Dynamic Brittle Fracture from Nonlocal Double-Well Potentials: A State-Based Model

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Abstract

We introduce a regularized model for free fracture propagation based on nonlocal potentials. We work within the small deformation setting, and the model is developed within a state-based peridynamic formulation. At each instant of the evolution, we identify the softening zone where strains lie above the strength of the material. We show that deformation discontinuities associated with flaws larger than the length scale of nonlocality δ can become unstable and grow. An explicit inequality is found that shows that the volume of the softening zone goes to zero linearly with the length scale of nonlocal interaction. This scaling

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is consistent with the notion that a softening zone of width proportional to δ converges to a sharp fracture set as the length scale of nonlocal interaction goes to zero. Here the softening zone is interpreted as a regularization of the crack network. Inside quiescent regions with no cracks or softening, the nonlocal operator converges to the local elastic operator at a rate proportional to the radius of nonlocal interaction. This model is designed to be calibrated to measured values of critical energy release rate, shear modulus, and bulk modulus of material samples. For this model one is not restricted to Poisson ratios of $1/4$ and can choose the potentials so that small strain behavior is specified by the isotropic elasticity tensor for any material with prescribed shear and Lamé moduli.

Keywords

Free fracture model · Nonlocal interactions · Double-well potentials · State-based peridynamics

Introduction

We address the problem of free crack propagation in homogeneous materials. The crack path is not known a priori and is found as part of the problem solution. Our approach is to use a nonlocal formulation based on double-well potentials. We will work within the small deformation setting, and the model is developed within a state-based peridynamic formulation. Peridynamics (Silling, 2000; Silling et al., 2007) is a nonlocal formulation of continuum mechanics expressed in terms of displacement differences as opposed to spatial derivatives of the displacement field. These features provide the ability to simultaneously simulate both smooth displacements and defect evolution. Computational methods based on peridynamic modeling exhibit formation and evolution of sharp features associated with phase transformation (see Dayal and Bhattacharya 2006) and fracture (see Silling and Lehoucq 2008; Silling et al. 2010; Foster et al. 2011; Agwai et al. 2011; Du et al. 2013; Lipton et al. 2016; Bobaru and Hu 2012; Ha and Bobaru 2010; Silling and Bobaru 2005; Weckner and Abeyaratne 2005; Gerstle et al. 2007; Silling and Askari 2005). A recent review of the state of the art can be found in Bobaru et al. (2016).

In this work we are motivated by the recent models proposed and studied in Lipton (2014, 2016), and Lipton et al. (2016). Calibration has been investigated in Diehl et al. (2016). These models are defined by double-well two-point strain potentials. Here one potential well is centered at the origin and associated with elastic response, while the other well is at infinity and associated with surface energy. The rationale for studying these models is that they are shown to be well posed over the class of square-integrable non-smooth displacements, and in the limit of vanishing nonlocality, the dynamics localize and recover features of sharp fracture propagation (see Lipton 2014, 2016). In this work we extend this modeling approach to the state-based formulation. Our work is further motivated by the recent numerical-experimental study carried out in Diehl et al. (2016) demonstrating that the bond-based model is unable to capture the Poisson ratio for a sample of PMMA at room temperature. Here we develop a double-well state-based potential for which the Poisson ratio is no longer constrained to be $1/4$. We show that for this model we can choose the potentials so that the small strain behavior is specified by the isotropic elasticity tensor for any material with prescribed shear and Lamé moduli.

Nonlocal Dynamics

We formulate the nonlocal dynamics. Here we will assume displacements u are small (infinitesimal) relative to the size of the three-dimensional body D. The tensile strain is written as $S = S(y,x,t;u)$ and given by

$$S(y,x,t;u) = \frac{u(t,y) - u(t,x)}{|y-x|} \cdot e_{y-x}, \qquad e_{y-x} = \frac{y-x}{|y-x|}, \tag{1}$$

where e_{y-x} is a unit direction vector and $\cdot$ is the dot product. It is evident that $S(y,x,t;u)$ is the tensile strain along the direction e_{y-x}. We introduce the influence function $\omega^\delta(|y-x|)$ such that ω^δ is nonzero for $|y-x| < \delta$, zero outside. Here we will take $\omega^\delta(|y-x|) = \omega(|y-x|/\delta)$ with $\omega(r) = 0$ for $r > 1$ nonnegative for $r < 1$ and ω is bounded.

The spherical or hydrostatic strain at x is given by

$$\theta(x,t;u) = \frac{1}{V_\delta} \int_{D \cap B_\delta(x)} \omega^\delta(|y-x|) S(y,x,t;u) |y-x|\, dy, \tag{2}$$

where V_δ is the volume of the ball $B_\delta(x)$ of radius δ centered at x. Here we have employed the normalization $|y-x|/\delta$ so that this factor takes values in the interval from 0 to 1.

Motivated by potentials of Lennard-Jones type, we define the force potential for tensile strain given by

$$\mathcal{W}^\delta(S(y,x,t;u)) = \alpha \omega^\delta(|y-x|) \frac{1}{\delta |y-x|} f(\sqrt{|y-x|} S(y,x,t;u)) \tag{3}$$

and the potential for hydrostatic strain

$$\mathcal{V}^\delta(\theta(x,t;u)) = \frac{\beta g(\theta(x,t;u))}{\delta^2} \tag{4}$$

where $\mathcal{W}^\delta(S(y,x,t;u))$ is the pairwise force potential per unit length between two points x and y and $\mathcal{V}^\delta(\theta(x,t;u))$ is the hydrostatic force potential density at x. They are described in terms of their potential functions f and g (see Fig. 1). These two potentials are double-well potentials that are chosen so that the associated forces acting between material points x and y are initially elastic and then soften and decay to zero as the strain between points increases (see Fig. 2 for the tensile force).

