for prescribed motion

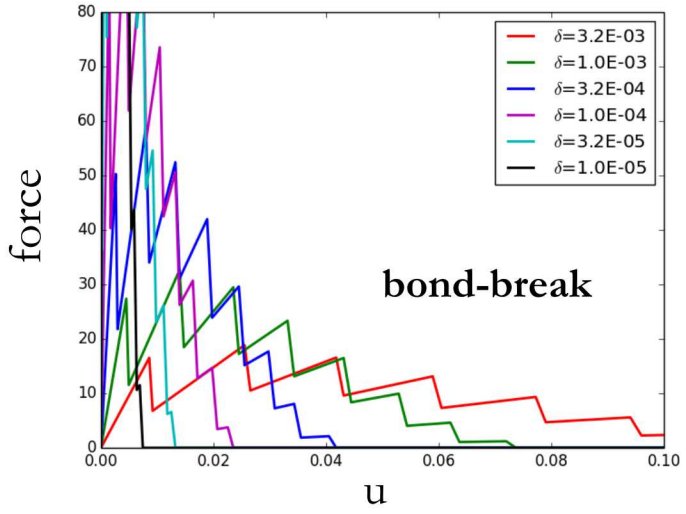


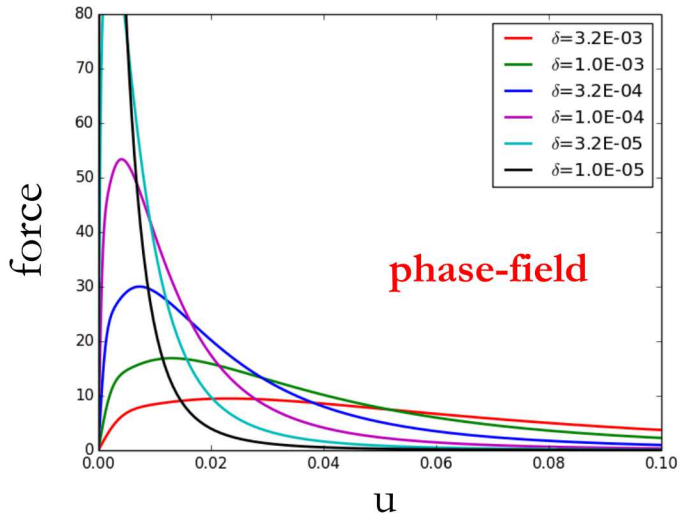


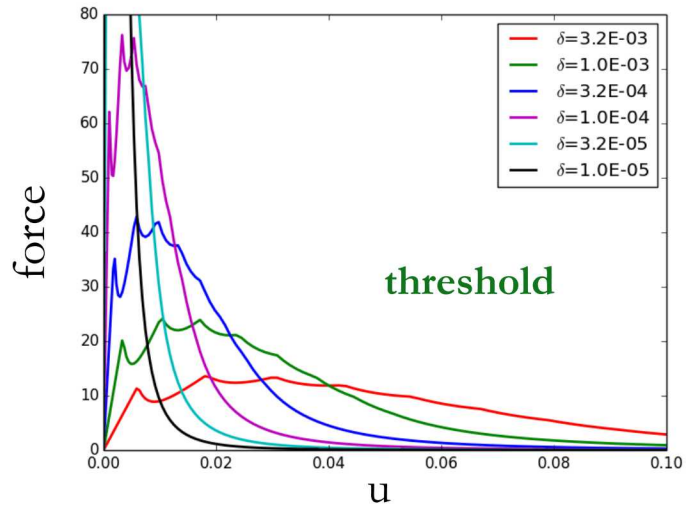


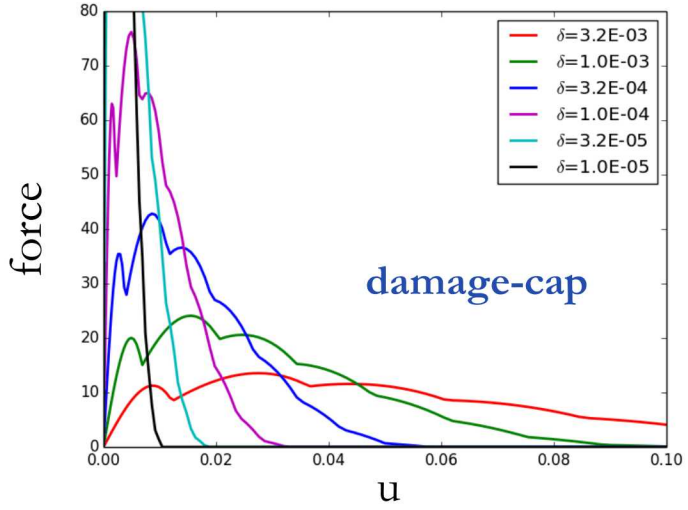


Effective traction-separation for prescribed motion (coarse mesh)

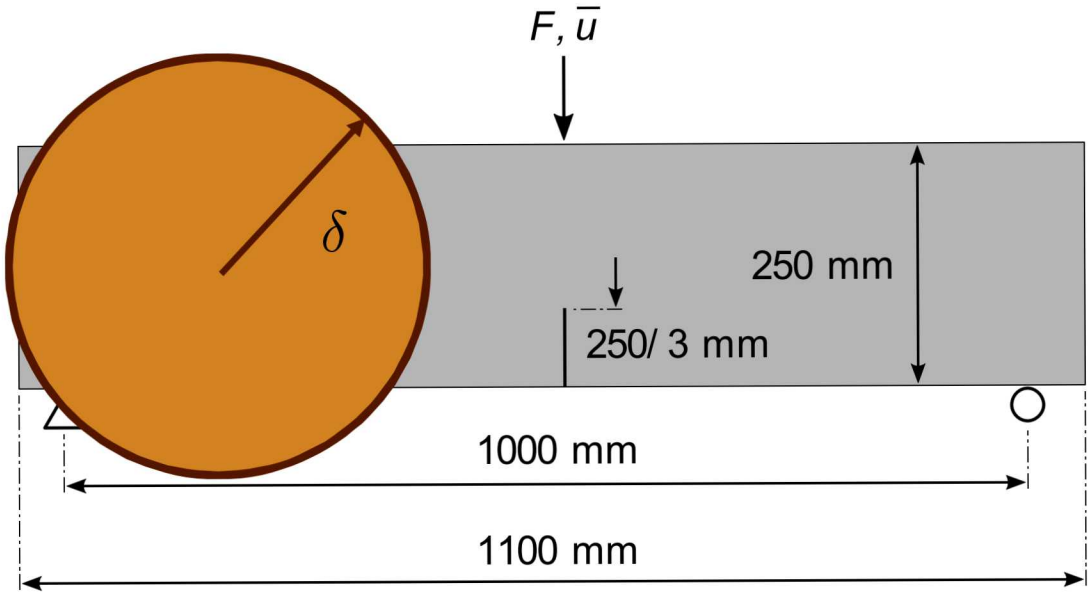








Quasi-brittle variational peridynamic fracture



Three-point bend test of concrete

Nominal bulk properties:

E = 32 GPa □ = 0.25 σ_c = 4.15 MPa G_c = 0.16 N/ mm

Critical stretch model says: $\varepsilon_c^2 = \frac{5G_c}{9\kappa\delta}$ → $\delta = 248$ mm

Roesler et al., 2007

Geelen et al., 2018

Cohesive degradation functions

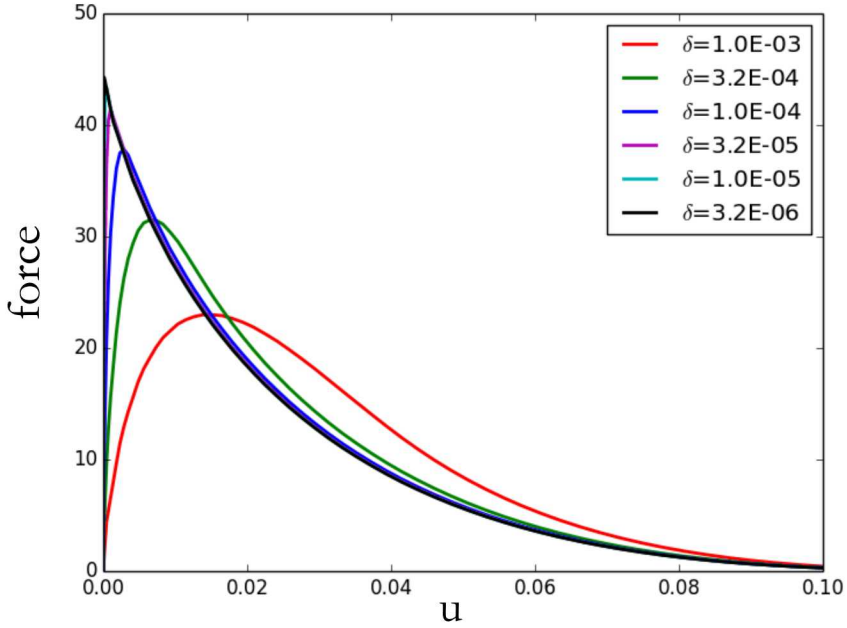
Bond-wise free energy: $\psi_\xi(d) = \bar{\psi}\, g(d) + \frac{\eta}{\delta} G_c\, d$

Stationarity: $\psi'_\xi(d) = \bar{\psi}\, g'(d) + \frac{\eta}{\delta} G_c = 0$

Cohesive degradation: $g'(0) = -m, \quad m = \frac{G_c\, \eta}{\bar{\psi}_c \delta}$

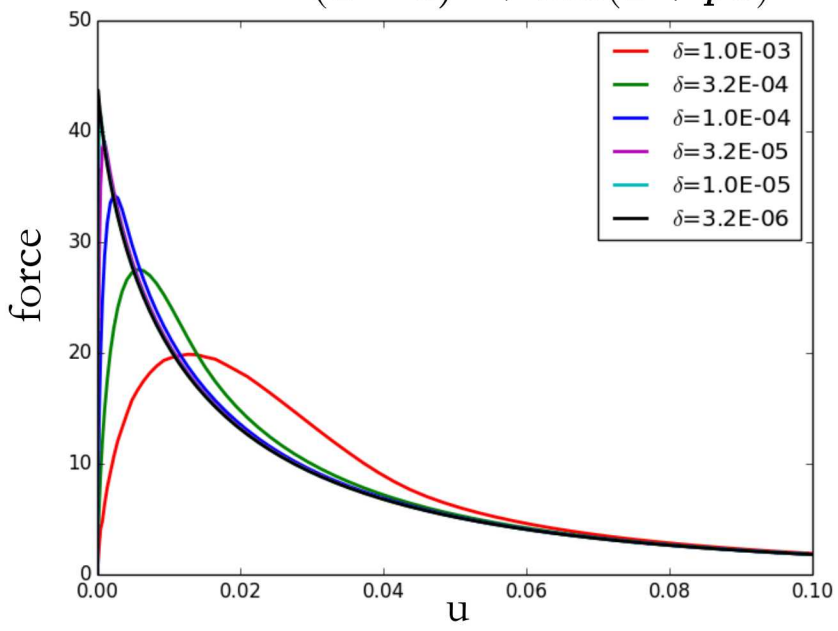
Quasi-linear degradation Geelen et al., 2018

$$g_l(d) = \frac{1-d}{1-d+md}$$

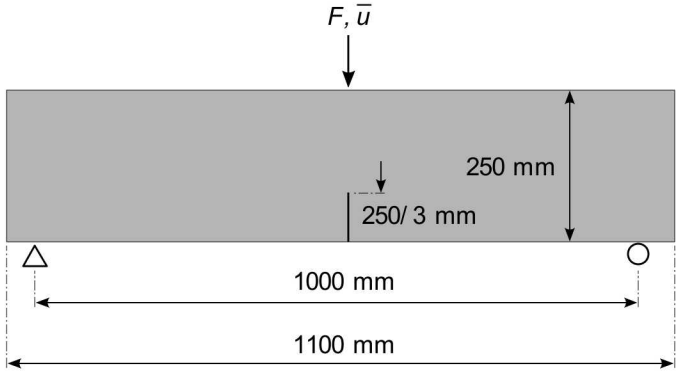


Lorentz degradation Lorentz et al., 2011

$$g_q(d) = \frac{(1-d)^2}{(1-d)^2 + md(1+pd)}$$



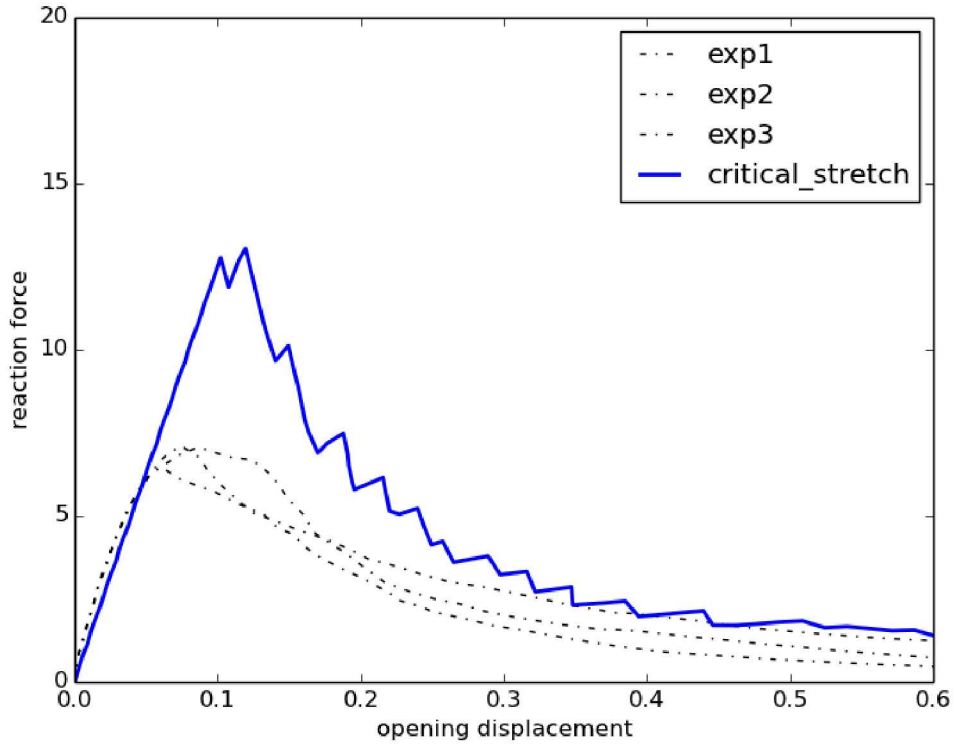
Three-point bend simulations (preliminary, 2D)



Implemented in Peridigm

initial state

final state



baseline $\delta = 15$ mm

smaller $\delta = 12$ mm

baseline mesh: 55,000 particles

finer mesh: 98,000 particles

Practical considerations

Irreversibility:

- Bond-damage only increases
- Modify constraint on the damage-state evolution

$$\mathcal{D} = \left\{ \underline{\mathrm{d}} \;\middle|\; \dot{d}_{[\mathbf{x}]}\langle\boldsymbol{\xi}\rangle \geq 0, \; 0 \leq \underline{\mathrm{d}}_{[\mathbf{x}]}\langle\boldsymbol{\xi}\rangle \leq 1, \; \forall\, \boldsymbol{\xi} \in \mathcal{H}(\mathbf{x}), \; \forall\, \mathbf{x} \in \Omega. \right\}$$

Tension/compression asymmetry

- Decompose bond-strain into positive and negative energetic contributions
- Only degrade the tensile part and only damage when in tension

$$\psi(\underline{\varepsilon}, \underline{\mathrm{d}}) = \frac{\kappa}{2} \int_{\mathcal{H}} \tilde{\omega}(\xi) \left(\underline{\varepsilon}_+^2\langle\boldsymbol{\xi}\rangle \, \hat{g}(\underline{\mathrm{d}}\langle\boldsymbol{\xi}\rangle) + \underline{\varepsilon}_-^2\langle\boldsymbol{\xi}\rangle \right) d\boldsymbol{\xi} + G_c \int_{\mathcal{H}} \tilde{\alpha}(\xi) \hat{h}(\underline{\mathrm{d}}\langle\boldsymbol{\xi}\rangle) \, d\boldsymbol{\xi}$$

$$\underline{\varepsilon}_+\langle\boldsymbol{\xi}\rangle = \begin{cases} \underline{\varepsilon}\langle\boldsymbol{\xi}\rangle & \text{for } \underline{\varepsilon}\langle\boldsymbol{\xi}\rangle \geq 0 \\ 0 & \text{otherwise} \end{cases}$$

$$\underline{\varepsilon}_-\langle\boldsymbol{\xi}\rangle = \underline{\varepsilon}\langle\boldsymbol{\xi}\rangle - \underline{\varepsilon}_+\langle\boldsymbol{\xi}\rangle.$$

