Propagation of complex fracture

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Results reported in:

Cohesive Dynamics and Fracture. arXiv:1411.4609v3 [math.AP] 11 Dec 2014. R. Lipton

Dynamic Brittle Fracture as a Small Horizon Limit of Peridynamics, *Journal of Elasticity* Jan, 2014, DOI 10.1007/s10659-013-9463-0, (Open access). R. Lipton

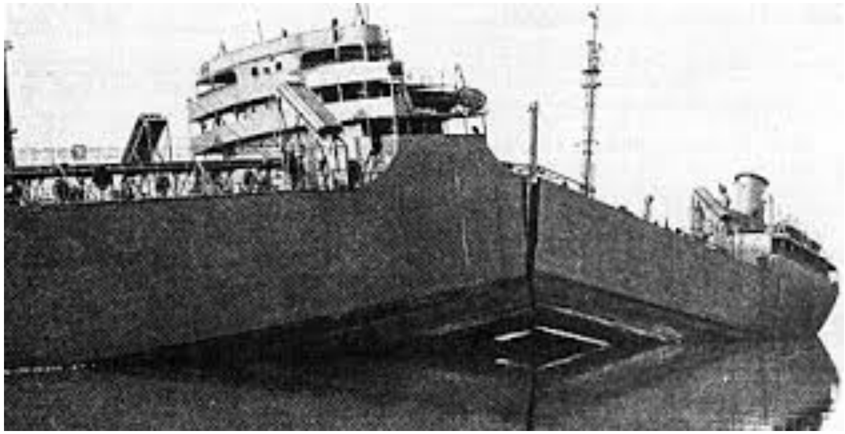
These results presented in the survey:

Peridynamics Fracture and Nonlocal Continuum Models, *SIAM News* April 2014, (Qiang Du – co author).

Dynamic fracture of Brittle Solids

Dynamic fracture of brittle solids is an example of collective interaction across disparate length and time scales.

Apply sufficient force to a sample of brittle material, atomistic-scale bonds will eventually snap, leading to fracture of the macroscopic specimen.

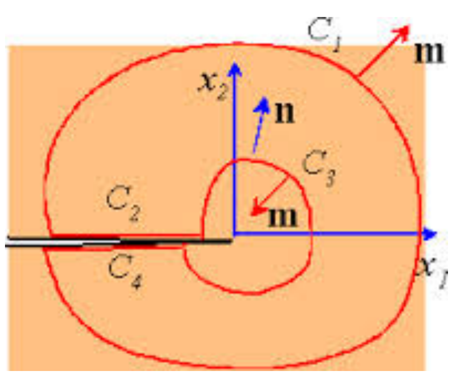


Classic theory of Dynamic Fracture Mechanics

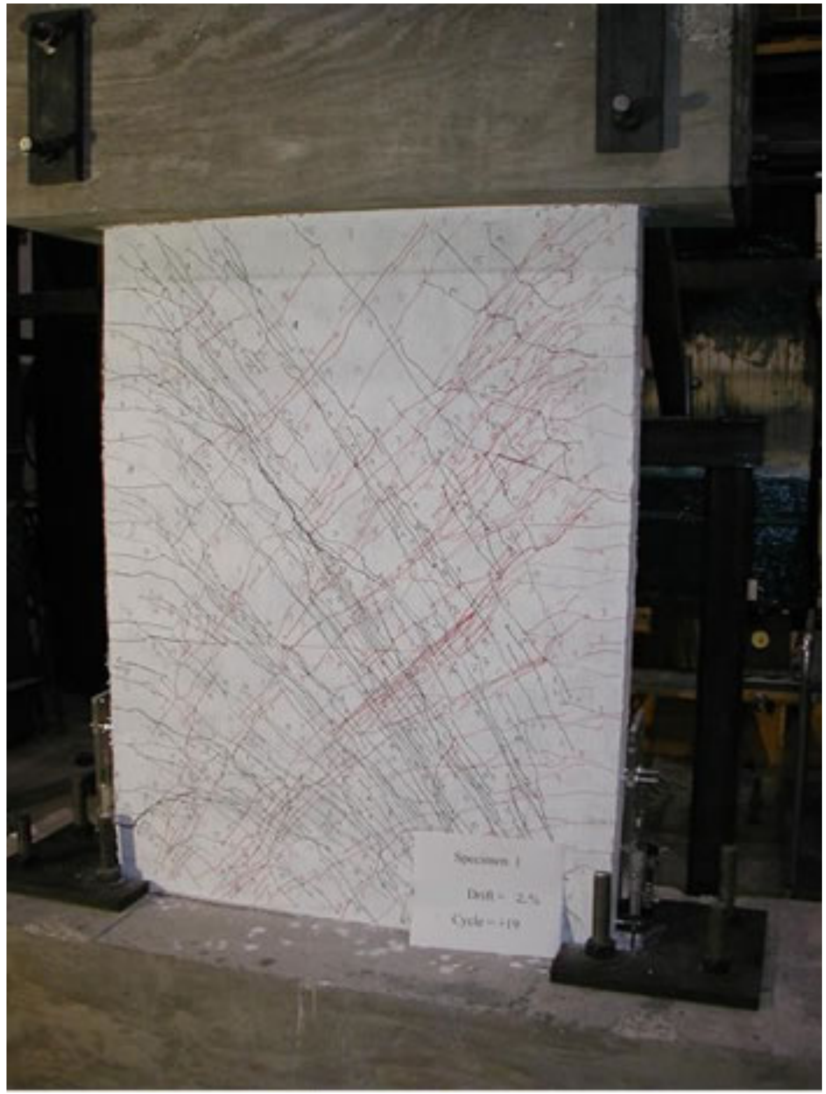
The theory of dynamic fracture is based on the notion of a deformable continuum containing a crack.