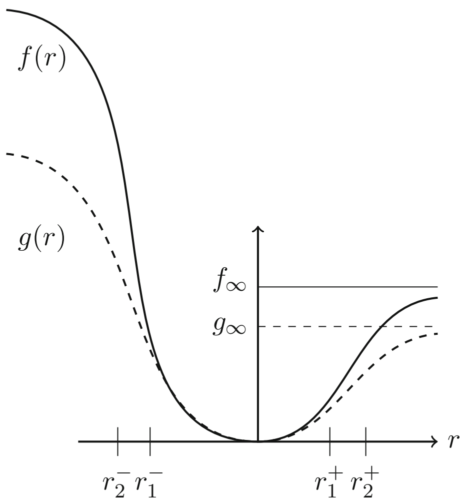

Fig. 1 Potential function $f(r)$ for tensile force and potential function $g(r)$ for hydrostatic force

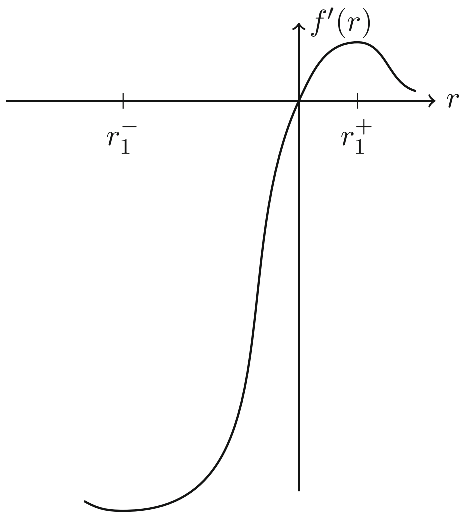

Fig. 2 Cohesive tensile force

This force is negative for compression, and a similar force hydrostatic strain law follows from the potential for hydrostatic strain. The first well for $\mathcal{W}^\delta(S(y,x,t;u))$ and $\mathcal{V}^\delta(\theta(x,t;u))$ is at zero tensile and hydrostatic strain, respectively. With this in mind, we make the choice

$$f(0) = f'(0) = g(0) = g'(0). \tag{5}$$

The second well is at infinite tensile and hydrostatic strain and is characterized by the horizontal asymptotes $\lim_{S\to\infty} f(S) = f_\infty$ and $\lim_{\theta\to\infty} g(\theta) = g_\infty$, respectively (see Fig. 1).

The critical tensile strain $S_c^+ > 0$ for which the force begins to soften is given by the inflection point $r_1^+ > 0$ of f and is

$$S_c^+ = \frac{r_1^+}{\sqrt{|y-x|}}. \tag{6}$$

The critical negative tensile strain is chosen much larger in magnitude than S_c^+ and is

$$S_c^- = \frac{r_1^-}{\sqrt{|y-x|}}, \tag{7}$$

with $r_1^- < 0$ and $r_1^+ << |r_1^-|$. The critical value $0 < \theta_c^+$ where the force begins to soften under positive hydrostatic strain for $\theta(x, t; u) > \theta_c^+$ is given by the inflection point r_2^+ of g and is

$$\theta_c^+ = r_2^+. \tag{8}$$

The critical compressive hydrostatic strain where the force begins to soften for negative hydrostatic strain is chosen much larger in magnitude than θ_c^+ and is

$$\theta_c^- = r_2^-, \tag{9}$$

with $r_2^- < 0$ and $r_2^+ < |r_2^-|$. For this model we suppose the inflection points for g and f satisfy the ordering

$$r_2^- < r_1^- < 0 < r_1^+ < r_2^+. \tag{10}$$

This ordering is chosen to illustrate ideas for a material that is weaker in shear strain than hydrostatic strain. With this choice and the appropriate influence function ω^δ, if the hydrostatic stress is positive at x and is above the critical value θ_c^+, then there are points y in the peridynamic neighborhood for which the tensile stress between x and y is above S_c^+. This aspect of the model is established and addressed in section "Control of the Softening Zone".

The potential energy is given by

$$\begin{aligned} PD^\delta(u) =& \frac{1}{V_\delta} \int_D \int_{D \cap B_\delta(x)} |y-x| \mathcal{W}^\delta(S(y, x, t; u))\, dy dx \\ &+ \int_D \mathcal{V}^\delta(\theta(x, t; u))\, dx. \end{aligned} \tag{11}$$

The material is assumed homogeneous, and the density is given by ρ, and the applied body force is denoted by $b(x, t)$. We define the Lagrangian

$$\mathrm{L}(u, \partial_t u, t) = \frac{\rho}{2}||\dot{u}||^2_{L^2(D;\mathbb{R}^3)} - PD^\delta(u) + \int_D b \cdot u dx,$$

here $\dot{u}$ is the velocity given by the time derivative of u, and $\|\dot{u}\|_{L^2(D;\mathbb{R}^3)}$ denotes the L^2 norm of the vector field $\dot{u} : D \to \mathbb{R}^3$. Applying the principle of least action together with a straightforward calculation gives the nonlocal dynamics

$$\rho\ddot{u}(x,t) = \mathcal{L}^T(u)(x,t) + \mathcal{L}^D(u)(x,t) + b(x,t), \text{ for } x \in D, \tag{12}$$

where

$$\mathcal{L}^T(u)(x,t) = \frac{2\alpha}{V_\delta}\int_{D\cap B_\delta(x)} \frac{\omega^\delta(|y-x|)}{\delta|y-x|}\partial_S f(\sqrt{|y-x|}S(y,x,t;u))e_{y-x}\,dy, \tag{13}$$

and

$$\mathcal{L}^D(u)(x,t)=\frac{\beta}{V_\delta}\int_{D\cap B_\delta(x)} \frac{\omega^\delta(|y-x|)}{\delta^2}\left[\partial_\theta g(\theta(y,t;u))+\partial_\theta g(\theta(x,t;u))\right]e_{y-x}\,dy. \tag{14}$$

The dynamics is complemented with the initial data

$$u(x,0) = u_0(x), \qquad \partial_t u(x,0) = v_0(x). \tag{15}$$

It is readily verified that this is an ordinary state-based peridynamic model. The forces are defined by the derivatives of the potential functions, and the derivative associated with the tensile strain potential is sketched in Fig. 2. We show in the next section that this initial value problem is well posed.