State-based bond-breaking criterion

Elastic free energy density: $\hat{A}(\mathbf{x}) = \frac{1}{2}\left(\mathrm{tr}\hat{E}\left(\underline{\varepsilon}\right)\right)^2 + \mu\,\mathrm{tr}\hat{E}\left(\underline{\varepsilon}^2\right)$

Bond integrity: $\underline{\mu}(\boldsymbol{\xi}) = \{1 \text{ for intact bonds}, \quad 0 \text{ for severed bonds}\}$

There are multiple ways to define the bond-energy:

Average bond-energy

$$\underline{s}_{ave}(\boldsymbol{\xi}) := \frac{1}{2}\mathrm{tr}\hat{E}\left(\underline{\varepsilon}\right) + \mu\underline{\varepsilon}(\boldsymbol{\xi})$$

Instantaneous bond-energy

$$\underline{s}_{inst}(\boldsymbol{\xi}) := \mathrm{tr}\hat{E}\left(\underline{\varepsilon}\right) + \mu\underline{\varepsilon}(\boldsymbol{\xi})$$

Foster, et al. 2011 proposed the work done on the bond:

$$\underline{s}_{work}(\boldsymbol{\xi})(t) := \int_0^t \underline{\mathbf{T}}(\boldsymbol{\xi}) \cdot \underline{\dot{\mathbf{Y}}}(\boldsymbol{\xi})\, dt.$$

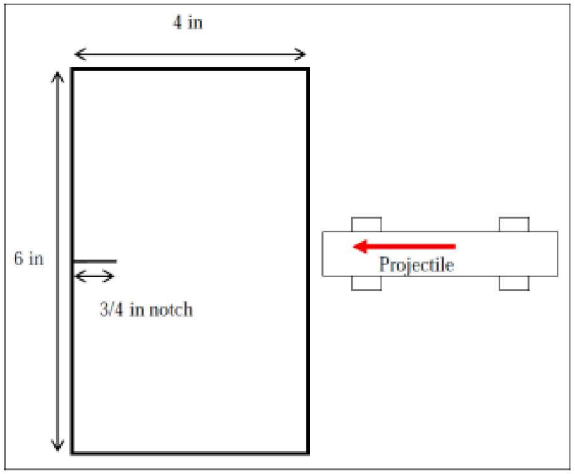
We use the **instantaneous bond-energy**: $\underline{s}_{inst}(\boldsymbol{\xi}) := \hat{A}_{,\varepsilon}\underline{\varepsilon}(\boldsymbol{\xi})$

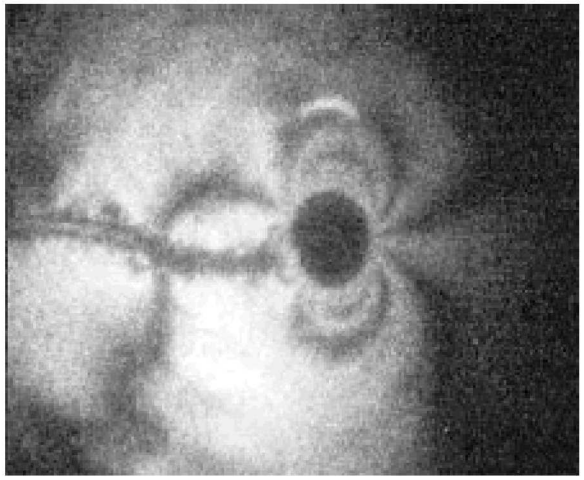
- The instantaneous bond-energy is the energy dissipated when severing a single bond (all other bonds held fixed).
- In general: $\underline{s}_{inst} \neq \underline{s}_{work}$.

Sandia National Laboratories

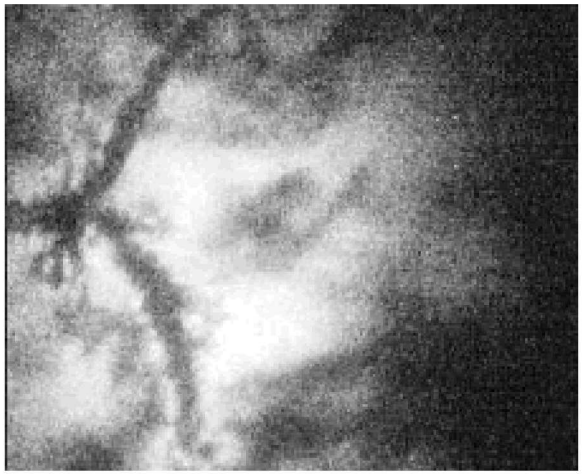
Beyond bond-based

- Mode-I crack propagation for low impact velocities
- Crack branching at higher velocities
- ρ = 1180 kg/ m^3, E = 3.5 GPa, ν = 0.35, G_c = 400 J/ m^2





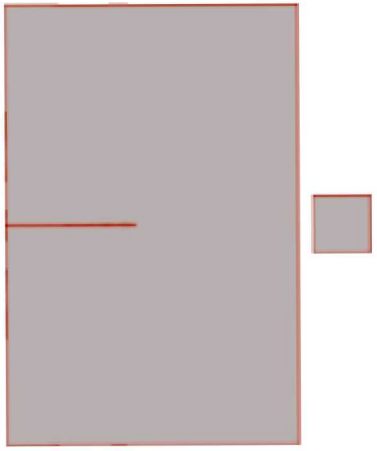
v_0 = 50.5 m/ s



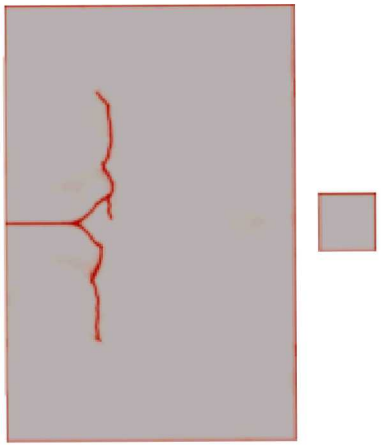
v_0 = 65.9 m/ s

Coherent gradient sensing: experimental results of Umberger and Love, 2010.

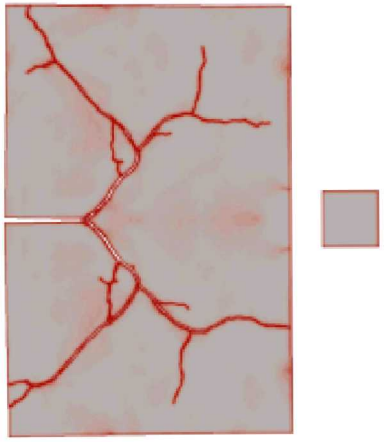
Crack branching vs. impact velocity



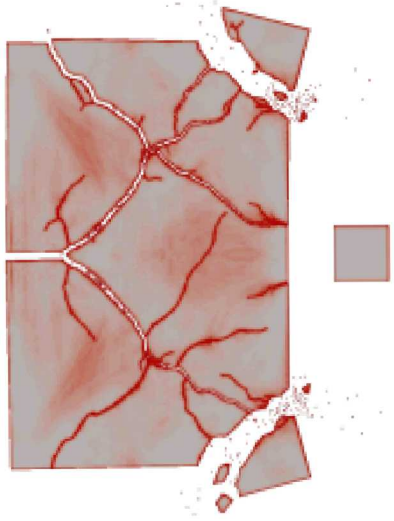
v_0 = 15 m/ s



v_0 = 25 m/ s

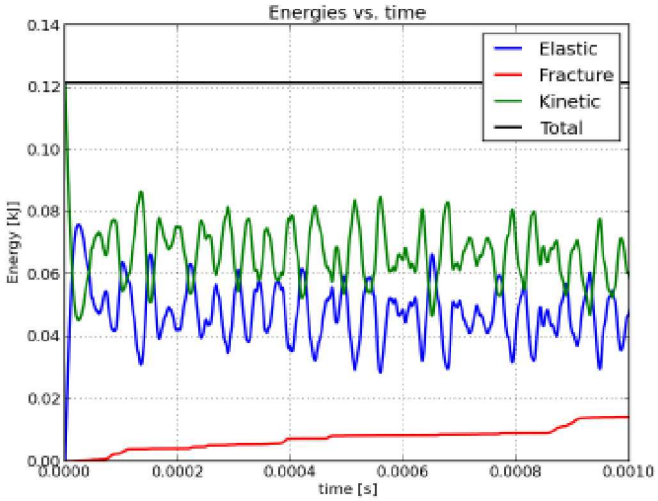


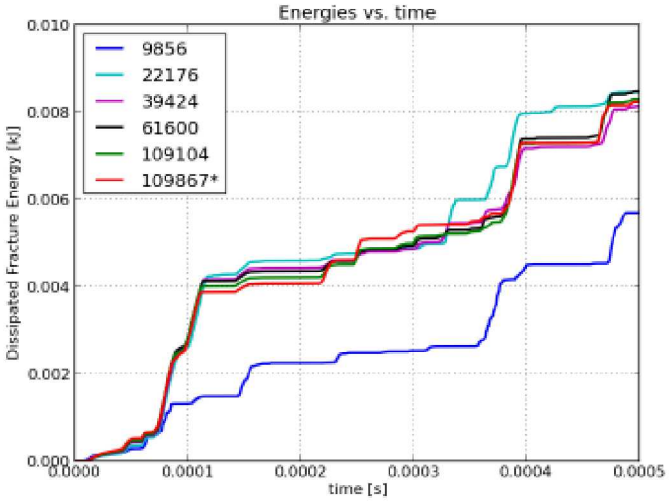
v_0 = 35 m/ s



v_0 = 50 m/ s

Beyond bond-based peridynamics

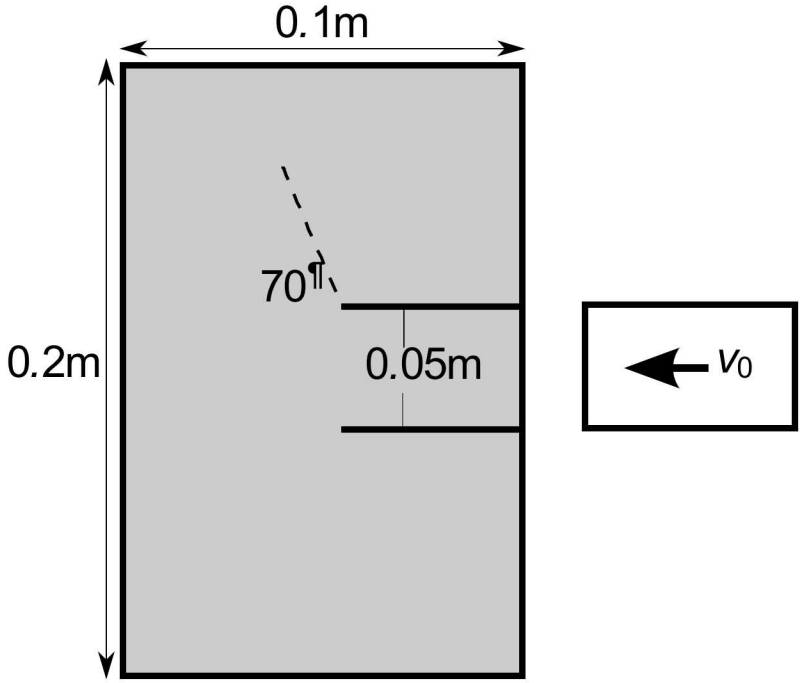




Dissipated energy over time for varying particle densities, with v_0 = 15 m/ s.

number of discrete particles	crack length	dissipated energy	cohesive energy
9,856	4 mm	2.5 J	**620 J/ m^2**
22,176	12 mm	4.6 J	**400 J/ m^2**
39,424	11 mm	4.4 J	**420 J/ m^2**
61,600	11 mm	4.4 J	**410 J/ m^2**
109,104	10 mm	4.2 J	**420 J/ m^2**
109,867 (unstructured)	10 mm	4.1 J	**410 J/ m^2**

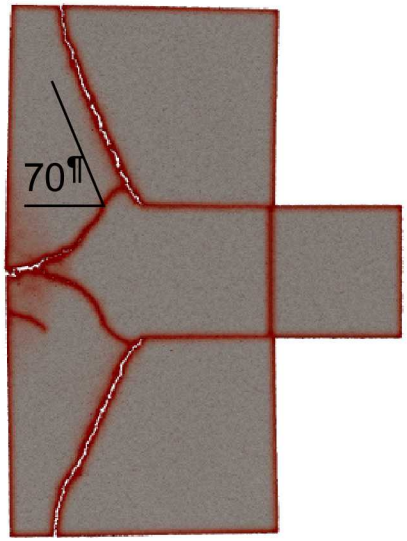
Kalthoff-Winkler Test



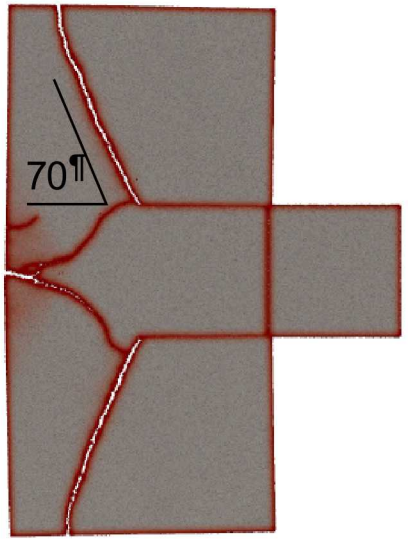
- Based on experiments by Kalthoff, Winkler 1987.
- $\rho = 8000\ \mathrm{kg/m^3}$, $E = 190$ GPa, $\nu = 0.3$ and $G_c = 22{,}000\ \mathrm{J/m^2}$.
- Impact velocity: $v_0 = 16\ \mathrm{m/s}$.
- Experimental crack propagation angle of 70¶.

Kalthoff-Winkler Validation

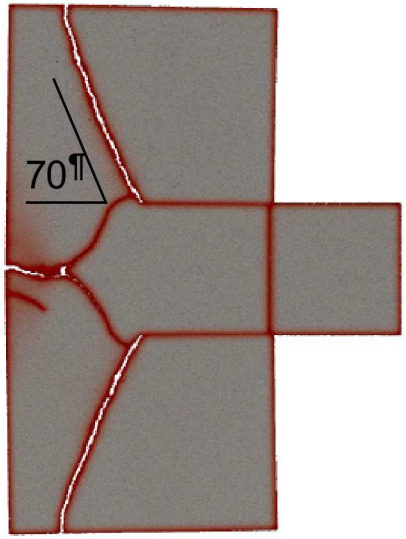
h = 1.2 mm
” = 5.0 mm



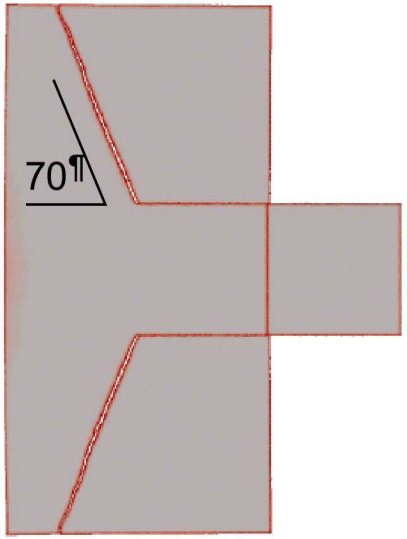
h = 1.0 mm
” = 5.0 mm



h = 0.8 mm
” = 5.0 mm



h = 0.4 mm
” = 1.8 mm



Beyond bond-based peridynamics

Extension to state-based is obvious … but *not trivial* to implement!

Most straightforward extension (linear peridynamic solid with damage):

$$\psi(\underline{\varepsilon}, \underline{\mathrm{d}}) = \frac{\bar{\kappa}}{2}\left(\int_{\mathcal{H}} \tilde{\omega}(\xi)\, \underline{\varepsilon}\langle \boldsymbol{\xi}\rangle\, \hat{g}(\underline{\mathrm{d}}\langle \boldsymbol{\xi}\rangle)\, d\boldsymbol{\xi}\right)^2 + \frac{\bar{\lambda}}{2}\int_{\mathcal{H}} \tilde{\omega}(\xi)\, \underline{\varepsilon}^2\langle \boldsymbol{\xi}\rangle\, \hat{g}(\underline{\mathrm{d}}\langle \boldsymbol{\xi}\rangle)\, d\boldsymbol{\xi} + G_c \int_{\mathcal{H}} \tilde{\alpha}(\xi)\hat{h}(\underline{\mathrm{d}}\langle \boldsymbol{\xi}\rangle)\, d\boldsymbol{\xi}$$

$$\nu \neq \frac{1}{4}$$

Requires solving a *quadratic programming problem* over each horizon!

Also seems to imply that neither

- Foster 2011 bond-work criterion
- Tupek 2014 instantaneous energy criterion

will asymptotically dissipate G_c as $\delta \to 0$ (under general loadings).

Undiscussed features and opportunities

- Other features not covered
  - Evidence of numerical convergence (more work needed)
  - Obvious how to incorporate irreversibility
  - Obvious how to decompose into positive and negative strains
- Opportunities (challenges)
  - Leverage optimization structure for better performance/robustness
  - Mathematical analysis
  - Mixed-mode cohesive models
  - Anisotropy
  - ***Plasticity***

Established a clear connection between peridynamic and phase-field fracture modeling!