The crack is mathematically modeled as a branch cut that begins to move when an infinitesimal extension of the crack releases more energy than needed to create a fracture surface.

Fracture mechanics, together with experiment, has been enormously successful in characterizing and measuring the resistance of materials to crack growth and thereby enabling engineering design.



Challenges – quantitative modeling of the state of a solid body containing a complex of freely propagating cracks.



Given a damaged Shear panel: how much more load can it sustain before failure ?

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On modeling multiple cracks: top down approach

Classic top down approach. Find the state of deformation in the cracking body by:

Starting with a PDE model (the wave equation) away from the crack

+

Provide a description of the physics in the process zone in the vicinity of the crack

+

Provide an equation for the time evolution of the crack

On modeling multiple cracks: top down approach

Application of cohesive zone elements:
Xu and A. Needleman, *Numerical simulations of fast crack growth in brittle solids*, J. Mech. Phys. Solids, 42 (1994), 1397– 1434.
A. Hillerborg, M. Modeer, and P.E. Petersson, *Analysis of crack formation and growth by means of fracture mechanics and finite elements*, Cem. Concr. Res., 6 (1976), 731–781.

Extended finite element XFEM, as Partition of unity methods to eliminate effects of mesh dependence on cohesive zone modeling of freely propagating cracks. (Material softening models-ductile materials).

T. Belytschko and T. Black, *Elastic crack growth in finite elements with minimal remeshing*, Int. J. Numer. Meth. Eng., 45 (1999), 601–620.

C.A. Duarte and J.T. Oden. *An hp adaptive method using clouds*. Computer Methods in Applied Mechanics and Engineering, 139(1-4):237–262, 1996.

J.M. Melenk and I. Babuska. *The partition of unity finite element method: Basic theory and applications.* Computer Methods in Applied Mechanics and Engineering, 39:289–314, 1996.

Phase field methods – free crack propagation

Quasistatic:
Francfort, G., Marigo, J.-J.: *Revisiting brittle fracture as an energy minimization problem*. J. Mech. Phys. Solids **46**, 1319–1342 (1998)

B. Bourdin, G. Francfort, J.-J. Marigo, Numerical experiments in revisited brittle fracture, J. Mech. Phys. Solids 48 (2000) 797–826.

Dynamic:
Bourdin, B., Larsen, C., Richardson, C.: *A time-discrete model for dynamic fracture based on crack regularization*. Int. J. Fract. **168**, 133–143 (2011)

Borden, M., Verhoosel, C., Scott, M., Hughes, T., Landis, C.: A phase-field description of dynamic brittle fracture. Comput. Methods Appl. Mech. Eng. **217–220**, 77–95 (2012)

Mikelic, M.F. Wheeler, T. Wick*. A quasistatic phase field approach to pressurized fractures. Nonlinearity 28(5), 1371-1399 (2015)*

Lattice models: bottom up approaches

Insight into crack tip instabilities and branching by modeling discreteness of fracture at the smallest length scales (breaking of atomic bonds).

M. Marder and S. Gross,
Origin of crack tip instabilities, J. Mech. Phys. Solids, 43 (1995),

M. Marder,
Supersonic rupture of rubber,
J. Mech. Phys. Solids, 54 (2006), 491–532.

M.J. Buehler, F.F. Abraham, and H. Gao
Hyperelasticity governs dynamic fracture at a critical length scale,
Nature, 426 (2003), 141–146.

Nonlocal models: bottom up approaches

Modeling discreteness of fracture at atomistic length scales through nonlocal models & upscaling to classic fracture mechanics.

Quasi-static models:

A.Braides & M.S. Gelli, *Limits of Discrete Systems with Long-Range Interactions,* Journal of Convex Analysis, 2002 9:363–399.

Alicandro Focardi and Gelli, *Finite-difference Approximtion of Energies in Fracture Mechanics, Annali della Scuola Normale Superiore di Pisa, 2000 29:671-709.*

L. Truskinovsky*, Fracture as a phase transition*, In: ``Contemporary research in mechanics and mathematics of materials.'' R. Batra, M. Beatty(eds.), CIMNE, Barcelona, 1996, 322-332.

Peridynamics - Fracture & Atomistics

S.A. Silling. Reformulation of Elasticity Theory for Discontinuities and Long-Range Forces. J. Mech. Phys. Solids 48 (2000) 175209.

S.A. Silling, M. Epton, O. Weckner, J. Xu, and E. Askari. Peridynamic states and constitutive modeling. J. Elasticity, 88 (2007) 151–184.

F. Bobaru and W. Hu. The meaning, selection, and use of the Peridynamic horizon and its relation to crack branching in brittle materials. Int. J. Fract. 176 (2012) 21-222.

J. Foster, S.A. Silling, and W. Chen. An energy based failure criterion for use with peridynamic states. International Journal for Multiscale Computational Engineering. 9 (2011) 675–688.