Existence of Solutions

The regularity and existence of the solution depends on the regularity of the initial data and body force. In this work we choose a general class of body forces and initial conditions. The initial displacement u_0 and velocity v_0 are chosen to be integrable and belonging to $L^\infty(D;\mathbb{R}^3)$. The body force $b(x,t)$ is chosen such that for every $t \in [0, T_0]$, b takes values in $L^\infty(D, \mathbb{R}^3)$ and is continuous in time. The associated norm is defined to be $\|b\|_{C([0,T_0];L^\infty(D,\mathbb{R}^3))} = \max_{t\in[0,T_0]}\|b(x,t)\|_{L^\infty(D,\mathbb{R}^3)}$. The space of continuous functions in time taking values in $L^\infty(D;\mathbb{R}^3)$ for which this norm is finite is denoted by $C([0, T_0]; L^\infty(D, \mathbb{R}^3))$. The space of functions twice differentiable in time taking values in $L^\infty(D, \mathbb{R}^3)$ such that both derivatives belong to $C([0, T_0]; L^\infty(D, \mathbb{R}^3))$ is written as $C^2([0, T_0]; L^\infty(D, \mathbb{R}^3))$.

We will establish existence and uniqueness for the evolution by writing the second-order ODE as an equivalent first-order system. The nonlocal dynamics (12) can be written as a first-order system. Set $y = (y_1, y_2)$ where $y_1 = u$ and $y_2 = u_t$. Now, set $F^\delta(y,t) = \Big(F_1(y,t), F_2(y,t)\Big)^T$ where:

$$
\begin{aligned}
F_1(y,t) &= y_2 \\
F_2(y,t) &= \mathcal{L}^T(y_1)(t) + \mathcal{L}^D(y_1)(t) + b(t)
\end{aligned}
\tag{16}
$$

And the initial value problem is given by the equivalent first-order system

$$
\begin{aligned}
\frac{d}{dt} y^\delta &= F^\delta(y^\delta, t) \\
y(0) = (y_1(0), y_2(0)) &= (u_0, v_0)
\end{aligned}
\tag{17}
$$

The existence of a unique solution to the initial value problem is asserted in the following theorem.

Theorem 1. *For a body force $b(t,x)$ in $C^1\Big([0,T]; L^\infty(D,\mathbb{R}^3)\Big)$ and initial data $y_1(0)$ and $y_2(0)$ in $L_0^\infty(D;\mathbb{R}^3) \times L_0^\infty(D;\mathbb{R}^3)$, there exists a unique solution $y(t)$ such that $y_1 = u$ is in*
$C^2\Big([0,T]; L^\infty(D,\mathbb{R}^3)\Big)$ for the dynamics described by (17) with initial data in $L^\infty((D;\mathbb{R}^3) \times L^\infty(D;\mathbb{R}^3)$ and body force $b(t,x)$ in $C^1\Big([0,T]; L^\infty(D,\mathbb{R}^3)\Big)$.

Proof. We will show that the model is *Lipschitz continuous* and then apply the theory of ODE in Banach spaces, e.g., Driver (2003), to guarantee the existence of a unique solution. It is sufficient to show that

$$
||\mathcal{L}^T(u)(x,t)+\mathcal{L}^D(u)(x,t)-(\mathcal{L}^T(v)(x,t)+\mathcal{L}^D(v)(x,t))||_{L^\infty(D)} \leq C||u-v||_{L^\infty(D)}
\tag{18}
$$

For ease of notation, we introduce the following vectors

$$
\vec{U} = u(y) - u(x),
$$

$$
\vec{V} = v(y) - v(x).
$$

We write

$$
\mathcal{L}^T(u)(x,t) + \mathcal{L}^D(u)(x,t) - (\mathcal{L}^T(v)(x,t) + \mathcal{L}^D(v)(x,t)) = \mathcal{I}_1 + \mathcal{I}_2. \tag{19}
$$

Here

$$
\begin{aligned}
\mathcal{I}_1 =& \frac{2\alpha}{\delta V_\delta} \int_{D\cap B_\delta(x)} \frac{\omega^\delta(|y-x|)}{\sqrt{|y-x|}} \Big\{ f'(\sqrt{|y-x|}S(y,x,t;u)) \\
&- f'(\sqrt{|y-x|}S(y,x,t;v)) \Big\} e_{(y-x)} dy \\
\mathcal{I}_2 =& \frac{\beta}{\delta^2 V_\delta} \int_{D\cap B_\delta(x)} \omega^\delta(|y-x|) \Big(g'(\theta(y,t;u)) + g'(\theta(x,t;u)) \\
&- (g'(\theta(y,t;v)) + g'(\theta(x,t;v))) \Big) e_{(y-x)} dy
\end{aligned} \tag{20}
$$

Since f'' is bounded a straightforward calculation gives:

$$
\begin{aligned}
&|f'(\sqrt{|y-x|}S(y,x,t;u)) - f'(\sqrt{|y-x|}S(y,x,t;v)) \\
&\leq \sqrt{|y-x|} \sup_{s\in\mathbb{R}}\{|f''(s)|\}|S(y,x,t;u) - S(y,x,t;v)|,
\end{aligned}
$$

and $|e_{y-x}| = 1$, so we can bound $\mathcal{I}_1$ by

$$
|\mathcal{I}_1| \leq \frac{2\alpha}{\delta V_\delta} \int_{D\cap B_\delta(x)} \omega^\delta(|y-x|) \sup_{x\in D}\{|f''(x)|\}|S(y,x,t;u) - S(y,x,t;v)|\, dy. \tag{21}
$$