Developments in one field can now easily be ported to the other
Demonstrated how to decouple the horizon size from process zone size

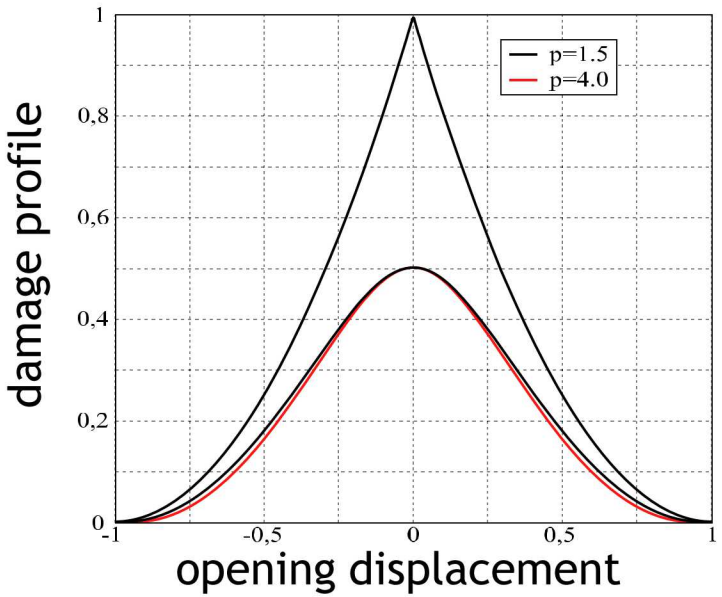
A phase field cohesive model

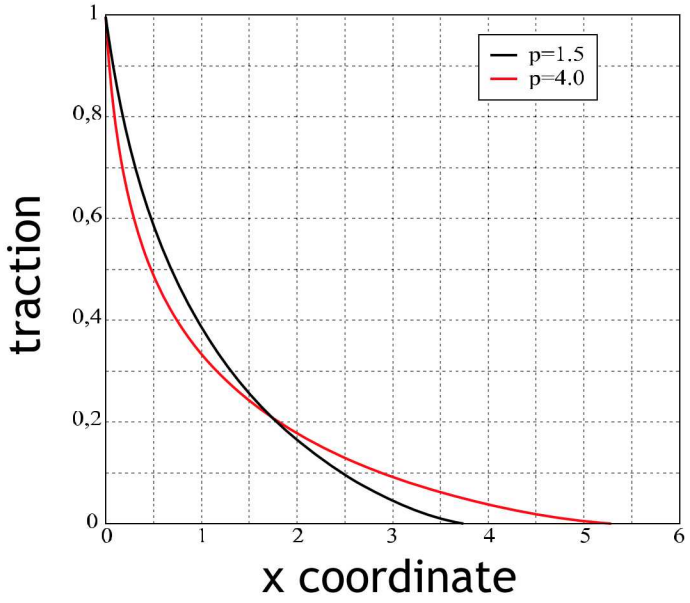
- Regularized phase field model by Lorentz, et al. 2011
- Shown to converge to cohesive zone model as $L \to 0$

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

$$g'(d)\psi_e^+ + k = c\nabla^2\phi$$ Phase field equation

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





Parameters of damage model

Depends on cohesive fracture parameters:

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

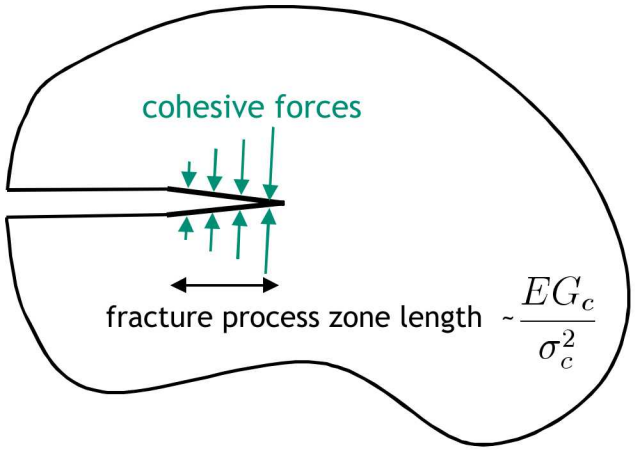
Physically justified constraints on the parameters ensure

- Regularization length scale resolves fracture process zone

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

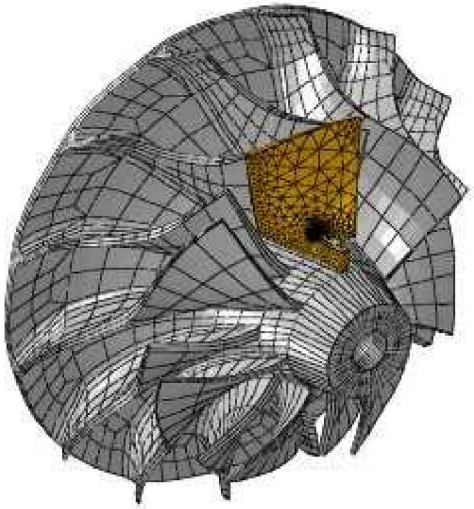
- Monotonic stress decay

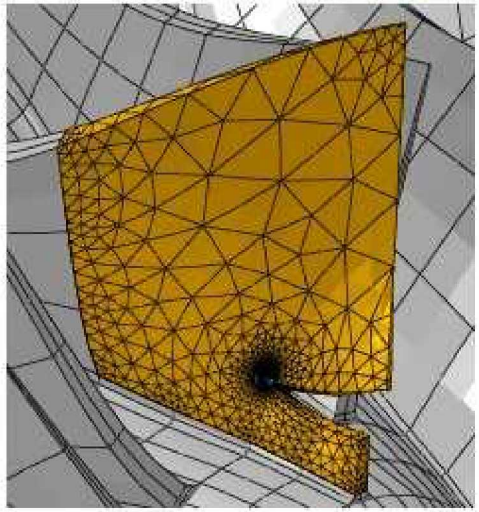
$$p \geq 1$$

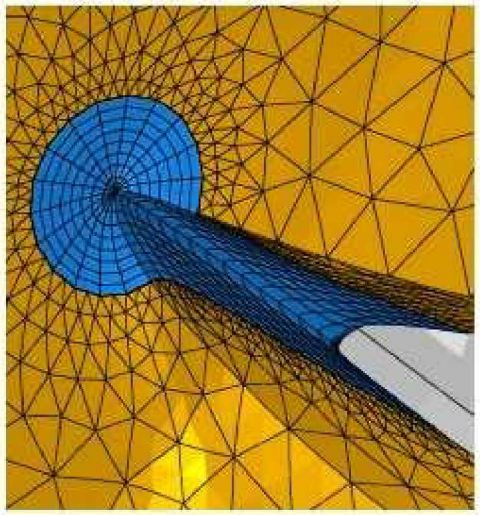


Computational challenges of fracture

- **Fracture is characterized by the separation/failure of material, leading to the formation of new surfaces!**
- **Both the mechanics of fracture and the geometry of the cracks are difficult to model and simulate with finite elements, especially in three dimensions**



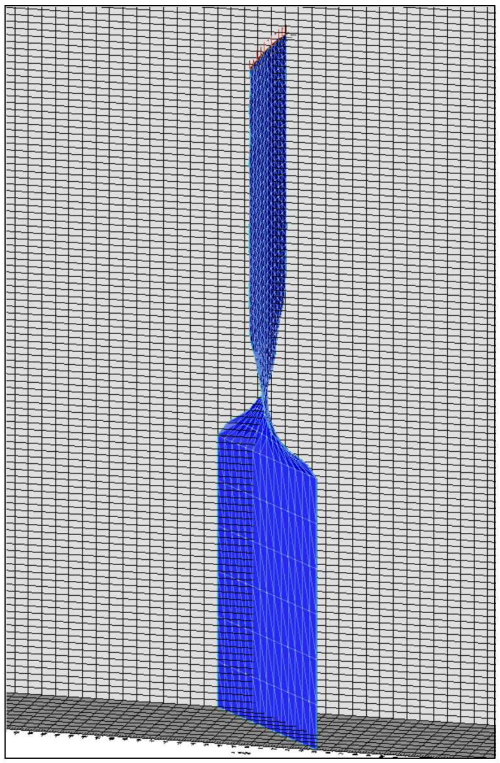




Slide borrowed from Prof. John Dolbow

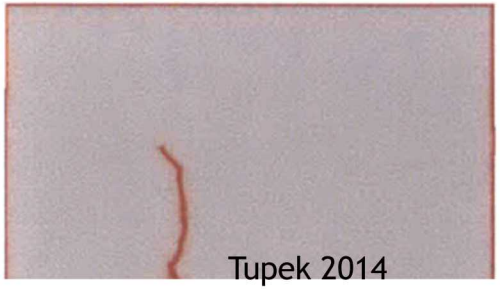
Numerical Fracture Renaissance

Several promising fracture methods have emerged in recent years



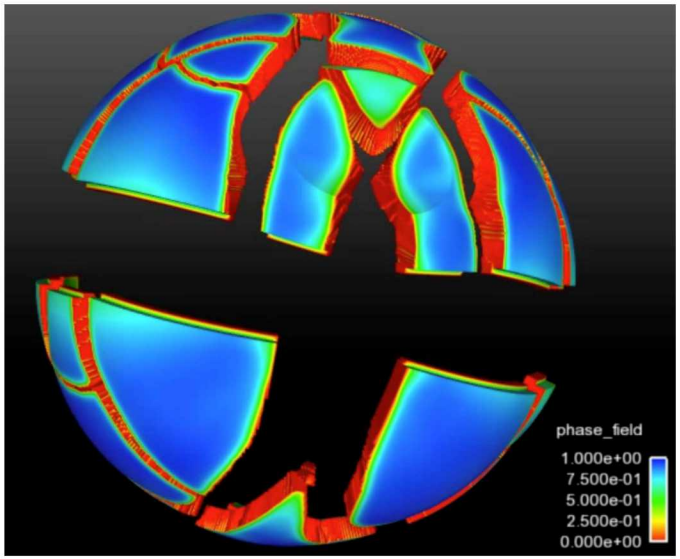
Duarte 2011

GFEM / XFEM



Tupek 2014

Peridynamics



Dolbow, Stevens 2015

Phase field

Overview

Motivations for phase-field fracture

- Regularization of ill-posed local damage models
- Regularization of variational fracture mechanics

Connections to

- LEFM
- gradient damage models
- cohesive models

Some results

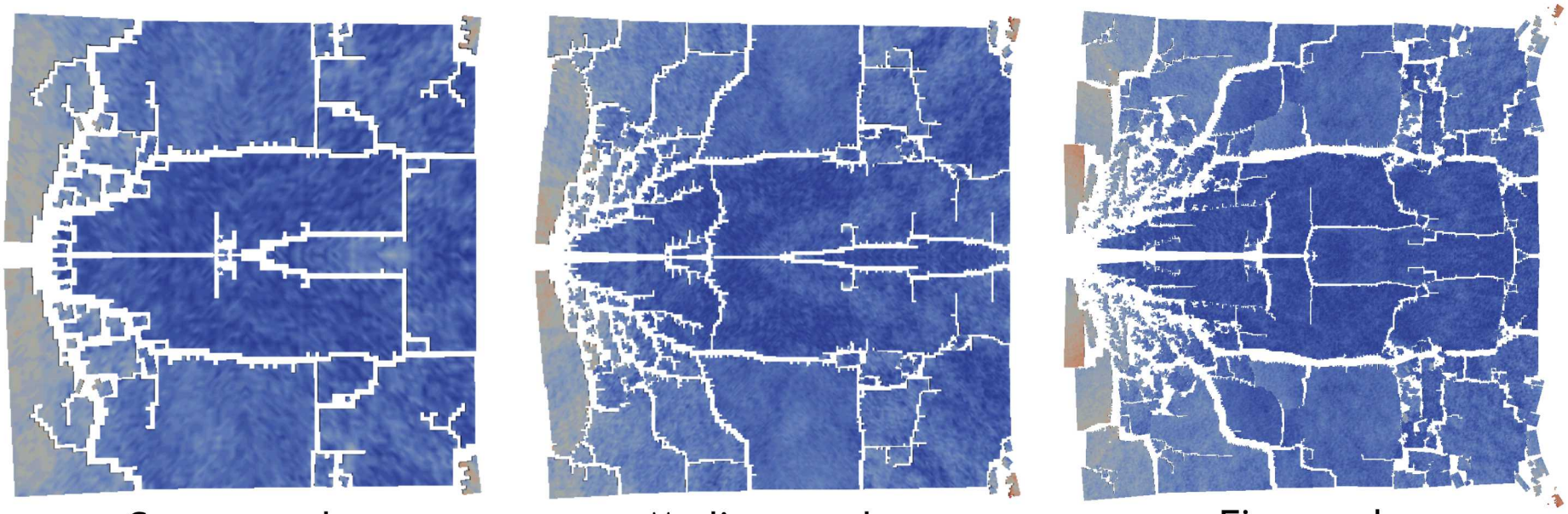
Ongoing work

Classical damage models: ill-posed

Fracture modeling is critical to predicting the performance and reliability of many Sandia components and systems

Most local damage 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 local damage model

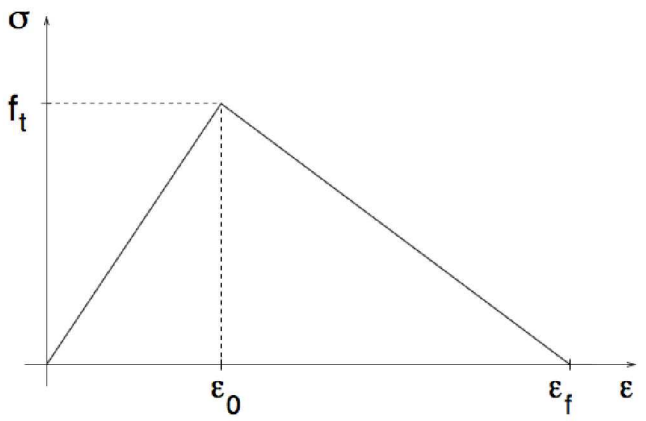
Consider a purely local model of damage

Stress-strain relationship

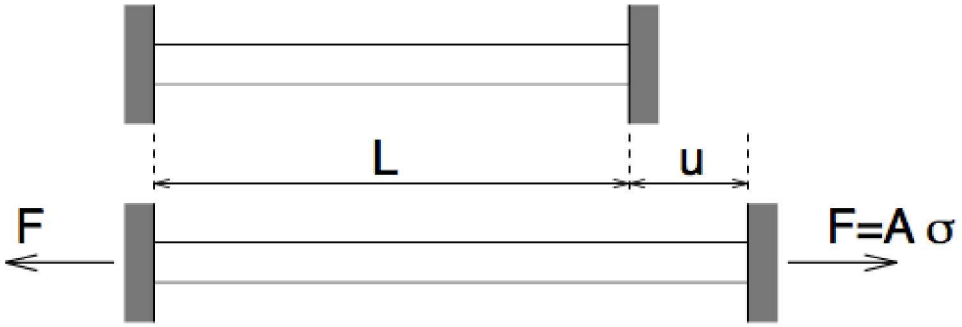
$$\sigma(x,t) = (1 - d(x,t))C\varepsilon(x,t)$$

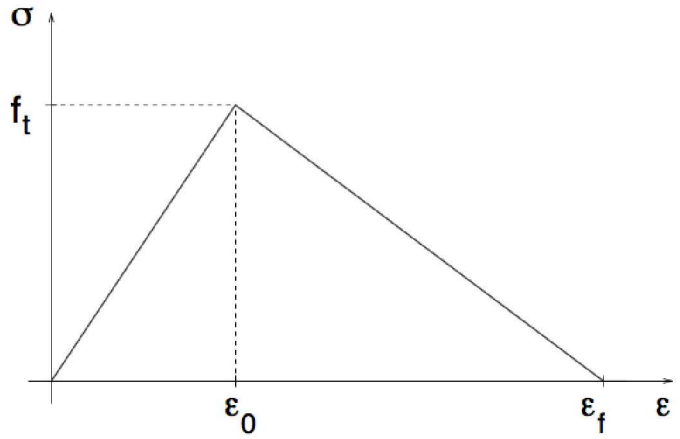
Strain-displacement

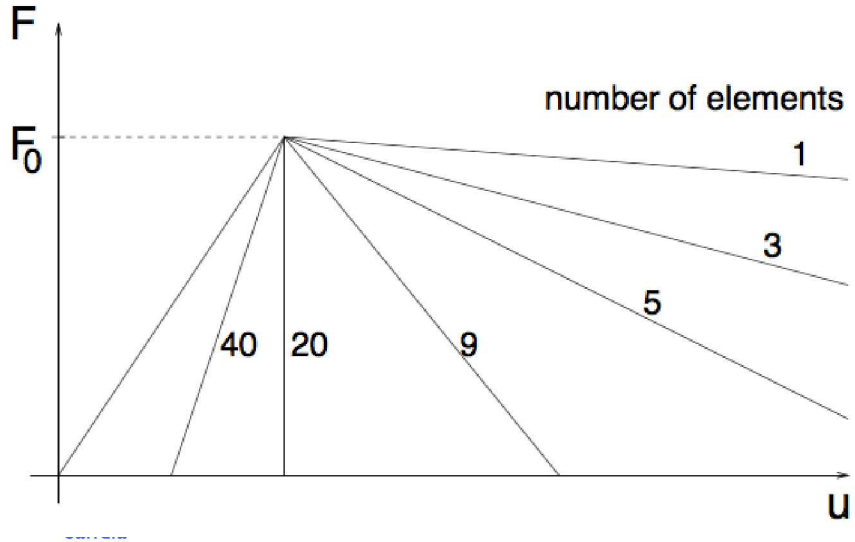
$$\varepsilon(x,t) = \nabla^{s} u(x,t)$$