P. Seleson, M. Parks, M. Gunzburger, R. Lehoucq. Peridynamics as an upscaling of molecular dynamics. SIAM Multiscale Modeling and Simulation. 8 (2009) 204-227.

The Challenge – quantitative modeling of complex fracture and residual strength

Given a damaged
Shear panel:
how much
more load can
it sustain before
failure ?

Bottom up meso-approach:
Can we get quantitative predictions from a self consistent – well posed dynamic, mesoscopic continuum theory, informed by atomistic Simulations – AND, at the same time, be consistent with Macroscopic parameters, such as Shear modulus, & Energy release rate?

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Cohesive peridynamic model

Unstable meso-scopic dynamics

Brittle fracture
As non-locality goes to zero

Nonlocal Cohesive Evolution with Dynamic Instability for Brittle fracture

Convergence to a PDE Based Model for Dynamic Brittle Fracture Characterized by μ and G

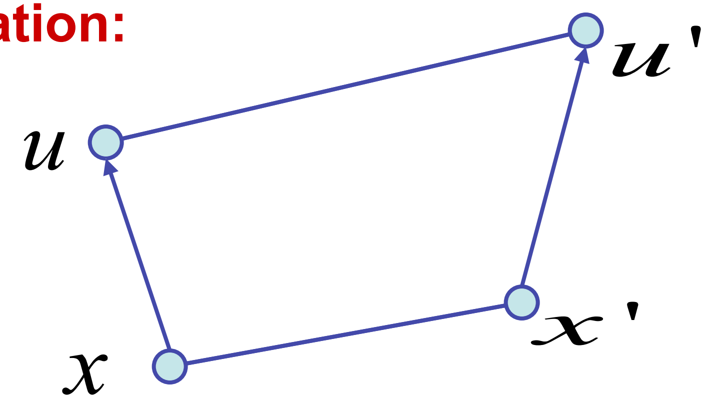
Cohesive dynamics as an Up-scaling of atomistic simulations

For nonlocal linear spring and Lennard-Jones MD models:
P. Seleson, M. Parks,
M. Gunzburger, R. Lehoucq
SIAM, MMS (2009)

Cohesive-dynamics in Peridynamic Formulation: Background:

A general nonlinear-nonlocal formulation:

S.A. Silling, *Reformulation of elasticity theory for discontinuities and long-range forces*, J. Mech. Phys. Solids, 48 (2000), 175–209. ``**Peridynamic Formulation**.''



Small displacement theory ``u'' is displacement, x denotes position. Shear strain ``S''

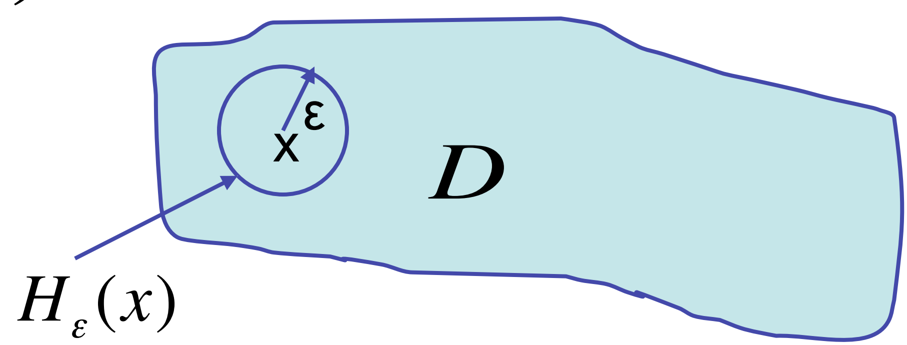
$$S = ((u(x') - u(x))/|x' - x|) * e$$

$$e = (x' - x)/|x' - x|$$

ε is length of nonlocal interaction in units taken relative to sample size. Limit of vanishing nonlocality corresponds to ε→0

Force depends on shear strain S

$$\rho \ddot{u} = \int_{H_\varepsilon(x)} k^\varepsilon(S, x' - x)\,dx' + b$$



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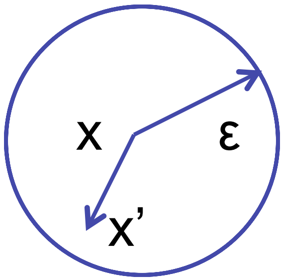
We identify the effect of horizon length scale relative to sample size on the dynamics

Neighborhood about x



1. We will introduce a family of peridynamic models parameterized by the radius of their horizon ε

2. Here fracture can be considered as a material phase transformation from linear elastic behavior into softening. In this model the dynamics drives the ``phase transformation.''

3. We will provide an analysis of the dynamics and identify its dependence upon the radius of the peridynamic horizon ε.

Main Point: We recover size effects that arise from the relative size of the peridynamic horizon with respect to the size of the sample of the material sample undergoing loading.