In what follows $C_1 = \sup_{s\in\mathbb{R}}\{|f''(s)|\} < \infty$ and we make the change of variable

$$
\begin{aligned}
y &= x + \delta\xi \\
|y-x| &= \sigma|\xi| \\
dy &= \delta^3 d\xi,
\end{aligned}
$$

and a straightforward calculation shows

$$
\mathcal{I}_1 \leq \frac{2\alpha C_1}{\delta^2} \int_{H_1(0)\cap\{x+\delta\xi\in D\}} |\omega(\xi)| \frac{|u(x+\delta\xi) - u(x) - (v(x+\delta\xi) - v(x))|}{|\xi|}\, d\xi \tag{22}
$$

Which leads to the inequality

$$
||\mathcal{I}_1||_{L^\infty(D;\mathbb{R}^3)} \leq \frac{4\alpha C_1 C_2}{\delta^2} ||u-v||_{L^\infty(D;\mathbb{R}^3)}, \tag{23}
$$

with $C_2 = \int_{H_1(0)} |\xi|^{-1}\omega(|\xi|)\, d\xi$. Now we can work on the second part, where we follow a similar approach. Noting that g'' is bounded, we let $C_3 = \sup_{\theta\in\mathbb{R}}\{|g''(\theta)|\} < \infty$ and $C_4 = \int_{H_1(0)} |\xi|\omega(|\xi|) d\xi$, to find that

$$
\begin{aligned}
|g'(\theta(y,t;u)) - g'(\theta(y,t;v))| &\leq C_3|\theta(y,t;u) - \theta(y,t;v)| \\
&\leq \frac{2C_3C_4}{\delta^2}\|u - v\|_{L^\infty(D;\mathbb{R}^3)},
\end{aligned}
$$

and

$$
\begin{aligned}
|g'(\theta(x,t;u)) - g'(\theta(x,t;v))| &\leq C_3|\theta(x,t;u) - \theta(x,t;v)| \\
&\leq \frac{2C_3C_4}{\delta^2}\|u - v\|_{L^\infty(D;\mathbb{R}^3)},
\end{aligned}
$$

so

$$
\|\mathcal{I}_2\|_{L^\infty(D;\mathbb{R}^3)} \leq \frac{4\beta C_3C_4}{\delta^2}\|u - v\|_{L^\infty(D;\mathbb{R}^3)}. \tag{24}
$$

Adding (23) and (24) gives the desired result

$$
\begin{aligned}
&||\mathcal{L}^T(u)(x,t) + \mathcal{L}^D(u)(x,t) - (\mathcal{L}^T(v)(x,t) + \mathcal{L}^D(v)(x,t))||_{L^\infty(D;\mathbb{R}^3)} \\
&\quad \leq \frac{4(\alpha C_1C_2 + \beta C_3C_4)}{\delta^2}\|u - v\|_{L^\infty(D;\mathbb{R}^3)}.
\end{aligned} \tag{25}
$$

□

Stability Analysis

In this section we identify a source for crack nucleation as a material defect represented by a jump discontinuity in the displacement field. To illustrate the ideas, we assume the defect is in the interior of the body and at least δ away from the boundary. This jump discontinuity can become unstable and grow in time. We proceed with a perturbation analysis and consider a time-independent body force density b and a smooth equilibrium solution u. Now assume that the defect perturbs u in the neighborhood of a point x by a piecewise constant vector field s that represents a jump in displacement across a planar surface with normal vector ν. We assume that this jump occurs along a defect of length 2δ on the planar surface.

The smooth equilibrium solution $u(x,t)$ is a solution of

$$
0 = \mathcal{L}^T(u)(x,t) + \mathcal{L}^D(u)(x,t) + b(x) \tag{26}
$$

Now consider a perturbed solution $u^P(x,t)$ that differs from equilibrium solution $u(x,t)$ by the jump across the planar surface which is specified by unit normal vector ν. We suppose the surface passes through x and extends across the peridynamic neighborhood centered at x. Points y for which $(y-x)\cdot\nu < 0$ are denoted by $\mathcal{E}_\nu^-$ and points for which $(y-x)\cdot\nu \geq 0$ are denoted by $\mathcal{E}_\nu^+$, see Fig. 3.

The perturbed solution u^P satisfies

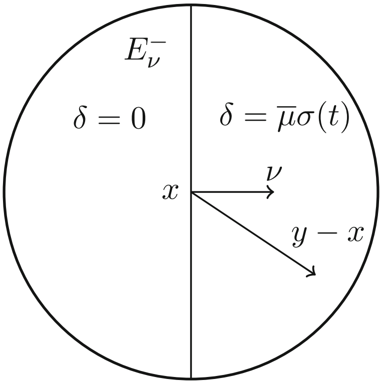

Fig. 3 Jump discontinuity

$$\rho \ddot{u^P} = \mathcal{L}^T(u^P)(x,t) + \mathcal{L}^D(u^P)(x,t) + b(x) \tag{27}$$

Here the perturbed solution $u^P(x,t)$ is given by the equilibrium solution plus a piecewise constant perturbation and is written

$$u^P(y,t) = u(y,t) + s(y,t) \tag{28}$$

Where

$$s(y,t) = \begin{cases} 0 & y \in \mathcal{E}_\nu^- \\ \bar{\mu}\sigma(t) & y \in \mathcal{E}_\nu^+ \end{cases} \tag{29}$$

Subtracting (26) from (27) gives

$$\rho \ddot{u^P} = \mathcal{L}^T(u^P)(x,t) + \mathcal{L}^D(u^P)(x,t) - \mathcal{L}^T(u)(x,t) + \mathcal{L}^D(u)(x,t) \tag{30}$$