Classical local damage models: non-convergent







Jirasek, 2002

Gradient damage

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

$$d(\cdot, t)) = D \quad \max_{x \in \Omega, \tau \le t} \tilde{Y}(x, \tau)$$

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)

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

Variational fracture mechanics

Direct extension of Griffith's original idea

Emphasizes energy dissipation due to surface creation

(vs. fracture toughness)

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

Large literature with validation and existence/uniqueness proofs

Similar to max-energy-release-rate crack direction criteria

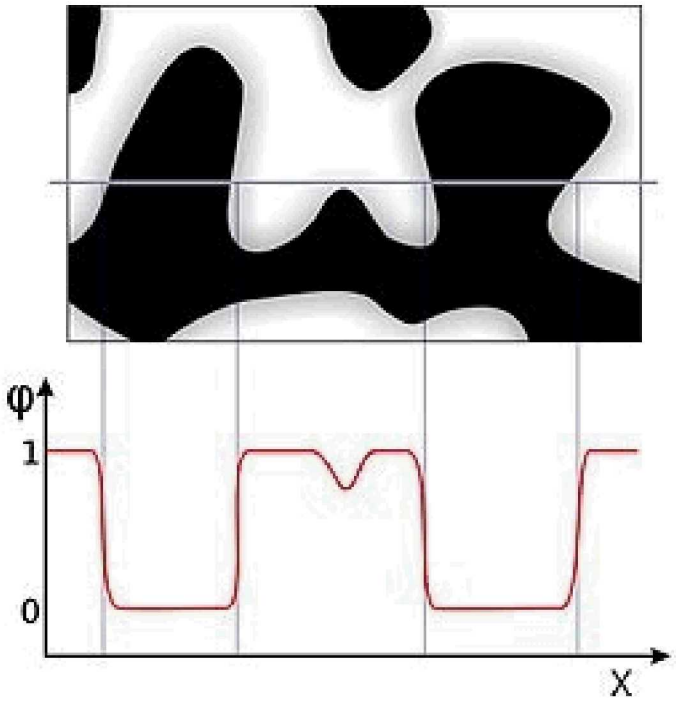
Generalizes to branching, discrete crack jumps, etc.

Reduces to LEFM in applicable cases

"The variational approach to fracture", Bourdin, Francfort, Marigo, 2008

Phase field models

- **Phase field models are mathematical models for solving interfacial problems!**
- **The method substitutes boundary conditions at the interface by a PDE for an auxiliary field, called the phase field, that takes the role of an order parameter!**
- **Values of the phase field are used to identify regions of the domain!**
- **As the phase field is evolved in time, the geometry of the interface (or crack) is likewise evolved**



A two-phase microstructure (top) and the phase-field variable along a horizontal line (bottom)

Phase field fracture

Variational fracture potential energy:

$$\Pi_{pot}(u, \Gamma) = \int_{\Omega} \psi_e(\varepsilon(u))\, dV + \int_{\Gamma} G_c\, dA$$

Approximate surface integral by a volume integral

Elliptically regularized potential energy:

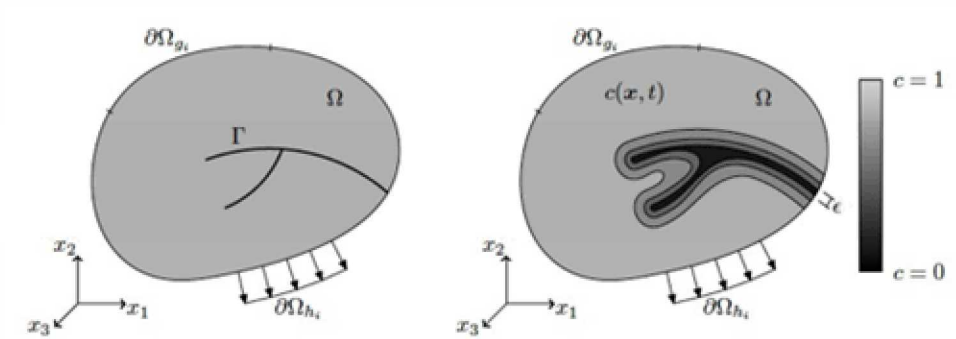
$$\Pi_l(u, d) = \int_{\Omega} \psi_e(\varepsilon(u))\, dV + \int_{\Omega} G_c \gamma_l\, dV$$

Common crack density:

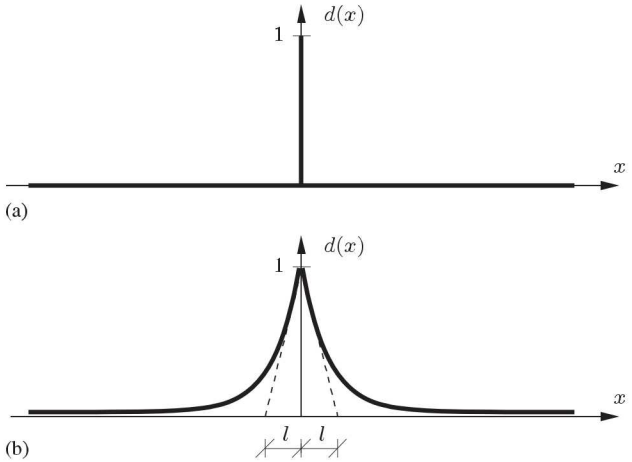
$$\gamma_l = \frac{1}{2l} d^2 + \frac{l}{2} |\nabla d|^2$$

Stress degradation:

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



Surface regularization intuition

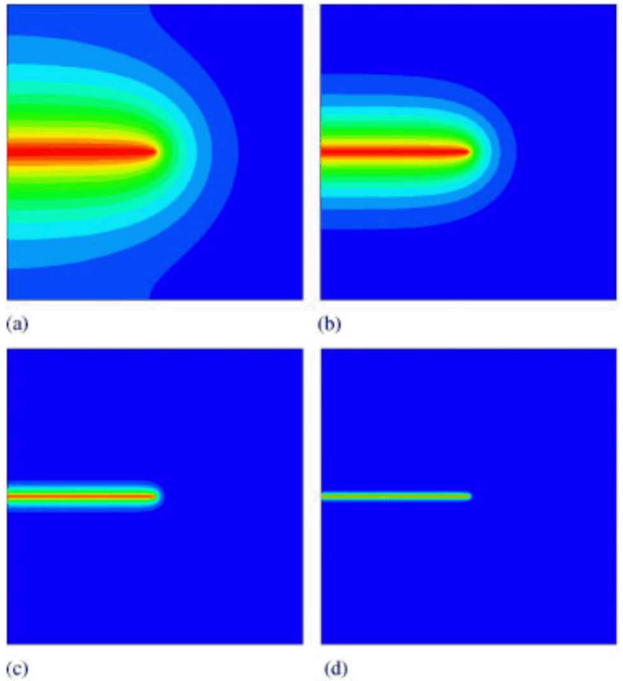


$$d(x) = \mathrm{e}^{-|x|/l}$$

$$d(x) - l^2 d''(x) = 0 \quad \text{in } \mathscr{B}$$

$$I(d) = \frac{1}{2}\int_{\mathscr{B}} \{d^2 + l^2 d'^2\}\,\mathrm{d}V$$

$$I(d = \mathrm{e}^{-|x|/l}) = l\Gamma$$



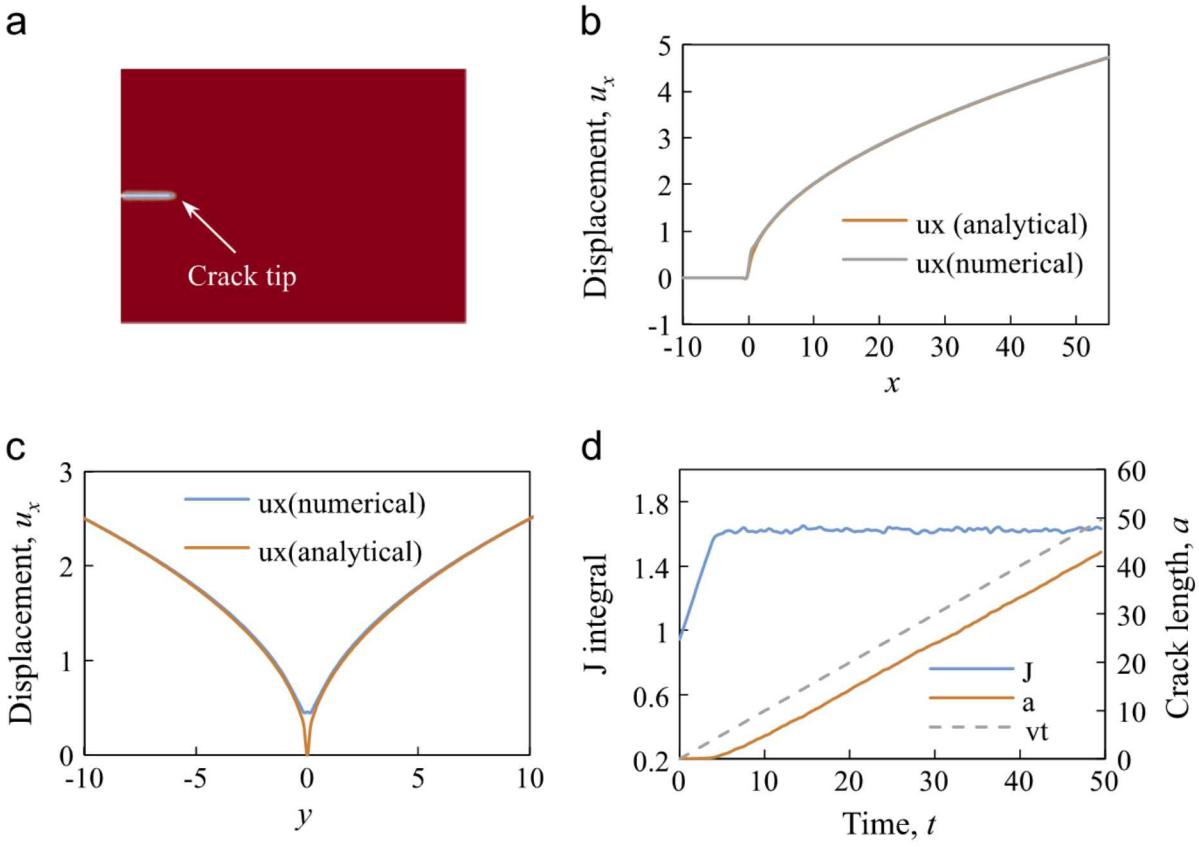
Regularized crack geometry with different length scale

Miehe, 2010

Crack "surface area": $\Gamma_l(d) := \dfrac{1}{2l}\displaystyle\int_{\mathscr{B}} \{d^2 + l^2 d'^2\}\,\mathrm{d}V$

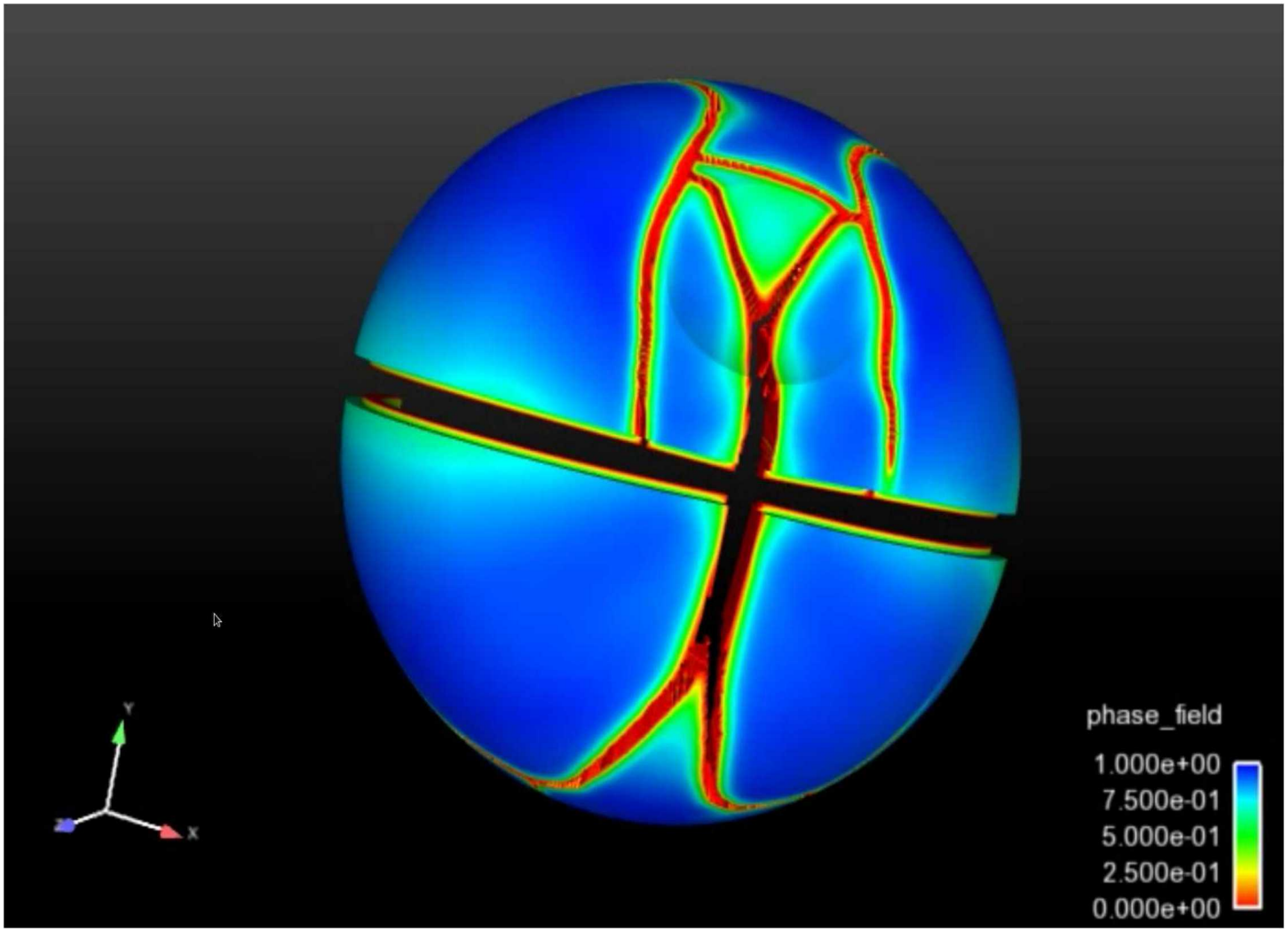
Relation to LEFM

- Example J integral calculation using phase field models
- Stable propagation at J ~ G_c = 1.5 (error decreases as $L \to 0$)