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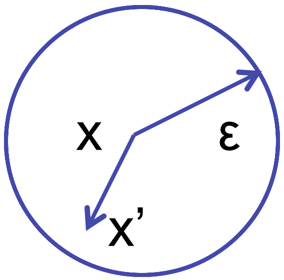
Choice of Potential Energy with Unstable Bonds



Peridynamic potential is a function of the strain along the direction `` x’-x ”

$$S = ((u(x') - u(x))/|x' - x|) * e \qquad e = (x' - x)/|x' - x|$$

$$W^{\varepsilon}(S, x' - x) = \frac{1}{\varepsilon} f\left(|x' - x| * |S|^2\right)$$

Non local law: Force between x and x’ depends on the strain

$$force = k^{\varepsilon}(S, x' - x) = \partial_S W^{\varepsilon}(S, x' - x)$$

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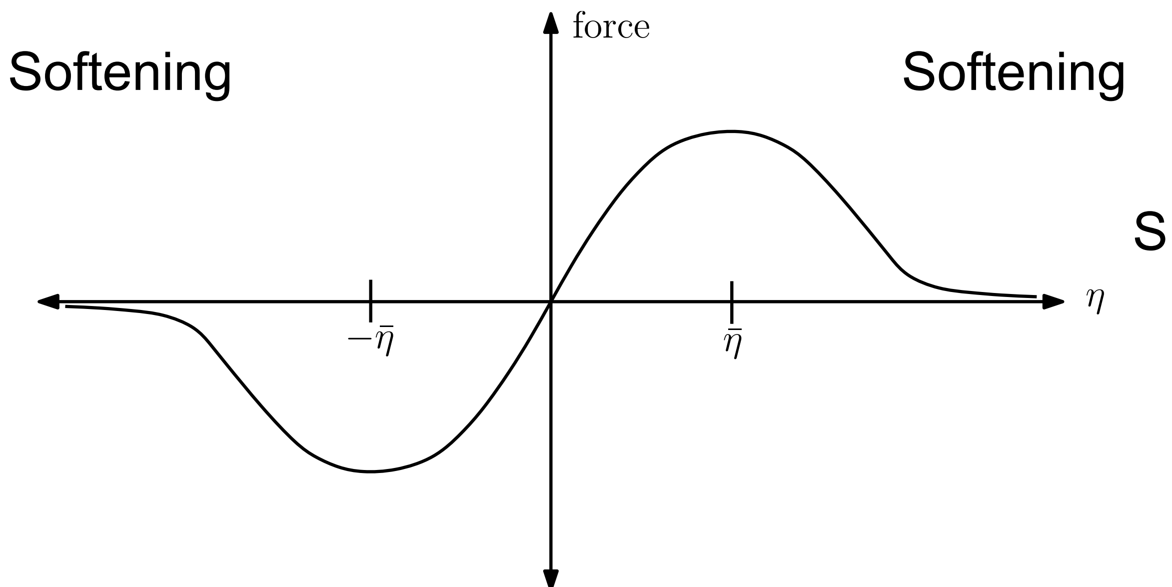
Introduce a cohesive dynamics via an unstable ``force vs. displacement'' law (L., J. Elast. 2014, ArXiv 2014)

$$force = \partial_S W^{\varepsilon}(S, x' - x)$$



$\bar{\eta} = \bar{r} / \sqrt{|x' - x|}$ $\quad \bar{r}$ is inflection point of $r \rightarrow f(r^2)$

Softening corresponding to square root concentration of strain

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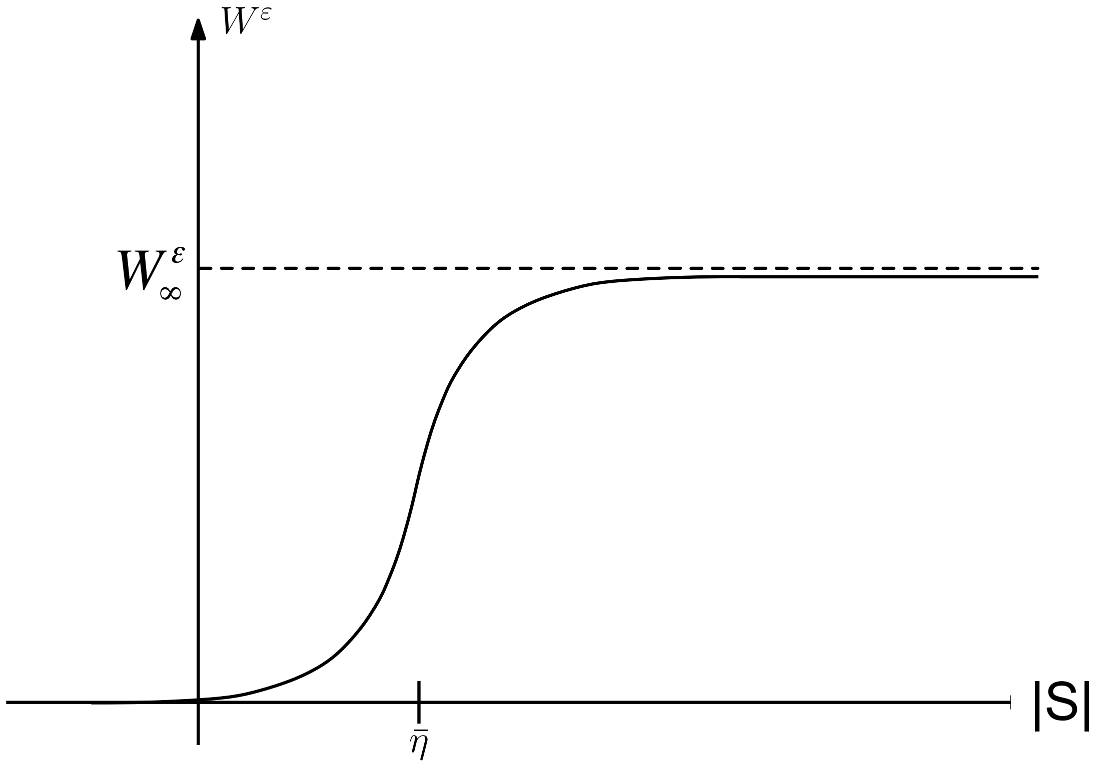
Convex – concave potential



$$|S| \mapsto W^{\varepsilon}(S, x' - x)$$

Cohesive Energy, Kinetic, Energy, Action Integral and Dynamics

Formulation of Cohesive potential energy:

Energy density

$$W^{\varepsilon}(S,x)=\frac{1}{Vol(H_{\varepsilon})}\int_{H_{\varepsilon}(x)} W^{\varepsilon}(S,x'-x)dx'$$

Potential Energy

$$PD^{\varepsilon}(u)=\int_D W^{\varepsilon}(S,x)\,dx$$

Kinetic Energy

$$K(\partial_t u)=\frac{1}{2}\int_D \rho\,|\,\partial_t u\,|^2\,dx$$

Externally applied energy

$$U(u(t))=\int_D b(t,x)u(t,x)\,dx$$

Initial conditions

$$u(0,x)=u_0(x) \qquad \partial_t u(0,x)=v_0(x)$$

Initial data doesn't depend on ε

Cohesive Energy, Kinetic, Energy, Action Integral and Dynamics at Mesoscale

Lagrangian $$L^{\varepsilon}(u(t),\partial_t u(t),t) = K(\partial_t u) - PD^{\varepsilon}(u) + U(u(t))$$

Action integral $$I(u) = \int_0^T L^{\varepsilon}(u(t),\partial_t u(t),t)\,dt$$

Least action principle delivers the Euler Lagrange equation

$$\rho \ddot{u}^{\varepsilon} = -\nabla PD^{\varepsilon}(u^{\varepsilon}) + b$$

Dynamics described by

$$\rho \ddot{u}^{\varepsilon}(t,x) = -2 \int_{H_{\varepsilon}(x)} (\partial_S W^{\varepsilon}(S^{\varepsilon}, x'-x)dx' + b(x,t)$$

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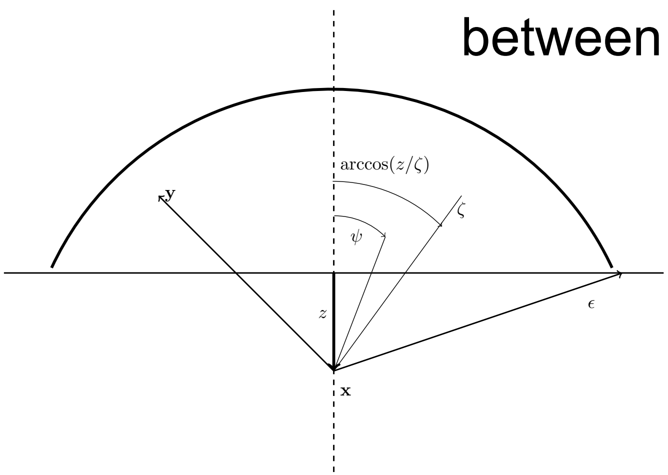
Calibrating the cohesive (bond softening) family of peridynamic models parametrized by ε

Calculate the fracture toughness G of the material using the peridynamic model, i.e. calculate the work per unit crack length to soften all bonds across both sides of the fracture surface.

The work required to completely soften the force between points x and y.

$$\frac{f_\infty}{\varepsilon} J\left(\left(\frac{|y-x|}{\varepsilon}\right)\right)$$



The total work required to completely soften the force between points x and y on either side of the surface:

$$G = 2\left(2\int_0^\varepsilon \frac{1}{V}\int_z^\varepsilon \int_0^{ar\cos(z/\zeta)} J\left(\frac{\zeta}{\varepsilon}\right)\frac{f_\infty}{\varepsilon}\zeta\, d\varphi\, d\zeta\, dz\right) = (4/\pi) f_\infty \int_0^1 r^2 J(r)\,dr$$

Total work independent of horizon and ε now becomes a modeling parameter.

Calibrating the cohesive (bond softening) family of peridynamic models parametrized by ε part II

Calculate the elastic moduli of the material from the peridynamic model. To do this calculate the Peridynamic energy density of a homogeneous strain that is small relative to the critical strain necessary for softening, i.e., suppose the deformation is linear at the length scale of the horizon: u(x)=Fx, so

$$S = \frac{Fy - Fx}{|y-x|} \bullet \left(\frac{y-x}{|y-x|} \right) = Fe \bullet e \qquad e = \frac{y-x}{|y-x|}$$

here $S = Fe \bullet e << S_c$ and to leading order the peridynamic energy density is

$$W^{\varepsilon}(S,x) = \frac{1}{Vol(H_{\varepsilon})} \int_{H_{\varepsilon}(x)} W^{\varepsilon}(S, x'-x)dx' = 2\mu |F|^2 + \lambda (trF)^2 + O(\varepsilon)$$

with $\lambda = \mu = (1/4)f'(0)\int_0^1 r^2 J(r)dr$

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Study the dependence of dynamics with respect to horizion size