Here the second term in $\mathcal{L}^D(u)$ vanishes as we are away from the boundary, and the integrand is odd in the y variable with respect to the domain $B_\delta(x)$. Since $u^P = u + s$ and s is small, we expand $f'(\sqrt{|y-x|}(S(y,x,t;u+s)))$ in Taylor series in s. Noting that $\theta(x,t;u+s) = \theta(x,t;u) + \theta(x,t;s)$ and $\theta(x,t;s)$ is initially infinitesimal, we also expand $g'(\theta(x,t;u+s))$ in a Taylor series in $\theta(x,t;s)$. Applying the expansions to (30) shows that to leading order

$$\begin{aligned} \rho \ddot{u^P} = \rho\ddot{\sigma}\overline{\mu} = \frac{2\alpha}{\delta V_\delta} \int_{B_\delta(x)} \frac{\omega^\delta(|y-x|)}{\sqrt{|y-x|}} f''(\sqrt{|y-x|}S)(s(y,t) - s(x,t)) \cdot \\ e_{(y-x)} e_{(y-x)} dy + \frac{\beta}{V_\delta \delta^2} \int_{B_\delta(x)} \omega^\delta(|y-x|) g''(\theta(y,t;u)) \frac{1}{V_\delta} \\ \int_{B_\delta(y)} \omega^\delta(|z-y|)(s(z,t) - s(y,t)) \cdot e_{z-y}\, dz e_{y-x}\, dy = I_1 + I_2, \end{aligned} \tag{31}$$

where I_1 and I_2 are the first, second terms on the right-hand side of (31). A straightforward calculation using (29) shows that

$$I_1 = -\frac{2\alpha}{\delta V_\delta} \int_{B_\delta(x)\cap\mathcal{E}_\nu^-} \frac{J^\delta(|y-x|)}{|y-x|} f''(\sqrt{|y-x|}S) e_{(y-x)} \cdot \bar{\mu}\sigma(t) e_{(y-x)} dy \quad (32)$$

We next calculate I_2. A straightforward but delicate calculation gives

$$\frac{1}{V_\delta} \int_{B_\delta(y)} \frac{\omega^\delta(|z-y|)}{\delta} (s(z,t) - s(y,t)) \cdot e_{z-y}\, dz = b(y) \cdot \overline{\mu}\sigma(t) \quad (33)$$

where

$$b(y) = \frac{1}{V_\delta} \int_0^{2\pi} \int_a^\delta \int_0^{\overline{\phi}} \omega(|z-y|) e(\theta,\phi) |z-y|^2 \sin\phi \, d\phi \, d\theta \, d|z-y| \quad (34)$$

and the limits of the iterated integral are

$$a = |(y-x)\cdot\nu| \quad \overline{\phi} = \arccos\left(\frac{|(y-x)\cdot\nu|}{|z-y|}\right), \quad (35)$$

and $e(\theta,\phi)$ is the vector on the unit sphere with direction specified by the angles θ and ϕ. Calculation now gives

$$\begin{aligned} I_2 = &\frac{\beta}{V_\delta \delta^2} \left(\int_{B_\delta(x)\cap\mathcal{E}_\nu^-} \omega^\delta(|y-x|) g''(\theta(y,t;u)) b(y) \cdot \overline{\mu}\sigma(t) e_{y-x} dy \right. \\ &\left. - \int_{B_\delta(x)\cap\mathcal{E}_\nu^+} \omega^\delta(|y-x|) g''(\theta(y,t;u)) b(y) \cdot \overline{\mu}\sigma(t) e_{y-x} dy \right), \end{aligned} \quad (36)$$

where

$$\begin{aligned} &\int_{B_\delta(x)\cap\mathcal{E}_\nu^-} \frac{\omega^\delta(|y-x|)}{\delta} b(y) \cdot \overline{\mu} s(t) e_{y-x} dy \\ &= \int_{B_\delta(x)\cap\mathcal{E}_\nu^+} \frac{\omega^\delta(|y-x|)}{\delta} b(y) \cdot \overline{\mu} s(t) e_{y-x} dy. \end{aligned} \quad (37)$$

We now take the dot product of both sides of (31) with $\overline{\mu}$ to get

$$\rho\ddot{\sigma} = \frac{(\mathsf{A} + \mathsf{B}^{\mathrm{sym}})\overline{\mu}\cdot\overline{\mu}}{|\overline{\mu}|^2}\sigma(t), \quad (38)$$

where

$$\mathsf{A} = -\frac{2\alpha}{\delta V_\delta} \int_{B_\delta(x)\cap\mathcal{E}_v^-} \frac{J^\delta(|y-x|)}{|y-x|} f''(\sqrt{|y-x|}S) e_{(y-x)} \otimes e_{(y-x)} dy \tag{39}$$

and $\mathsf{B}^{\text{sym}} = (\mathsf{B} + \mathsf{B}^T)/2$ with

$$\mathsf{B} = \frac{\beta}{V_\delta \delta^2} \left(\int_{B_\delta(x)\cap\mathcal{E}_v^-} \omega^\delta(|y-x|) g''(\theta(y,t;u)) b(y) \otimes e_{y-x} dy \right.$$
$$\left. - \int_{B_\delta(x)\cap\mathcal{E}_v^+} \omega^\delta(|y-x|) g''(\theta(y,t;u)) b(y) \otimes e_{y-x} dy \right). \tag{40}$$

Inspection shows that

$$f''(\sqrt{|y-x|}S) < 0, \text{ when } S > S_c^+. \tag{41}$$

Thus the eigenvalues of A can be nonnegative whenever the tensile strain is positive and greater than S_c^+ so that the force is in the softening regime for a preponderance of points y inside $B_\delta(x)$. In general the defect will be stable if all eigenvalues of the stability matrix $\mathsf{A} + \mathsf{B}^{\text{sym}}$ are negative. On the other hand, the defect will be unstable if at least one eigenvalue of the stability matrix is positive.

We collect results in the following proposition.

Proposition 1 (Fracture nucleation condition about a defect). *A condition for crack nucleation at a defect passing through a point x is that the associated stability matrix $\mathsf{A} + \mathsf{B}^{\text{sym}}$ has at least one positive eigenvalue.*

If the equilibrium solution is constant, then $\theta(y,t;u) = \text{constant}$ and $\mathsf{B}^{\text{sym}} = 0$. For this case the fracture nucleation condition simplifies and depends only on the eigenvalues of the matrix A. In the next section, we analyze the size of the set where the tensile strain is greater than S_c^+ so that the tensile force is in the softening regime for points y inside $B_\delta(x)$.