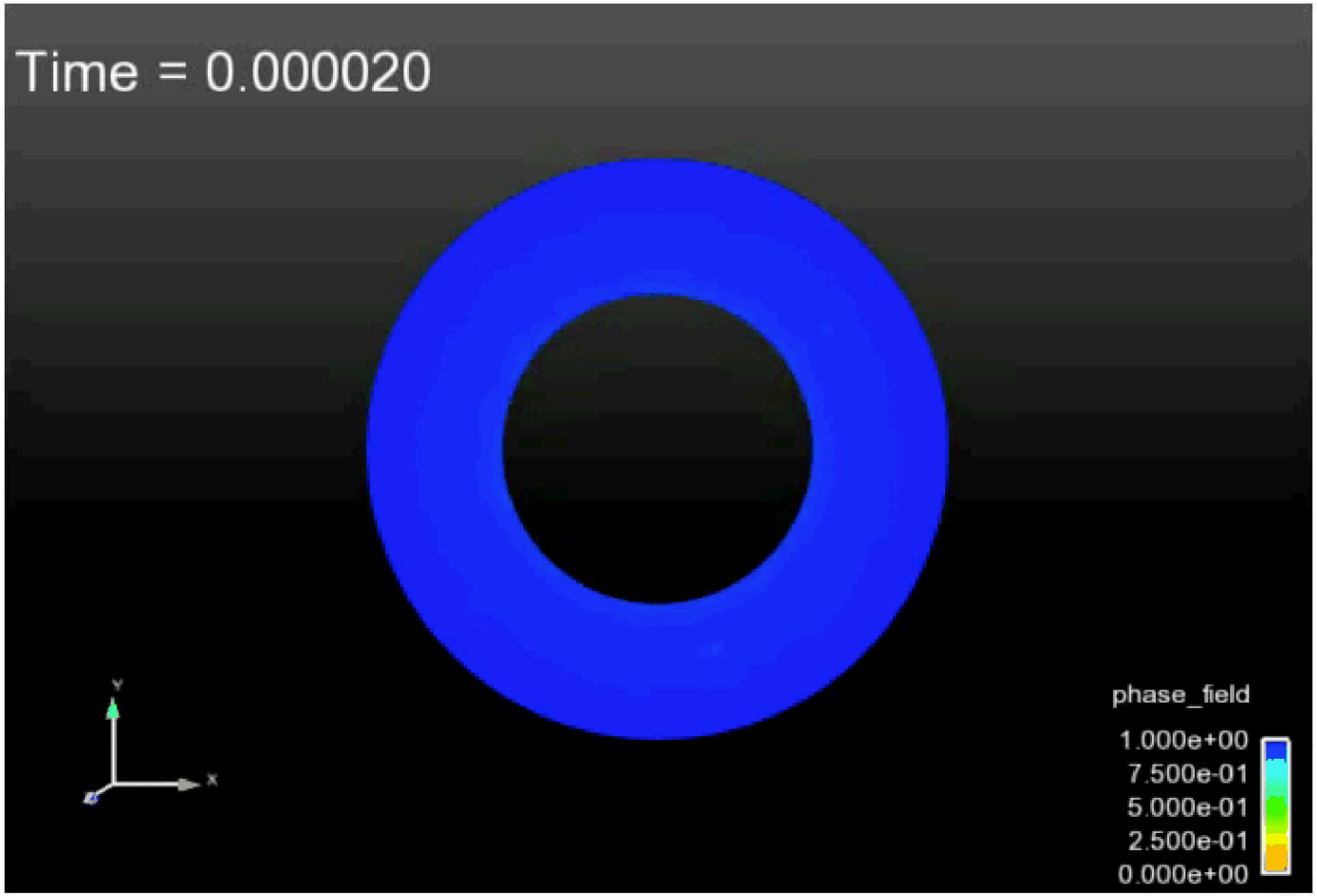


Hossain, 2014

SM demo: Thick “Moon”



SM demo: hollow cylinder



Anatomy of a phase field model

Helmholtz free energy density:

$$\Psi = g(d)\psi_e^+ + \psi_e^- + \frac{G_c}{l}h(d) + \frac{\alpha}{2}G_c\, l\, |\nabla d|^2$$

degradation

Undamaged tensile strain energy

Undamaged compressive strain energy

damage potential

damage gradient potential

Anatomy of a phase field model

Euler-Lagrange: $$g'(d)\psi_e^+ + \frac{G_c}{l}h'(d) = \alpha G_c\, l\nabla^2 d$$

A specific form of more general class of "***gradient damage***" models

A very classic gradient damage model:
(related to integral nonlocal regularization) $$\tilde{d} - l^2\nabla^2\tilde{d} = d$$

Proposed definition for phase field fracture models:

"***A gradient damage model with a well defined surface energy as*** $L \to 0$ "

Damage potential

$$\Psi = g(d)\psi_e^+ + \psi_e^- + \frac{G_c}{l}h(d) + \frac{\alpha}{2}G_c\, l\, |\nabla d|^2$$

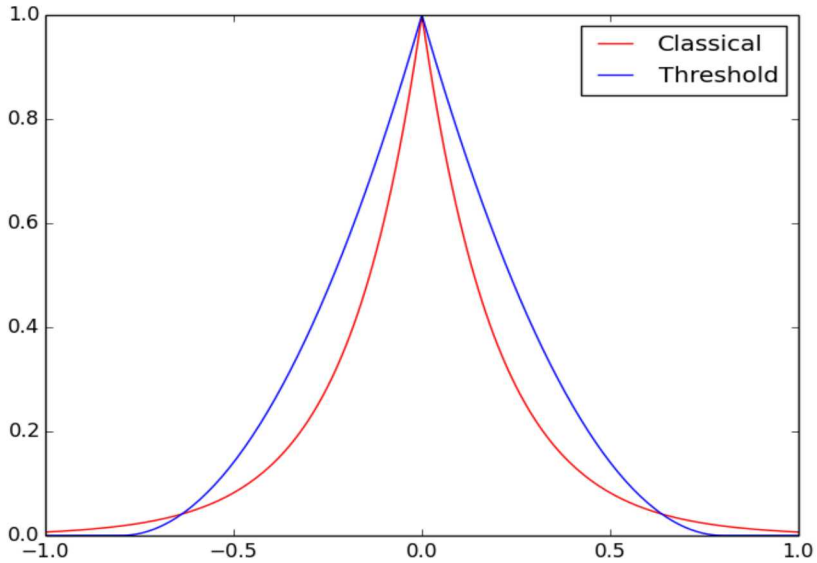
damage potential

classical: $h(d) = \frac{d^2}{2}$

$$d - l^2\nabla^2 d = 0$$

threshold: $h(d) = |d|$

$$1 - l^2\nabla^2 d = 0$$



Surface geometry
Euler-Lagrange equations

Influences through crack
damage profile

Degradation function

$$\Psi = g(d)\psi_e^+ + \psi_e^- + \frac{G_c}{l}h(d) + \frac{\alpha}{2}G_c\, l\, |\nabla d|^2$$

degradation

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

Borden Hughes: $g(d) = (1-d)^3$

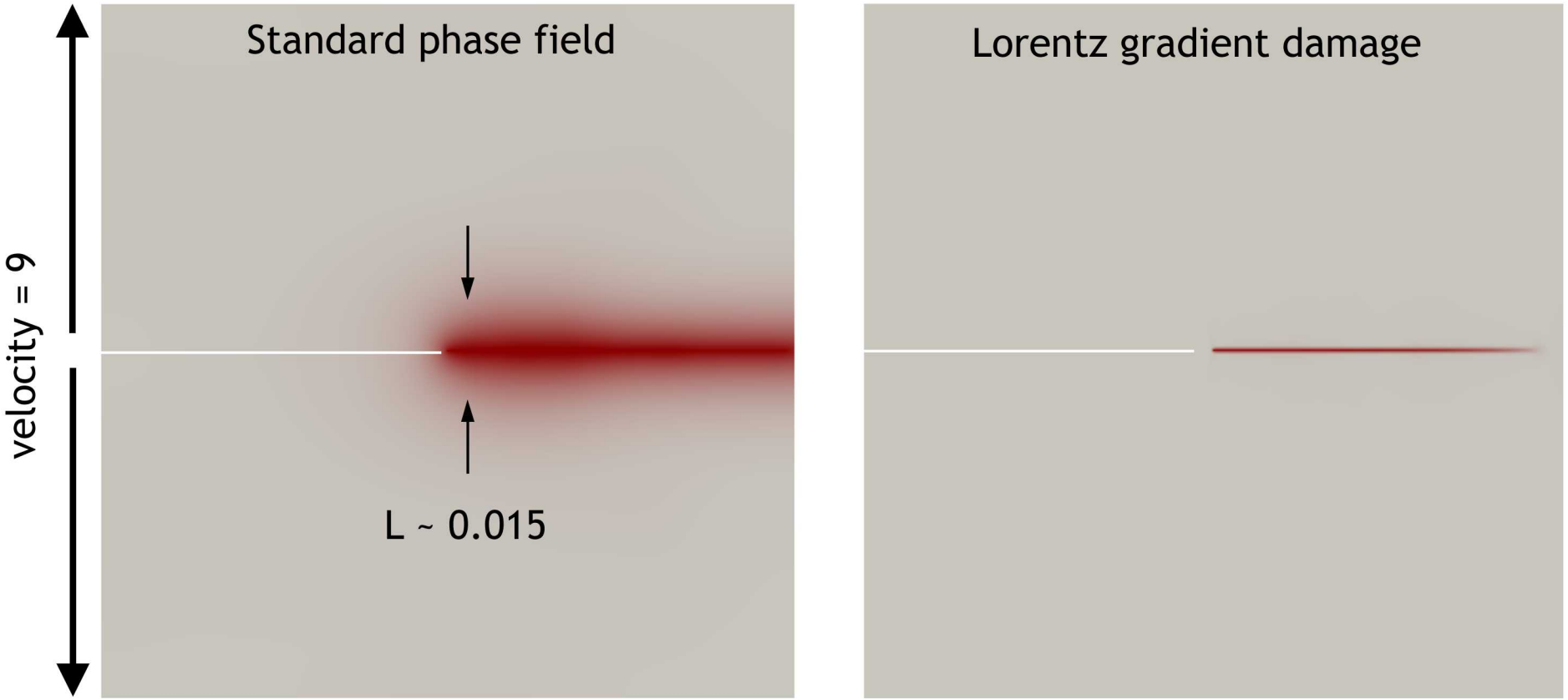
Lorentz: $g(d) = \dfrac{(1-d)^2}{1+(m-2)d+(1+pm)d^2}$

Newly proposed: $g(d) = \dfrac{1-d}{1+(\frac{G_c}{\psi_c l}-1)d}$

Influences stress decay shape

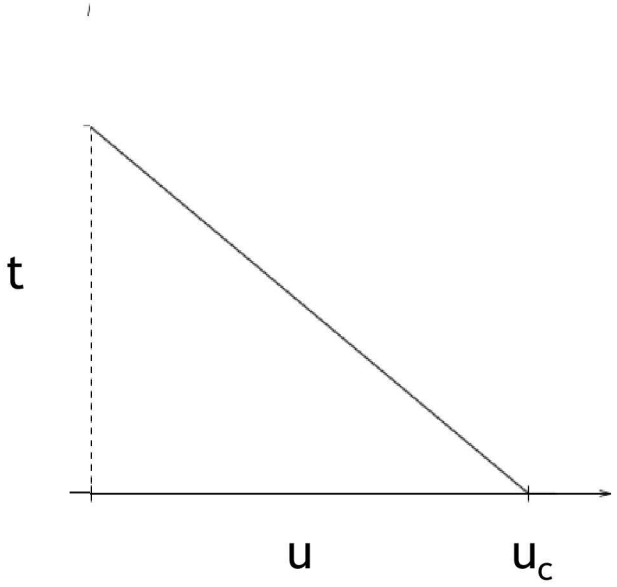
Limitations to standard phase field

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

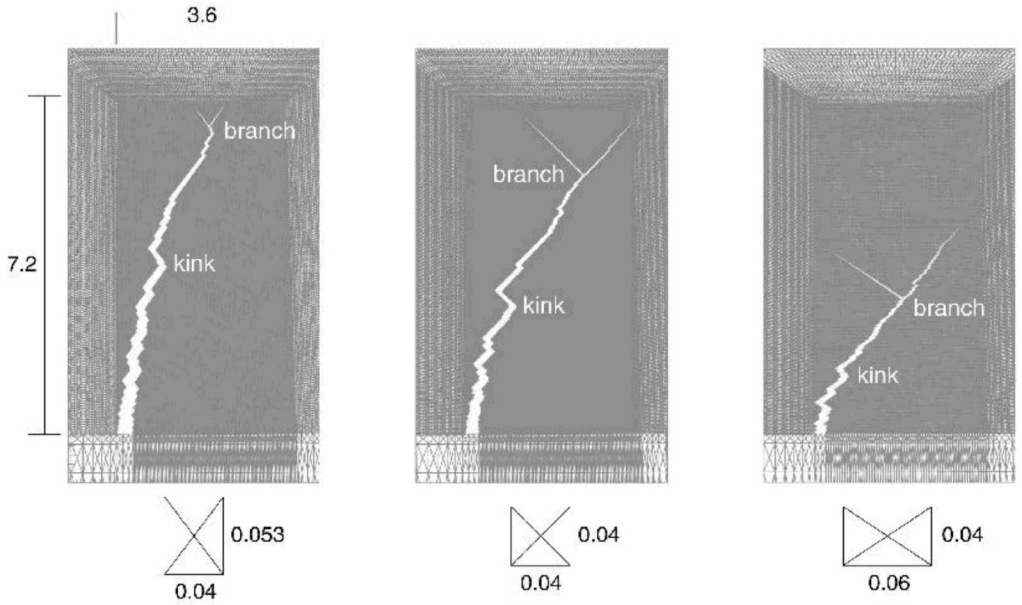


$$\sigma_{\max} = 250\text{e}6 \quad G_c = 100e3 \quad E = 200\text{e}9$$

Relationship to cohesive zone models



Traction separation law



Mesh dependence using cohesive networks

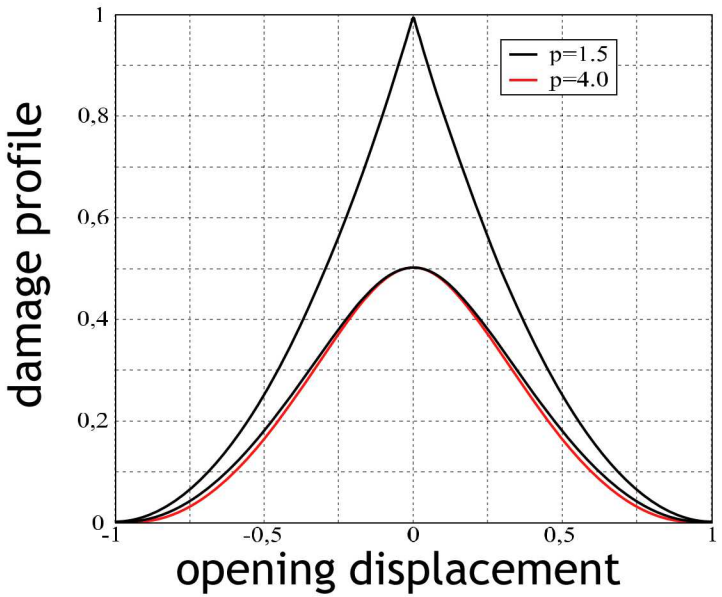
A phase field cohesive model

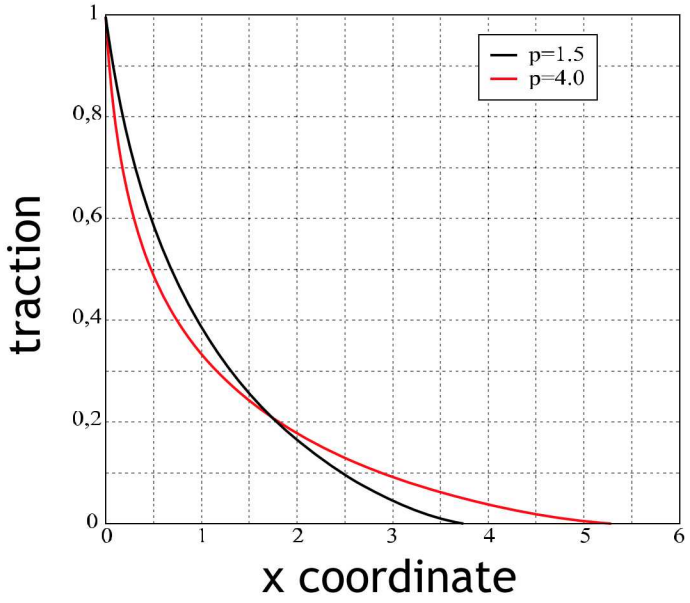
- Regularized phase field model by Lorentz, et al. 2011
- Shown to converge to cohesive zone model as $L \to 0$

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

$$g'(d)\psi_e^+ + k = c\nabla^2\phi$$ Phase field equation

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





Parameters of damage model

Depends on cohesive fracture parameters:

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

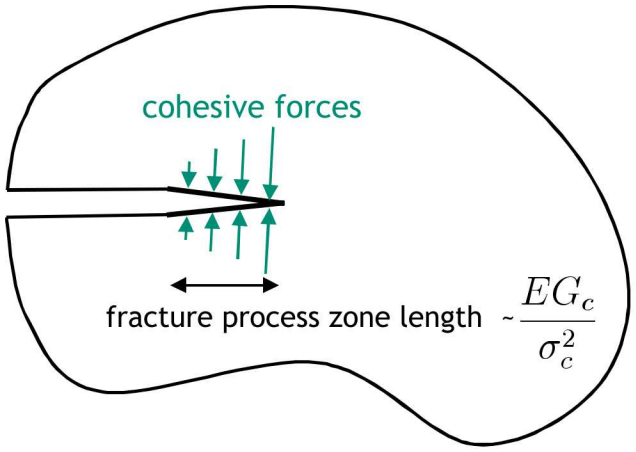
Physically justified constraints on the parameters ensure

- Regularization length scale resolves fracture process zone

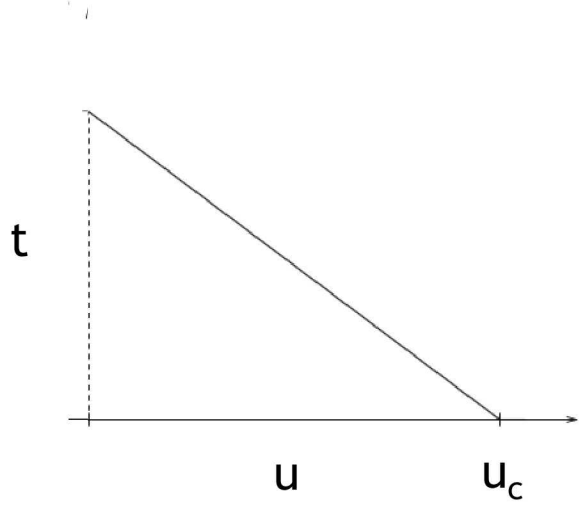
$$L < \frac{3}{2(p+2)}\frac{EG_c}{\sigma_c^2}$$

- Monotonic stress decay

$$p \geq 1$$

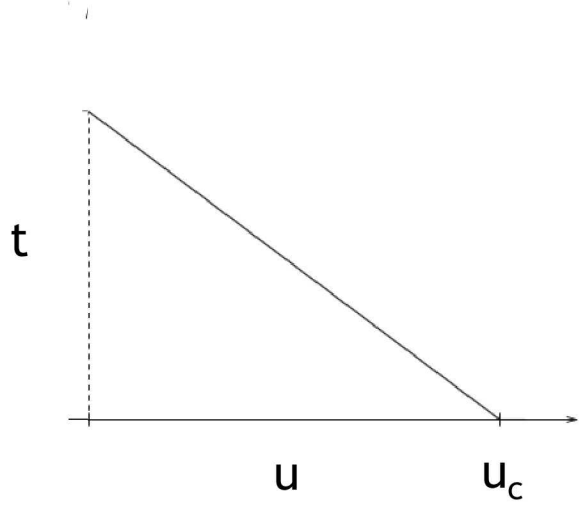


Designing a phase field model



Given an extrinsic cohesive model, can we design a phase field model?