For initial data $u(0,x)=u_0\,(x)$ and $u_t(0,x)=v_0(x)$ belonging to $L^2(D)$.

$$\rho\ddot{u}^{\varepsilon}(t,x) = -2\int_{H_\varepsilon(x)} (\partial_S W^{\varepsilon}(S^{\varepsilon}, x'-x)dx' + b(x,t)$$

This problem is well posed and has a solution $u^{\varepsilon}(t,x)$
That belongs to $C^2([0,T];L^2(D))$ Lipton. J. Elasticity 2014

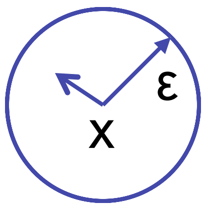
The force is a function of strain

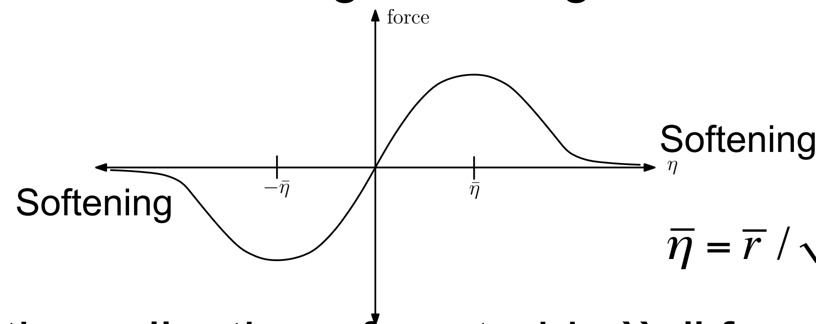
$$S = ((u(x') - u(x))/|x'-x|\ ) * e$$

``a generalized directional derivative''
so both continuous and discontinuous deformation
$u^{\varepsilon}(t,x)$ can participate in the dynamics.

Process zone:

Collection of neighborhoods containing softening behavior



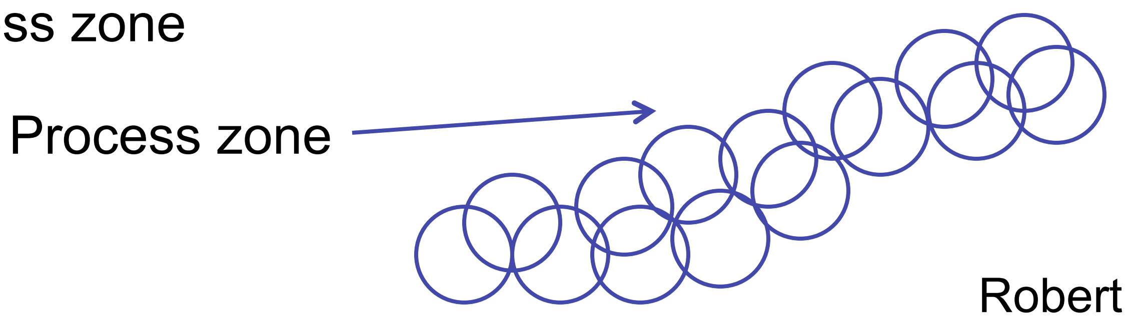


$\overline{\eta} = \overline{r} / \sqrt{|x' - x|}$

Process zone defined to be the collection of centroids ``x'' for which the proportion of bonds P with strain greater than critical value $\overline{\eta}$ is greater than α, $0 < \alpha < 1$, i.e., $P(\{y \in H_\varepsilon(x) : |S^\varepsilon| > \overline{\eta}\}) > \alpha$

Classic Barenblatt & Dugdale models feature a process zone collapsed onto a prescribed crack surface

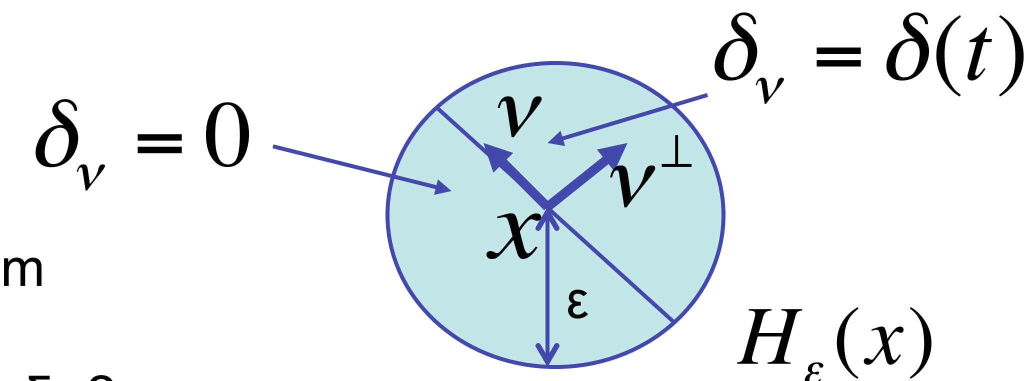
However for the cohesive bond model the dynamics selects which points lie in process zone



Lipton 2013

Rapid growth of small fissures from instability inside the process zone:

Linear stability of jump perturbation across the neighborhood at x



Given a smooth equilibrium solution u(x) is it stable under a jump perturbation δ_ν ?