Control of the Softening Zone

We define the softening zone in terms of the collection of centers of peridynamic neighborhoods with tensile strain exceeding S_c^+. In what follows we probe the dynamics to obtain mathematically rigorous and explicit estimates on the size of the softening zone in terms of the radius of the peridynamic horizon. In this section we assume $\omega^\delta = 1$, $\delta < 1$, and from the definition of the hydrostatic strain $\theta(x,t;u)$, we have the following lemma.

Lemma 1 (Hydrostatic softening implies tensile softening). *If $\theta_c^+ < \theta(x,t;u)$, then $S_c^+ < S(y,x,t;u)$ for some subset of points y inside the peridynamic neighborhood centered at x and*

$$\{x \in D : \theta(x) > \theta_c^+\} \subset \{x \in D : S(x,y,t;u) > S_c^+, \textit{ for some } y \textit{ in } B_\delta(x)\}. \tag{42}$$

Proof. Suppose $\theta_c^+ < \theta(x,t;u)$, then there are points y in $B_\delta(x)$ for which

$$\theta_c^+ < |y-x|S(y,x,t;u) < \sqrt{|y-x|}S(y,x,t;u), \tag{43}$$

so

$$S_c^+ < \frac{\theta_c^+}{\sqrt{|y-x|}} < S(y,x,t;u), \tag{44}$$

since $r_1^+ < r_2^+ = \theta_c^+$. This directly implies

$$\{x \in D : \theta(x) > \theta_c^+\} \subset \{x \in D : S(x,y,t;u) > S_c^+, \text{ for some } y \text{ in } B_\delta(x)\}, \tag{45}$$

and the lemma is proved. □

This inequality shows that the collection of neighborhoods where softening is due to the hydrostatic force is also subset of the neighborhoods where there is softening due to tensile force. Motivated by this observation, we focus on peridynamic neighborhoods where the tensile strain is above critical. We start by defining the *softening zone*. The set of points y in $B_\delta(x)$ with tensile strain larger than critical can be written as

$$A_\delta^+(x) = \{y \in B_\delta(x) : S(y,x,t;u) > \mathcal{S}_c^+\}.$$

From the monotonicity of the force potential f, we can also express this set as

$$A_\delta^+(x) = \{y \in B_\delta(x); f(\sqrt{|y-x|}S(y,x,t;u)) \geq f(r_1^+)\}.$$

We define the weighted volume of the set A_δ^+ in terms of its characteristic function $\chi_{A_\delta^+}(y)$ taking the value one for $y \in A_\delta^+$ and zero outside. The weighted volume of A_δ^+ is given by $\int_{B_\delta(x)} \chi_{A_\delta^+}(y)|y-x|\,dy$, and the weighted volume of $B_\delta(x)$ is $m = \int_{B_\delta(x)} |y-x|\,dy$. The weighted volume fraction $P_\delta(x)$ of $y \in B_\delta(x)$ with tensile strain larger than critical is given by the ratio

$$P_\delta(x) = \frac{\int_{B_\delta(x)} \chi_{A_\delta^+}(y)|y-x|\,dy}{m}.$$

Definition 1 (Softening zone). Fix any volume fraction $0 < \gamma \leq 1$, and with each time t in the interval $0 \leq t \leq T$, define the softening zone $SZ^\delta(\gamma, t)$ to be the collection of centers of peridynamic neighborhoods for which the weighted volume fraction of points y with strain $S(y, x, t; u)$ exceeding the threshold $\mathcal{S}_c$ is greater than γ, i.e.,

$$SZ^\delta(\gamma, t) = \{x \in D; P_\delta(x) > \gamma\}. \tag{46}$$

We now show that the volume of $SZ^\delta(\gamma, t)$ goes to zero linearly with the horizon δ for properly chosen initial data and body force. This scaling is consistent with the notion that a softening zone of width proportional to δ converges to a sharp fracture as the length scale δ of nonlocal interaction goes to zero. We define the sum of kinetic and potential energy as

$$W(t) = \frac{\rho}{2}||\dot{u}||^2_{L^2(D,\mathbb{R}^d)} + PD^\delta(u(t)) \tag{47}$$

and set

$$C(t) = \Big(\frac{1}{\sqrt{\rho}}\int_0^t ||b||_{L^2(D,\mathbb{R}^d)} d\tau + \sqrt{W(0)}\Big)^2. \tag{48}$$

Here $C(t)$ is a measure of the total energy delivered to the body from initial conditions and body force up to time t. The tensile toughness is defined to be the energy of tensile tension between x and y per unit length necessary for softening and is given by $f(r_1^+)/\delta$. We now state the geometric dependence of the softening zone on horizon.

Theorem 2. *The volume of the softening zone SZ^δ is controlled by the horizon δ according to the following relation expressed in terms of the total energy delivered to the system, the tensile toughness, and the weighted volume fraction of points y where the tensile strain exceeds S_c^+,*

$$\text{Volume}(SZ^\delta(\gamma, t)) \leq \frac{\delta C(t)}{\gamma m f(r_1^+)}. \tag{49}$$

Remark 1. It is clear that for zero initial data such that $u(0, x) = 0$ that $C(t)$ depends only on the body force $b(t, x)$ and initial velocity. For this choice we see that the softening zone goes to zero linearly with the horizon δ.