Designing a phase field model



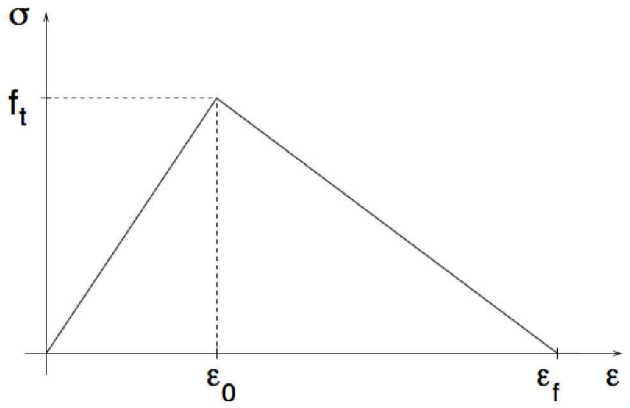
Given an extrinsic cohesive model, can we design a phase field model?

$$g(d) = \frac{1-d}{1+(\frac{G_c}{\psi_c l}-1)d}$$

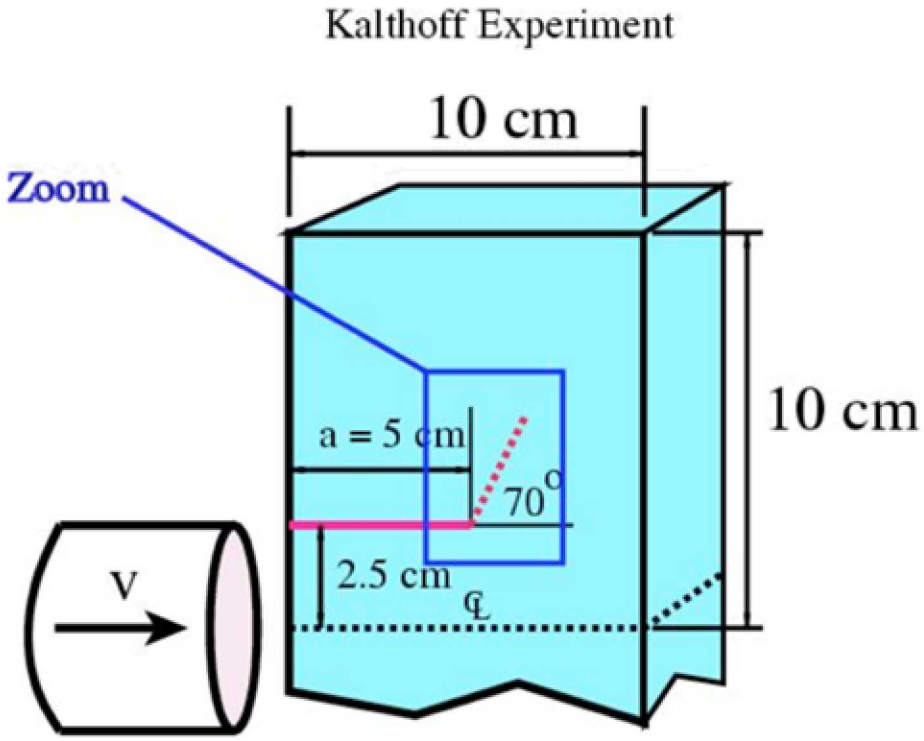
$$h(d) = |d|$$

$$g'(0)\psi_e^+ + \frac{G_c}{l} = 0 \;\Rightarrow\; \psi_e^+ = \psi_c$$

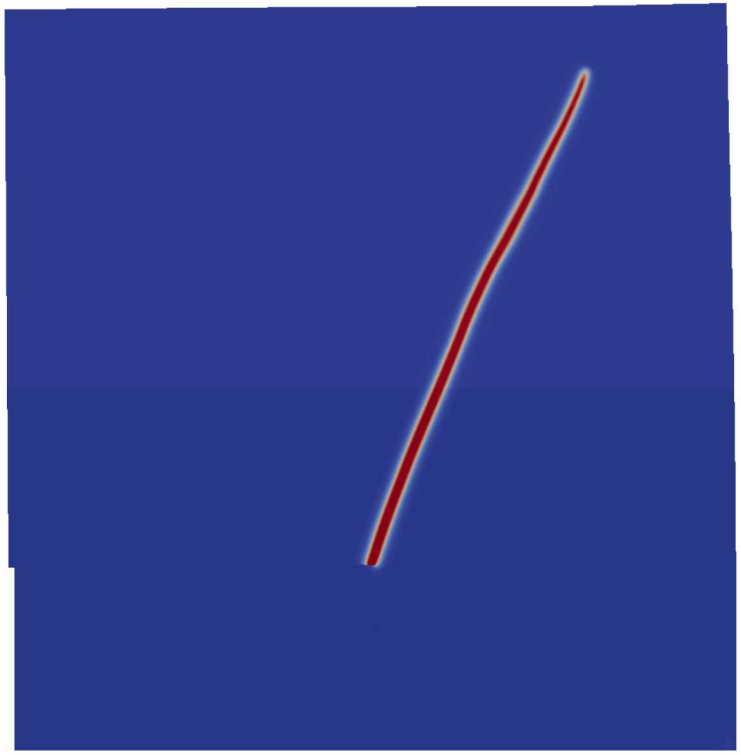
$$g'(1)\psi_e^+ + \frac{G_c}{l} = 0 \;\Rightarrow\; \psi_e^+ l^2 = \text{const}$$



Kalthoff "validation"



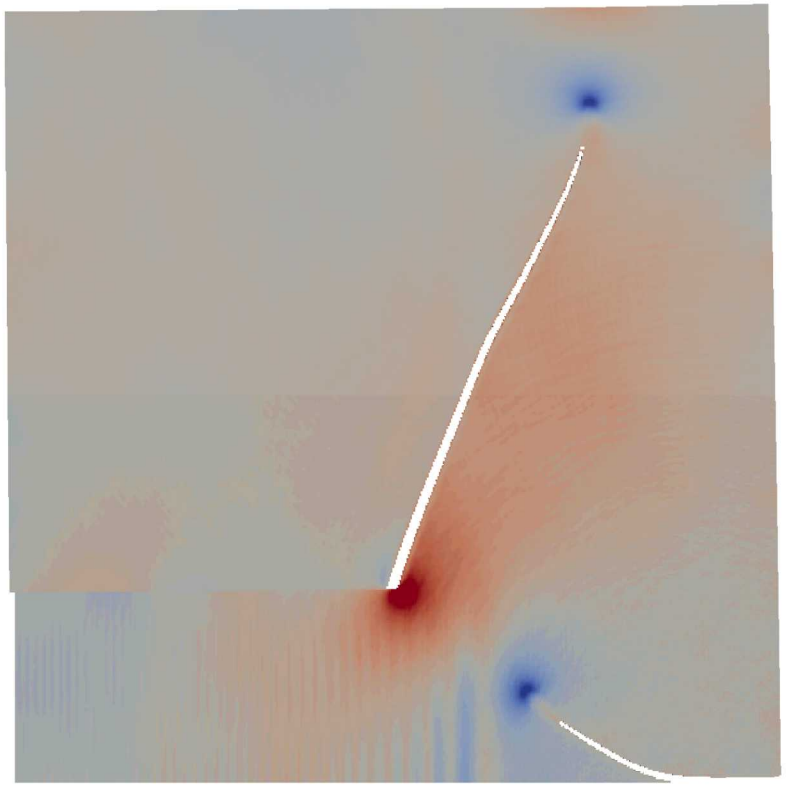
Damage contour



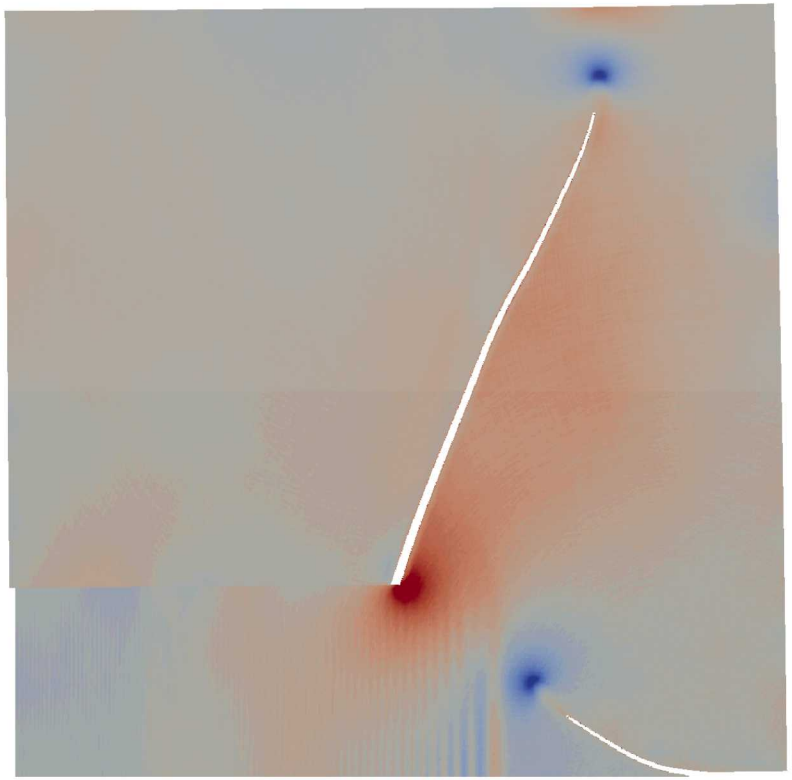
Achieves the expected crack propagation angle: ~70°