Calculation gives the condition for linear stability

$$\rho\delta_{tt} = A_\nu \delta \qquad A_\nu = \frac{1}{2}\int_{H_\varepsilon(x)} (-\partial_S^2 W^\varepsilon(S, x'-x))dx'$$

Unstable $\quad A_\nu > 0 \quad -\partial_S^2 W^\varepsilon(S) > 0 \ |S| > \bar{r}/\sqrt{|x'-x|}$ perturbation grows

Neutrally stable $\quad A_\nu < 0 \quad -\partial_S^2 W^\varepsilon(S) < 0 \ |S| < \bar{r}/\sqrt{|x'-x|}$ perturbation stable

Lipton 2013, 2014

Physical significance of process zone for cohesive model

Significance of process zone
(identified by stability analysis)

Points in process zone satisfy

$$P(\{y \in H_\varepsilon(x) : |S^\varepsilon| > \overline{\eta}\}) > \alpha$$

And ``small'' fissures on the length scale of the horizon can grow exponentially to become macroscopic cracks.

The fracture set: In this model the material can be torn apart, i.e., given sufficient force the material can soften and fail.
In this model there is **no bond breaking**: instead fracture can be thought of as a phase transition from a predominantly linear elastic phase within the horizon into a predominantly soft phase.

Here the fracture set corresponds all neighborhoods with α>0.5.

Dependence of the process zone with length scale of nonlocal interaction ε: Horizon as modeling parameter

The energy put into the system up to time t is given by

$$C(t) = (1 + 2LEFM(u_0) + \tfrac{\rho}{2}\|v_0\| + \tfrac{2}{\rho^2}[\int_0^t \|b(\tau)\| d\tau)]^2$$

Dependence of the process zone with length scale of nonlocal interaction ε: Horizon as modeling parameter

Dependence of the process zone with length scale of nonlocal interaction

The energy of the process zone is controlled by ε according to the following fundamental inequality derived directly from the equation of motion

$$\alpha f(\overline{r})VOL(PZ^{\varepsilon}) \leq \varepsilon C(t)$$

$f(\overline{r})$ is the energy per unit length needed to soften the bond
C(t) is the total energy put into the system up to time t
α is the proportion of bonds softened inside the neighborhood
ε is the ratio between the nonlocal interaction with respect to sample size

L. 2014

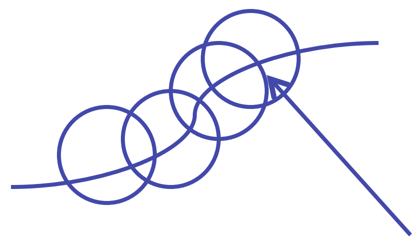
From a modeling perspective:
The estimate for the size of the process zone is consistent with the fracture toughness being the same for every choice ε

Collapse of the process zone with vanishing nonlocality ε & convergence to brittle fracture

Collapse/concentration of the process zone

The volume of the process zone goes to zero with ε uniformly in time and concentrates on a set of zero volume.

Lipton. 2013, 2014



Concentration set

I.e., the *process zones* concentrate on a set of zero volume for all times in the flow as $\varepsilon \to 0$.

Vanishing non-local limit of Cohesive flows

For initial data $u(0,x)=u_0(x)$ and $u_t(0,x)=v_0(x)$ belonging to $L^2(D)$

$$\rho\ddot{u}^{\varepsilon} = -2\int_{H_\varepsilon(x)} (\partial_S W^{\varepsilon}(S^{\varepsilon}, x'-x)dx' + b$$

Overview:

1. Start with nonlocal dynamics associated with horizon length scale ε,
2. Then pass to the limit of vanishing nonlocality ε → 0 in the dynamics to recover dynamics associated with a PDE based evolution describing brittle fracture. (L. 2014)

Here ε is the ratio of non local interaction length to sample size.

Cohesive evolution with bounded initial data

Initial displacement $u_0(x)$

$$\sup_{x\in D} |u_0| < \infty$$

Initial velocity $v_0(x)$

$$\sup_{x\in D} |v_0| < \infty$$

Initial data with bounded linear elastic energy

$$LEFM(u_0) = \int_D 2\mu |E(u_0)|^2 + \lambda |div(u_0)|^2 dx + G(H^1(S_{u_0}))$$

Energy inequality: In anticipation of small horizon limit

Recall the fracture toughness and linear elastic response of the family of PD models parameterized by ε are given by

$$\lambda = \mu = (1/4) f'(0) \int_0^1 r^2 J(r)\,dr \qquad G = (4/\pi) f_\infty \int_0^1 r^2 J(r)\,dr$$

Note that only $f'(0)$ and f_∞ determine the elastic moduli parameters μ, λ and G for this family of peridynamic models.