We now establish the theorem using Gronwall's inequality and Tchebychev's inequality. The peridynamic energy density at a point x is

$$E^\delta(x) = \frac{1}{V_\delta}\int_{D\cap B_\delta(x)} |y - x|\mathcal{W}^\delta(S(y, x, t; u))\, dy + \mathcal{V}^\delta(\theta(x, t; u)) \tag{50}$$

Which can also be rewritten with the following change of variable $y - x = \delta\xi$

$$E^{\delta}(x) = \frac{\alpha}{\delta V_1}\int_{D\cap B_1(0)} \omega(|\xi|) f(\sqrt{\delta|\xi|}S(x+\delta\xi, x, t; u))d\xi + \frac{\beta g(\theta(x,t;u))}{\delta^2} \quad (51)$$

Recall from the monotonicity of $f(r)$ that $r_1^+ < r$ implies $f(r_1^+) < f(r)$. Now define the set where the strain exceeds the threshold S_c^+

$$S^{+,\delta} = \left\{(\xi, x) \in B_1(0) \times D;\ x + \delta\xi \in D \text{ and } f(r_1^+) < f(\sqrt{\delta|\xi|}S(x+\delta\xi, x, t; u))\right\} \quad (52)$$

A straightforward calculation with $\omega(|\xi|) = 1$ shows that

$$\begin{aligned} \frac{f(r_1^+)}{\delta}\int_{S^{+,\delta}} |\xi| d\xi dx &\leq \int_{S^{+,\delta}} \frac{1}{\delta} f(\sqrt{\delta|\xi|}S(x+\delta\xi, x, t; u)d\xi dx \\ &\leq \int_D E^{\delta}(x)\,dx = PD^{\delta}(u(t)) \end{aligned} \quad (53)$$

We define the weighted volume of the set $S^{+,\delta}$ to be

$$\tilde{V}(S^{+,\delta}) = \int_{S^{+,\delta}} |\xi| d\xi dx \quad (54)$$

and inequality (53) becomes

$$\frac{f(r_1^+)}{\delta}\tilde{V}(S^{+,\delta}) \leq \int_{S^{+,\delta}} \frac{1}{\delta} f(\sqrt{\delta|\xi|}S(x+\delta\xi, x, t, u))d\xi dx \leq PD^{\delta}(u(t)) \quad (55)$$

Next we use Gronwall's inequality to prove the following theorem that shows that the kinetic and peridynamic energies of the solution $u(x,t)$ are bounded by the energy put into the system.

Theorem 3.

$$C(t) \geq \frac{\rho}{2}\|\dot{u}\|^2_{L^2(D;\mathbb{R}^2)} + PD^{\delta}(u(t)). \quad (56)$$

Proof. We start by multiplying both sides of (12) by $\dot{u}$ to get

$$\rho\ddot{u}(t)\cdot\dot{u}(t) = \left(\mathcal{L}^T(u)(x,t) + \mathcal{L}^D(u)(x,t)\right)\cdot\dot{u}(t) + b(t)\cdot\dot{u}(t).$$

Applying the product rule in the first term and integration by parts in the second term gives

$$\frac{1}{2}\frac{d}{dt}\Big[\rho||\dot{u}||^2_{L^2(D,\mathbb{R}^d)}+2PD^\delta(u(t))\Big]=\int_D b(t)\cdot\dot{u}(t)\,dx.$$

Application of Cauchy's inequality to the right-hand side gives

$$\begin{aligned}\frac{1}{2}\frac{d}{dt}\Big[\rho||\dot{u}||^2_{L^2(D,\mathbb{R}^d)}+2PD^\delta(u(t))\Big]&=\int_D b(t)\cdot\dot{u}(t)dx\\ &\leq ||b(t)||_{L^2(D,\mathbb{R}^d)}||\dot{u}(t)||_{L^2(D,\mathbb{R}^d)}.\end{aligned}\tag{57}$$

Now set $\tilde{W}(t)=\rho||\dot{u}||^2_{L^2(D,\mathbb{R}^d)}+2PD^\delta(u(t))+\zeta$ where ζ is a positive number and can be taken arbitrarily small and (57) becomes,

$$\begin{aligned}\frac{1}{2}\tilde{W}'(t)&=\leq ||b(t)||_{L^2(D,\mathbb{R}^d)}||\dot{u}(t)||_{L^2(D,\mathbb{R}^d)}\\ &\leq ||b(t)||_{L^2(D,\mathbb{R}^d)}\frac{\sqrt{\tilde{W}(t)}}{\sqrt{\rho}}\end{aligned}$$

Now we can write

$$\frac{1}{2}\int_0^t\frac{\tilde{W}'(\tau)}{\sqrt{\tilde{W}(\tau)}}d\tau\leq\frac{1}{\sqrt{\rho}}\int_0^t||b||_{L^2(D,\mathbb{R}^d)}d\tau$$

Which simplifies to

$$\sqrt{\tilde{W}(t)}-\sqrt{\tilde{W}(0)}\leq\frac{1}{\sqrt{\rho}}\int_0^t||b||_{L^2(D,\mathbb{R}^d)}d\tau.\tag{58}$$

Since ζ can be made arbitrarily small, we find that

$$\sqrt{W(t)}-\sqrt{W(0)}\leq\frac{1}{\sqrt{\rho}}\int_0^t||b||_{L^2(D,\mathbb{R}^d)}d\tau,\tag{59}$$

and (56) follows. □

We apply inequality (55) and Theorem 3 to get the fundamental inequality.

$$\tilde{V}(S^{+,\delta})\leq\frac{C(t)\delta}{f(\bar{r})}.\tag{60}$$

The fundamental inequality above is defined on $B_1(0)\times D$, and we now use it to bound the volume of the softening zone on D. Introducing the characteristic function $\chi^{S^{+,\delta}}(\xi,x)$ and taking the value 1 when $(\xi,x)\in S^{+,\delta}$ and 0 otherwise, we immediately have

$$mP_\delta(x) = \int_{B_1(0)} \chi^{S^{+,\delta}}(\xi, x)|\xi|d\xi.$$

So we can rewrite equation (54) as

$$\begin{aligned}\tilde{V}(S^{+,\delta}) &= \int_D \int_{B_1(0)} \chi^{S^{+,\delta}}(\xi, x)|\xi|d\xi dx \\ &= m \int_D P_\delta(x)\, dx.\end{aligned} \tag{61}$$

Now applying Tchebychev's inequality to (61) with $SZ^\delta(\gamma, t)$ defined by (46) gives the desired result

$$\text{Volume}(SZ^\delta(\gamma, t)) \le \frac{1}{\gamma} \int_D P_\delta(x)\, dx = \frac{\tilde{V}(S^{+,\delta})}{m\gamma} \le \frac{C(t)\delta}{m\gamma f(r_1^+)}. \tag{62}$$

Calibration of the Model

In this section we show how to calibrate this model using the known elastic properties and energy release rate of fracture associated with a given material.