Mesh insensitivity

Pressure contours for dynamic crack propagation



Medium mesh: 250k elements

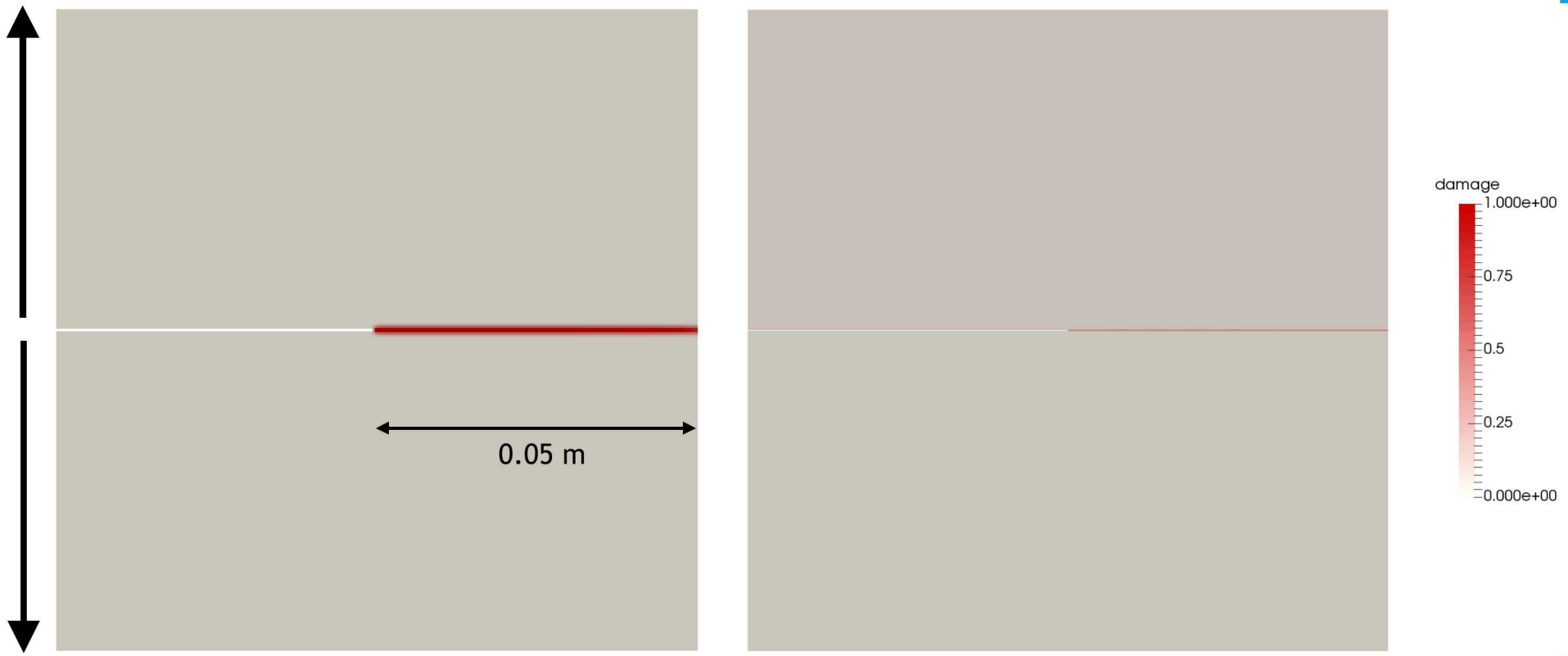


Fine mesh: 1,000k elements

Mode-I: Length scale refinement

Length-scale decreases with Δx

v = 25 m/s



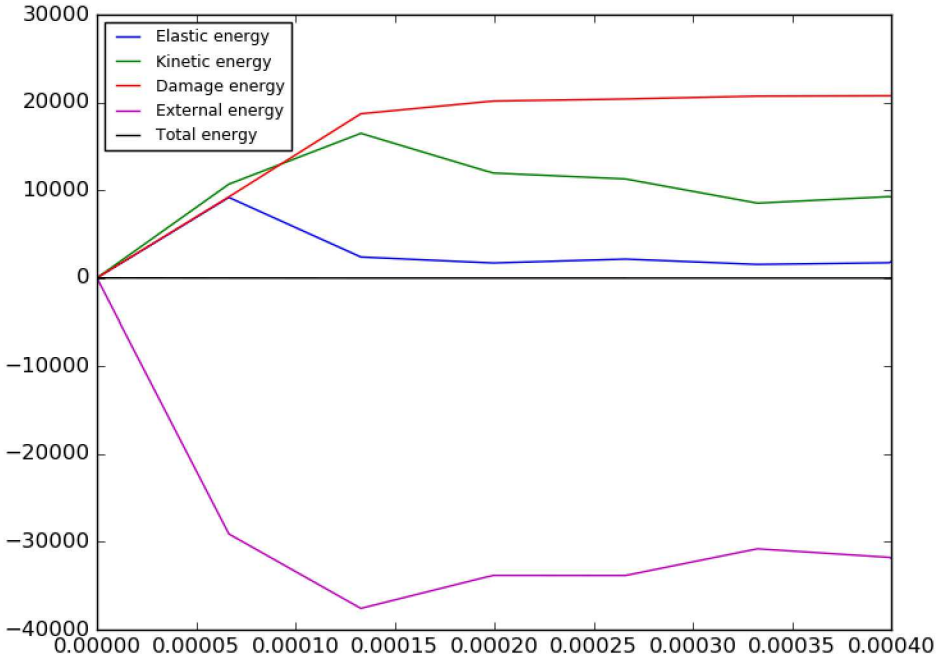
71.5 thousand elements

14.4 million elements

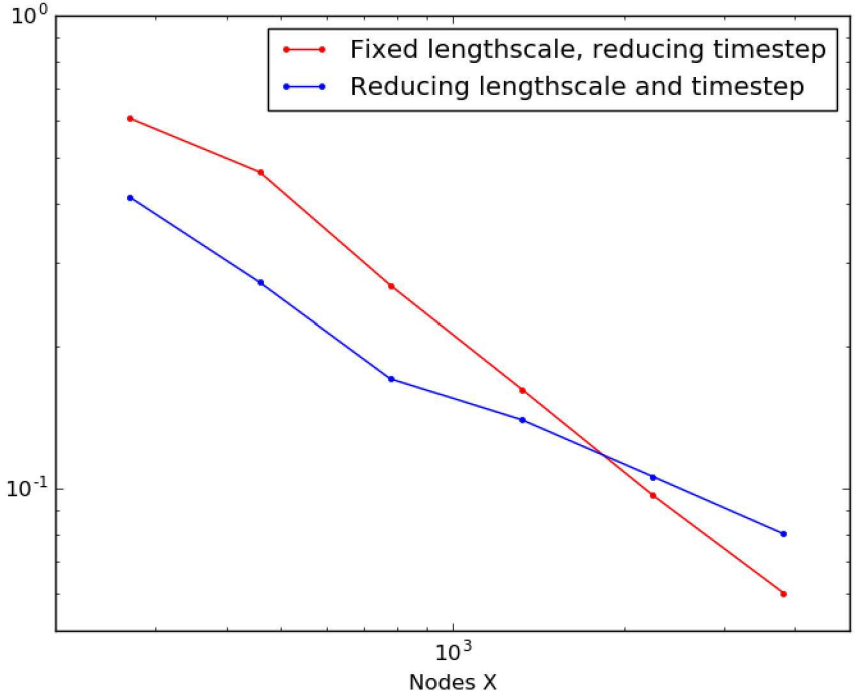
G_c = 4e5

Accuracy

Total numerical energy is preserved



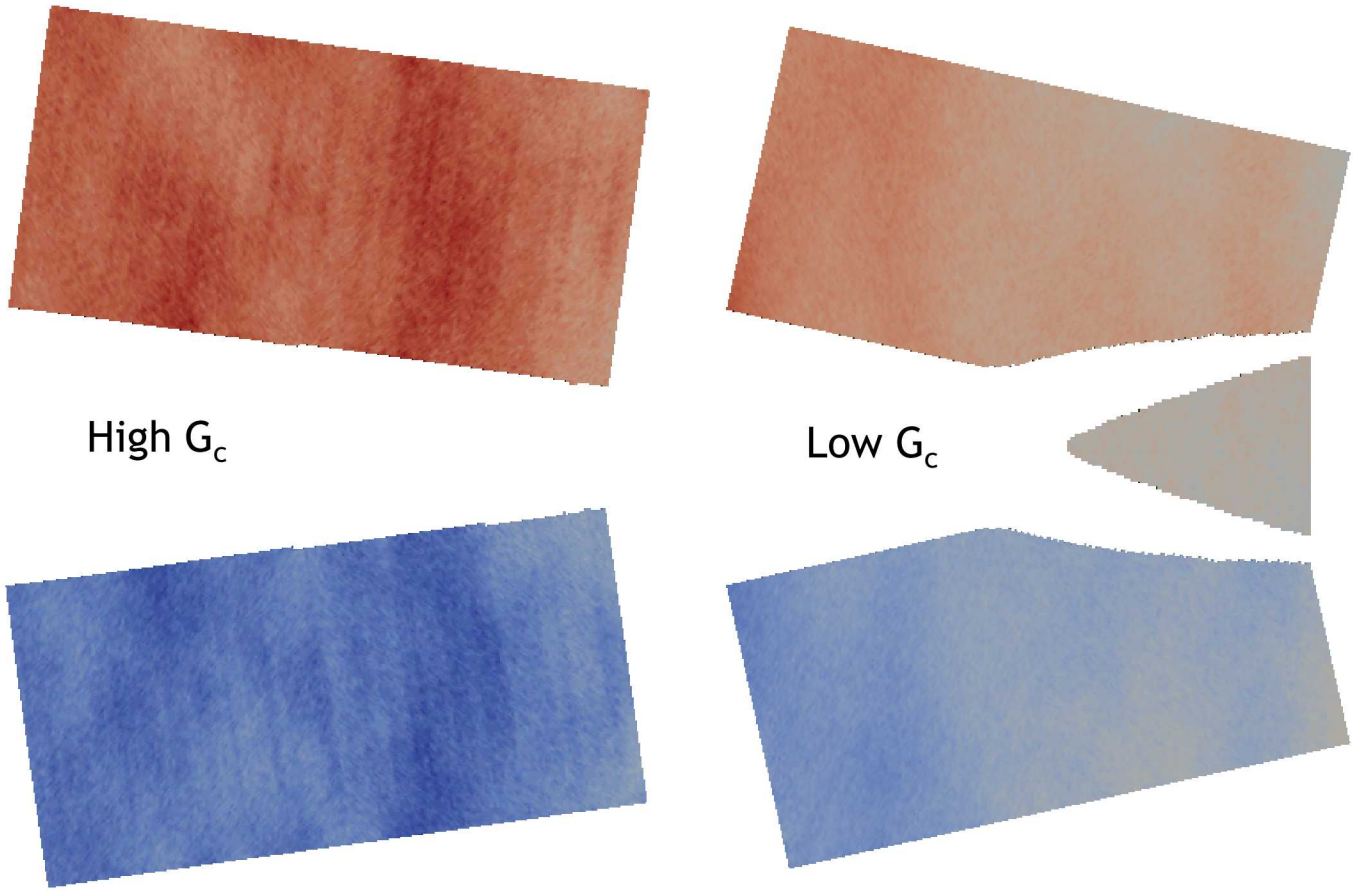
Dissipated fracture energy error



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

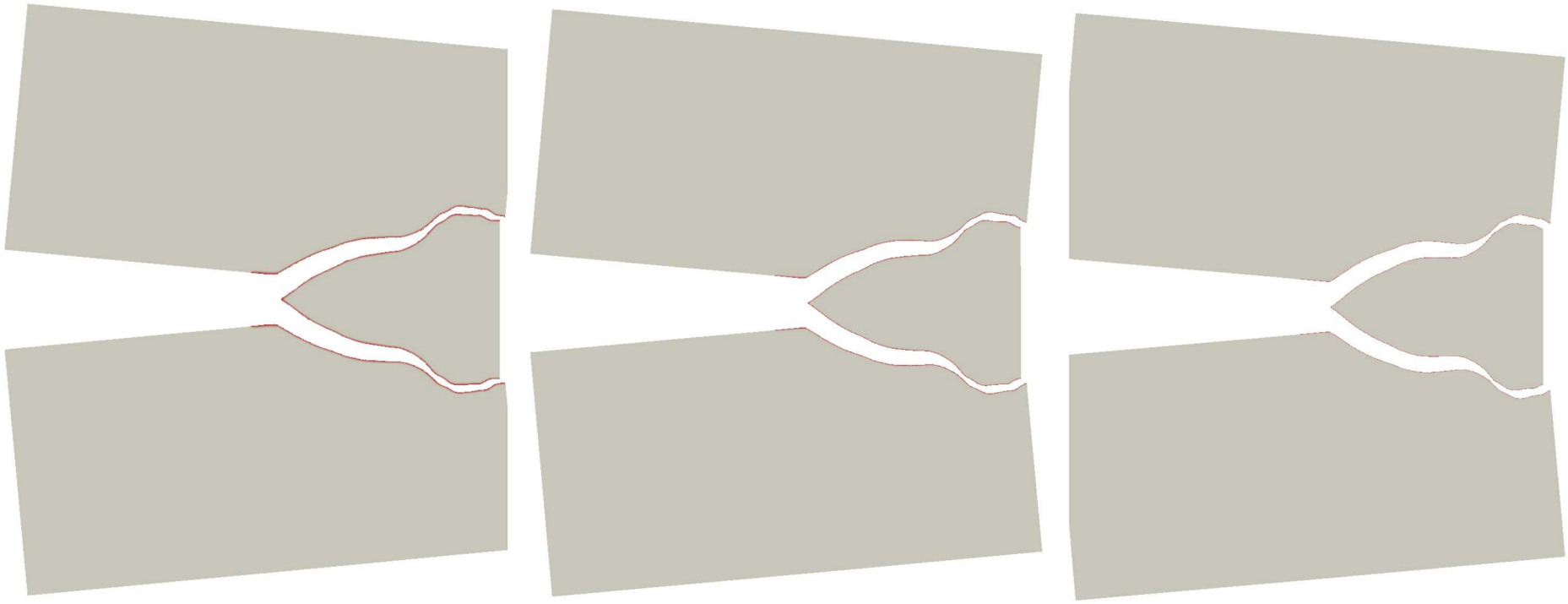
Importance of fracture energy

Mode-I crack transition to branching



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

Lo

Me

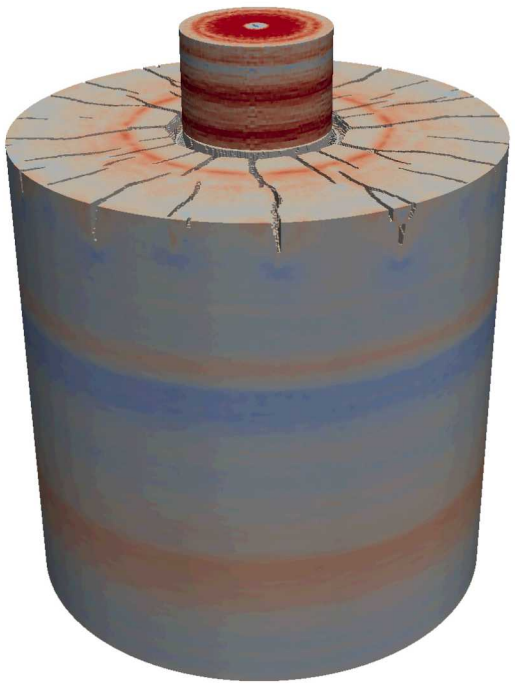
Initial vertical crack propagates upward

Eventually turns to run parallel to the glass-metal interface

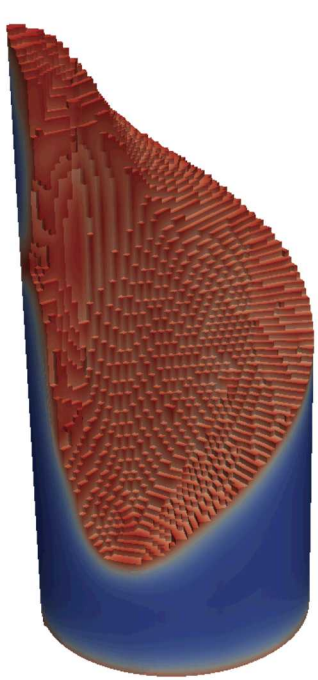
Experimentally observed crack path

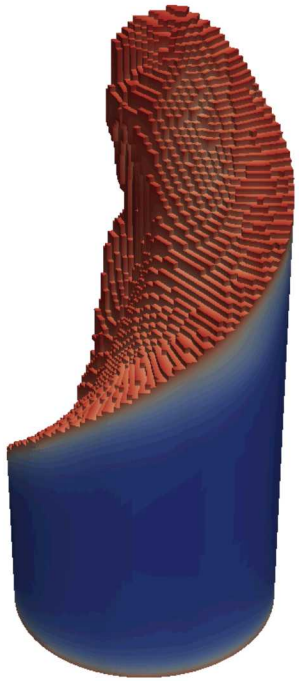
1.5 million element simulation runs in 6 hours on 1 GPU

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

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 time step constraint: $\Delta t \leq \frac{1}{s}\Delta x$
- Parabolic time step constraint: $\Delta t \leq \frac{\eta}{c}(\Delta x)^2$
- Can use hyperbolic time step if: $\eta \geq \frac{c}{s\Delta x} = \frac{3}{8}\frac{G_c}{s}\frac{L}{\Delta x}$

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.

Toward scalable multiscale failure modeling

The Problem:

Potential *pervasive fracture/failure* of NASA experimental equipment

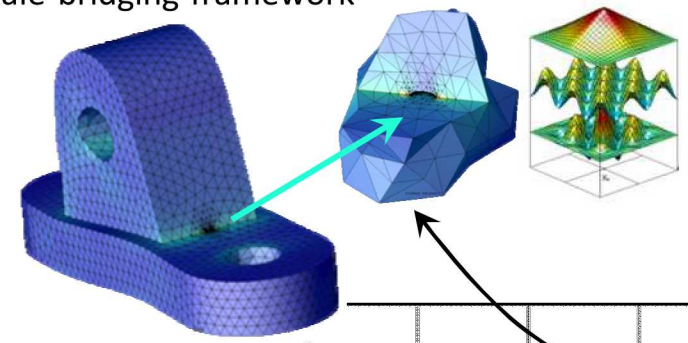
Figure D-3. The integrated spacecraft with Carrier and Lander elements provides reconnaissance, safe landing, and in-situ science in a single mission.

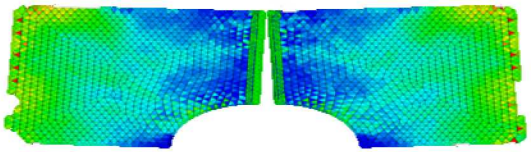
The Approach:

Develop a multiscale fracture simulation capability for accurately resolving fine-scale fractures *at scale*, based on…

GFEM^{gl}

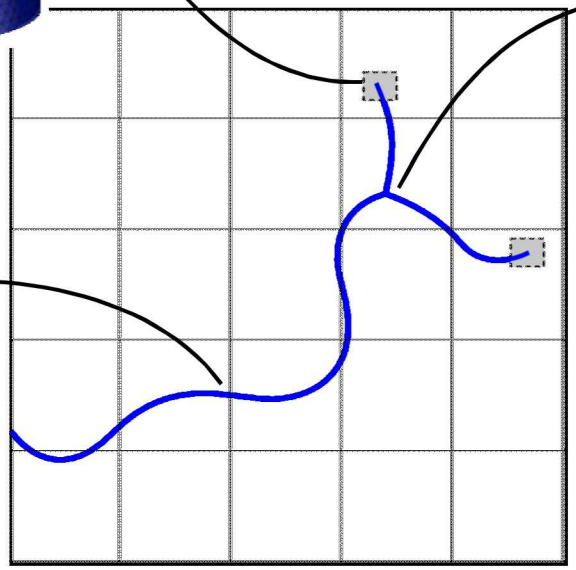
Scale-bridging framework



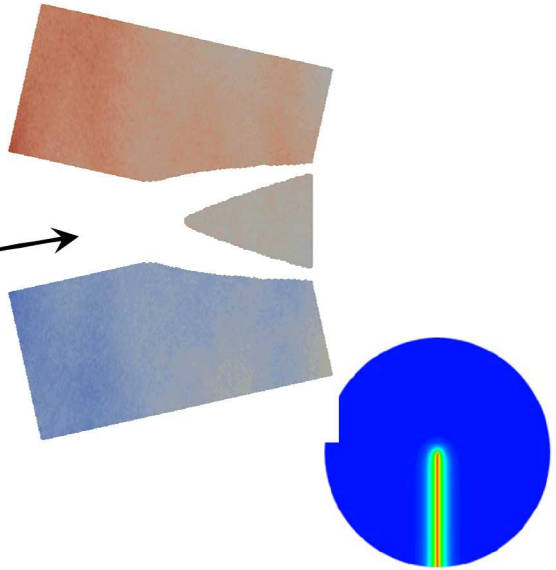


XFEM

Discontinuity representation



Cracked domain



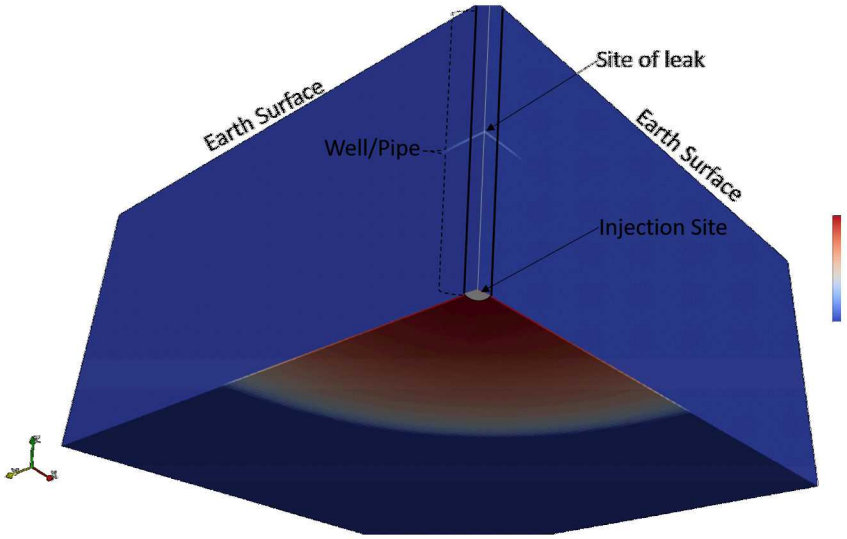
Phase field

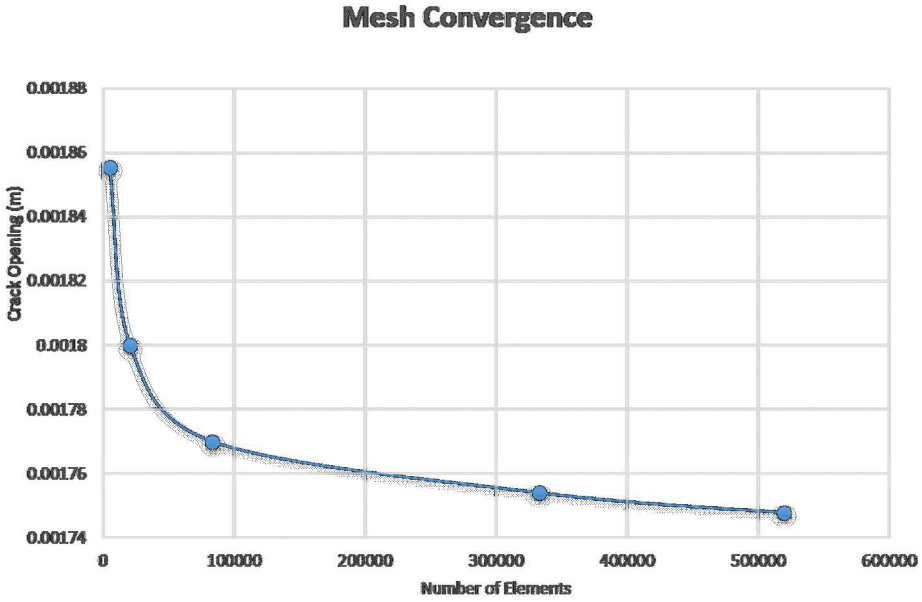
Detailed fracture path prediction

(Gupta et al. 2012, Tupek 2016)