Fundamental inequality:

$$LEFM(u_0) = \int_D 2\mu |E(u_0)|^2 + \lambda |div(u_0)|^2 dx + G(H^1(S_{u_0})) \geq$$

$$\geq PD^\varepsilon(u_0) = \int_D \int_{H_\varepsilon(x)} W^\varepsilon(S_0, x'-x)\,dx'\,dx$$

Lipton. J. ELAS 2015

Brittle fracture limit of cohesive evolutions

Compactness Theorem: (for small horizon limit of dynamics).
Let $u^{\varepsilon}(t,x)$ be a family of nonlocal cohesive evolutions associated with the same initial data. Then up to subsequences they converge to a limit evolution $u^{0}(t,x)$ that has bounded LEFM energy for [0,T]

Limiting evolution has bounded Linear Elastic Fracture Energy [0,T].

$$\int_D 2\mu |E(u^0)|^2 + \lambda |div(u^0)|^2 dx + G(H^1(S_{u^0})) \leq C$$

$$\lim_{\varepsilon \to 0} \{ \sup_{0<t<T} \left| \int_D |u^{\varepsilon}(t,x) - u^0(t,x)|^2 \, dx \right| \} = 0$$

$u^0(t,\bullet)$ in SBD(D)

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Recover classic wave equation in the small horizon limit theory for points not on crack set

Distinguished limit of vanishing nonlocality

Theorem. For $\lambda = \mu = (1/4) f'(0) \int_0^1 r^2 J(r)\, dr$

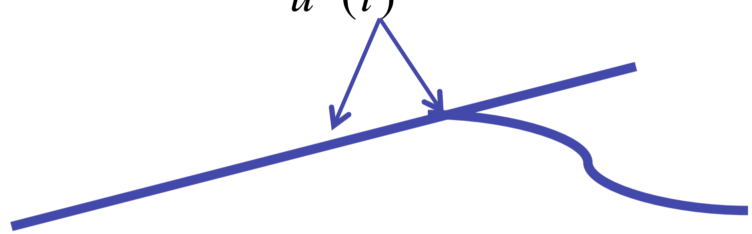
Limiting displacement u^0 evolves elastodynamically away from fracture

$$\rho \ddot{u}^0 = div(\sigma) + b \qquad \sigma = \lambda I Tr(Eu^0) + 2\mu E u^0$$

As $\varepsilon \to 0$ the cohesive evolution $u^\varepsilon(x,t)$ approaches PDE based fracture given by the deformation - jump set pair

$$u^0(t,x) \quad S_{u^0(t)}$$

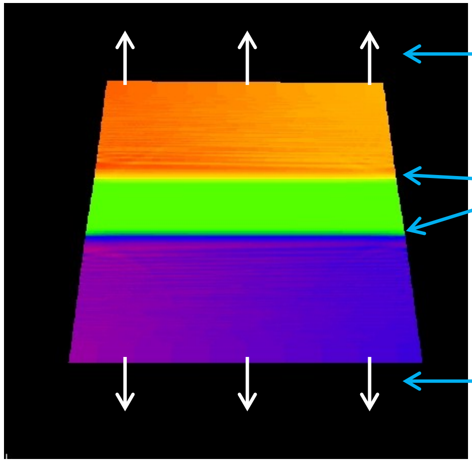
J. ELAS Lipton. 2014



Peridynamics simulation for Cohesive Evolution, Stewart Silling (Sandia) 2015

A well posed problem

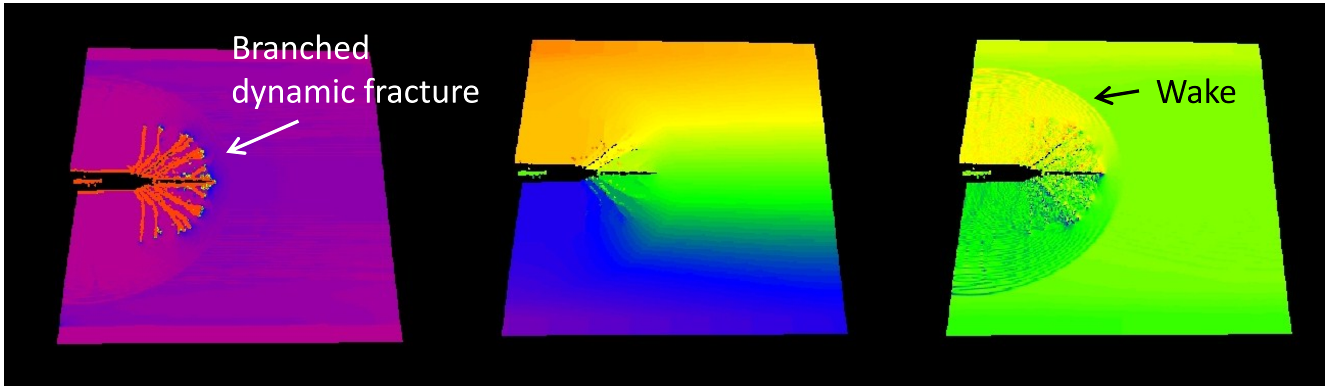
Crack nucleation within a continuous deformation



+ velocity applied at boundary

Incident waves

- velocity applied at boundary



Bond strain

Displacement

Velocity

Conclusions

- The nonlocal cohesive model in peridynamic formulation is mathematically well posed. It is a free process zone model providing nucleation and propagation of fracture surface driven by mesoscopic instability.

- Evolution of the process zone together with the the fracture set is governed by a single equation of motion consistent with Newton's second law - a hallmark of peridynamic models.

- The cohesive dynamics provides a-priori estimates for size of process zone in terms of horizon radius. Useful for calibrating the model to the material sample.

- These nonlocal models recover a brittle fracture limit with bounded Griffith fracture energy in the limit of vanishing nonlocality.

Publications:

Journal of Elasticity 2014,
DOI 10.1007/s10659-013-9463-0

General 3-d evolutions: ArXive 2014
J. Elasticity 2015, in revision