Poroelastic phase field fracture

Arpeggio coupled simulation:
pore pressure injection with pipe leak





Work with UC-Boulder collaborators, notably student David Culp

Research on ductile phase field fracture

Components:

- FeFp hyperelastic plasticity model
- Driving energy:
  max(undamaged strain energy + undamaged plastic work)
- Linear hardening model

Two models coded:

- "Classical"

$$\psi = \mathrm{c}^2 * \max_{\mathrm{t}} \left(\tilde{\psi}^{\mathrm{e}}(\varepsilon^e) + \tilde{\psi}^p(\varepsilon^p) \right) + \frac{G_c}{4l} \left((1-c)^2 + 4l^2 (\nabla c)^2 \right)$$

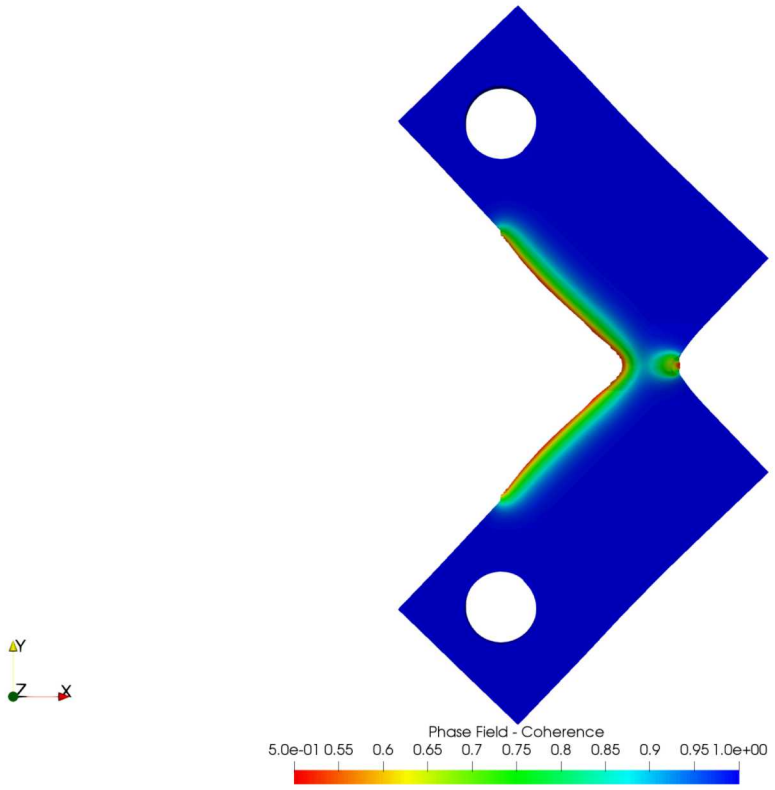
- "Threshold"

$$\psi = \mathrm{c}^2 * \max_{\mathrm{t}} \left(\tilde{\psi}^{\mathrm{e}}(\varepsilon^e) + \tilde{\psi}^p(\varepsilon^p) \right) + \psi_{crit} (2(1-c) + 4l^2 (\nabla c)^2)$$

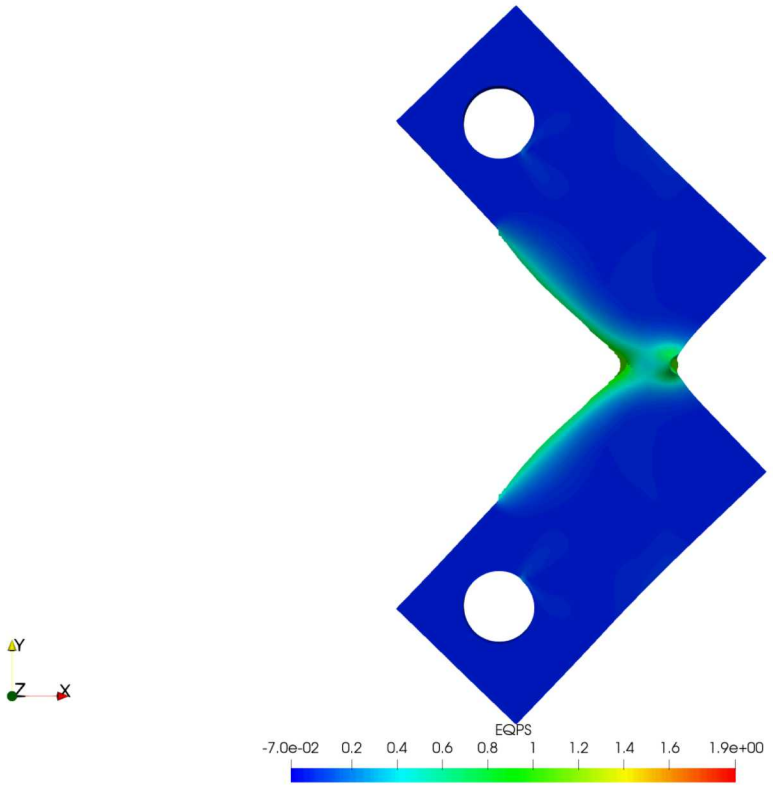
$$\psi_{crit} = \frac{G_c}{4l}$$

Output - Fields

Deformed View (Visual threshold at c=0.5):



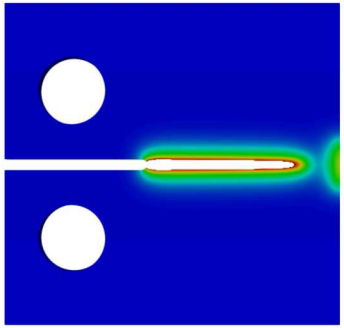
Phase Field

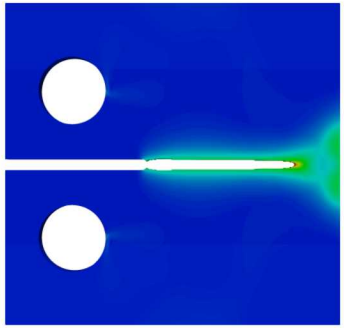


EQPS

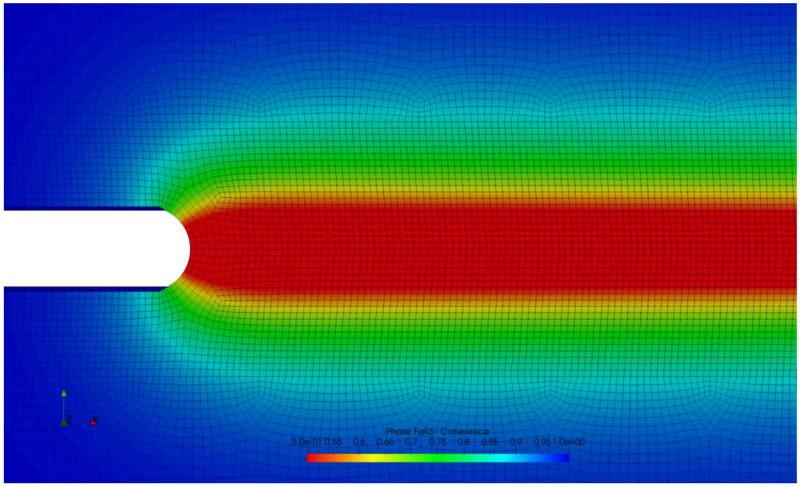
Output - Fields

Undeformed View (Visual threshold at c=0.5):

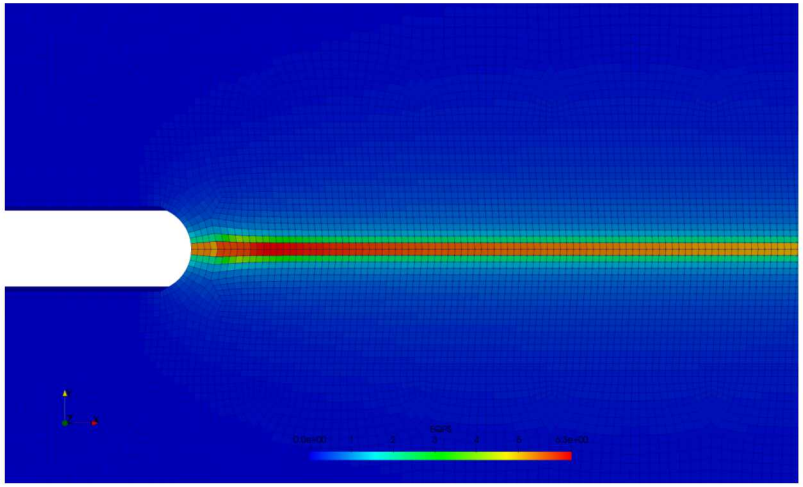




Undeformed View (No visual threshold, zoomed):



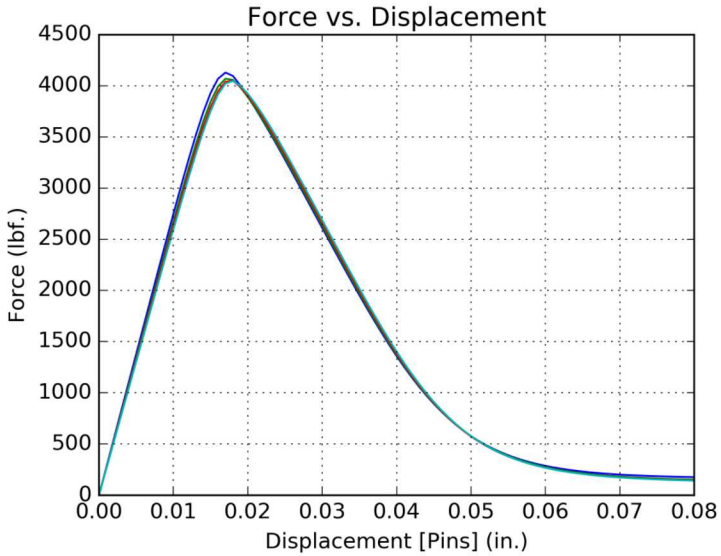
Phase Field

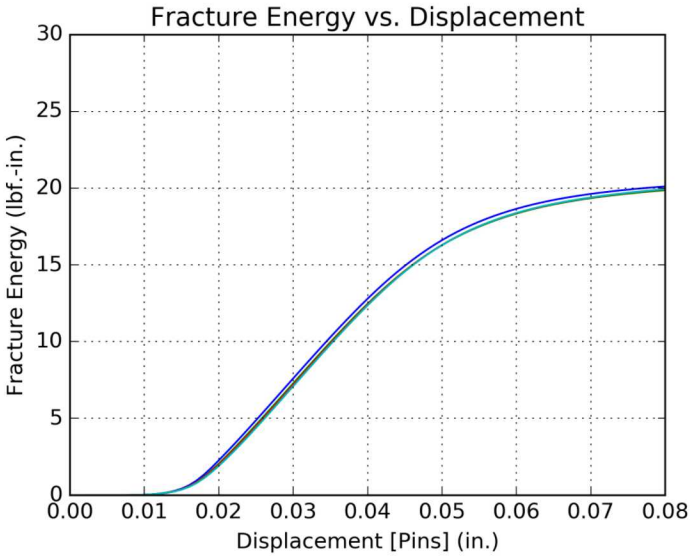


EQPS

Preliminary Results

Working toward getting convergent force-displacement results

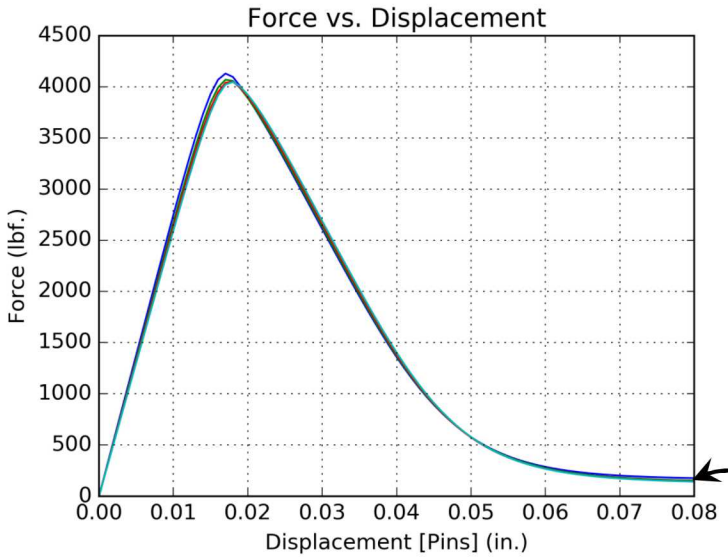


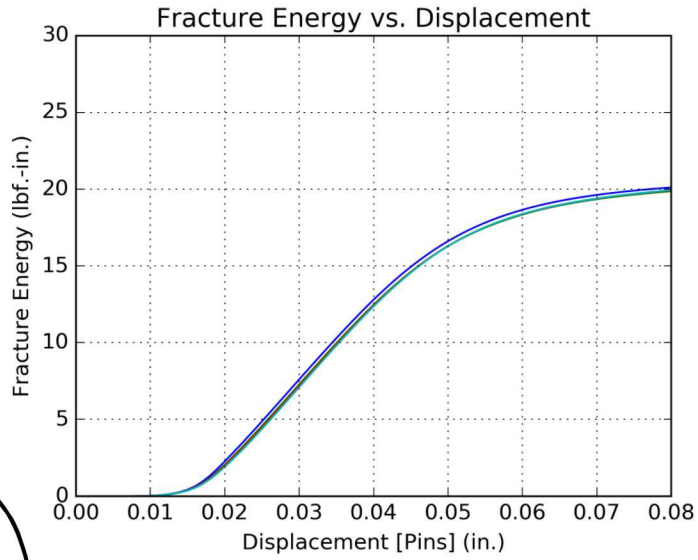


- There are a lot of caveats here that are still being worked out
- Illustrates the ultimate goal: convergent ductile fracture

Preliminary Results

Working toward getting convergent force-displacement results





e.g. is this left over stress acceptable?

- There are a lot of caveats here that are still being worked out
- Illustrates the ultimate goal: convergent ductile fracture

Conclusions and future work

Advantages

- Simple to implement
- Efficient phase-field models can be constructed which are either cohesive or LEFM
- Method is trivially thread scalable (and MPI scalable)
- Explicit time integration is possible and reasonably efficient
- No need for J-integrals or auxiliary propagation direction criterion
- Crack propagation, branching, coalescence is a prediction (not a prescription) of the model

Conclusions and future work

Disadvantages

- No explicit surfaces created
- Surprisingly significant dependence on
  - Degradation and damage potential model forms
  - Tensile/compressive strain energy split
  - Solver strategies (staggered, monolithic, etc.)
  - Conditioning coefficient
- Numerical damage smearing
- Requires resolving damage length scale
  - May be fracture process zone size, then similar or just slightly more expensive than other methods
  - If process zone size is small, length must be small compared to geometry
- Computationally expensive?