Calibrating the Peridynamic Energy to Elastic Properties

We start by considering a body D for which the strain S is small. Here *small* means for a fixed $|y-x|$ we have $|S| << |S_c^\pm|$, $|\theta| << |\theta_c^\pm|$. Now we proceed to calculate the peridynamic energy density inside the material due to the presence of a small deformation $u(x)$. Suppose that the *strain* at the length scale of a neighborhood of *horizon* δ is a linear function, i.e.,

$$\begin{aligned}S(u, y, x) &= \frac{u(y) - u(x)}{|y - x|} \cdot \frac{y - x}{|y - x|} \\ &= F \frac{y - x}{|y - x|} \cdot \frac{y - x}{|y - x|} = Fe \cdot e,\end{aligned} \tag{63}$$

here F is a 3 by 3 matrix. We expand the first potential with respect to S and the second in θ keeping in mind that

$$f(0) = f'(0) = g(0) = g'(0) = 0$$

to get

$$
\begin{aligned}
f\left(\sqrt{|y-x|}S\right) &= \frac{|y-x|}{2} f''(0)S^2 + O(S^3) \\
g\left(\theta(x,t;S)\right) &= \frac{1}{2} g''(0)\theta^2 + O(\theta^3)
\end{aligned}
\tag{64}
$$

So we write the *energy density* which was defined in Eq. (50) for points x of distance δ away from the boundary ∂D to leading order

$$
\begin{aligned}
E^\delta =& \frac{1}{V_\delta}\frac{\alpha f''(0)}{2\delta}\int_{H_\delta(x)} \omega^\delta(|y-x|)|y-x|(Fe\cdot e)^2 dy \\
&+ \frac{\beta g''(0)}{2\delta^2}\left(\frac{1}{V_\delta}\int_{H_\delta(x)} \omega^\delta(|y-x|)|y-x|Fe\cdot e\, dy\right)^2
\end{aligned}
\tag{65}
$$

The change of variable $\delta\xi = y - x$ gives to leading order

$$
\begin{aligned}
E^\delta =& \frac{\alpha f''(0)}{2V_1}\int_{H_1(0)} \omega(|\xi|)|\xi|(Fe\cdot e)^2 d\xi \\
&+ \frac{\beta g''(0)}{2V_1^2}\left(\int_{H_1(0)} \omega(|\xi|)|\xi|Fe\cdot e\, d\xi\right)^2
\end{aligned}
\tag{66}
$$

Observe that $(Fe\cdot e)^2 = \sum_{ijkl} F_{ij}F_{kl}e_ie_je_ke_l$ and the first term in (66) is given by

$$
\sum_{ijkl} \mathbb{M}_{ijkl} F_{ij} F_{kl} \tag{67}
$$

where

$$
\begin{aligned}
\mathbb{M}_{ijkl} =& \frac{\alpha f''(0)}{2V_1}\int_{\mathcal{H}_1(0)} |\xi|\omega(|\xi|)\, e_ie_je_ke_l\, d\xi = \frac{\alpha f''(0)}{2V_1}\int_0^1 |\xi|^3\omega(|\xi|)\, d|\xi| \\
&\int_{S^2} e_ie_je_ke_l\, de.
\end{aligned}
\tag{68}
$$

where de is an element of surface measure on the unit sphere. Next observe $Fe\cdot e = \sum_{kj} F_{kj}e_ke_j$ and the second term in (66) is given by

$$
\frac{\beta g''(0)}{2V_1^2}\left(\sum_{ij}\Lambda_{ij}F_{ij}\right)^2 = \frac{\beta g''(0)}{2V_1^2}\sum_{ijkl}\Lambda_{ij}\Lambda_{kl}F_{ij}F_{kl}. \tag{69}
$$

where

$$\Lambda_{jk} = \int_{\mathcal{H}_1(0)} |\xi|\omega(|\xi|)\, e_j e_k \, d\xi = \int_0^1 |\xi|^3\omega(|\xi|) d|\xi| \int_{S^2} e_j e_k \, de. \tag{70}$$

Focusing on the first term, we show that

$$\mathbb{M}_{ijkl} = 2\mu \left(\frac{\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}}{2} \right) + \lambda \delta_{ij}\delta_{kl} \tag{71}$$

where μ and λ are given by

$$\lambda = \mu = \frac{\alpha f''(0)}{10} \int_0^1 |\xi|^3\omega(|\xi|)\, d|\xi|. \tag{72}$$

To see this we write

$$\Gamma_{ijkl}(e) = e_i e_j e_k e_l, \tag{73}$$

to observe that $\Gamma(e)$ is a totally symmetric tensor valued function defined for $e \in S^2$ with the property

$$\Gamma_{ijkl}(Qe) = Q_{im}e_m Q_{jn}e_n Q_{ko}e_o Q_{lp}e_p = Q_{im}Q_{jn}Q_{ko}Q_{lp}\Gamma_{\mathrm{mnop}}(e) \tag{74}$$

for every rotation Q in SO^3. Here repeated indices indicate summation. We write

$$\int_{\mathcal{H}_1(0)} |\xi|^3\omega(|\xi|)\, e_i e_j e_k e_l \, d\xi = \int_0^1 |\xi|^3\omega(|\xi|) d|\xi| \int_{S^2} \Gamma_{ijkl}(e)\, de \tag{75}$$

to see that for every Q in SO^3

$$Q_{im}Q_{jn}Q_{ko}Q_{lp} \int_{S^2} \Gamma_{ijkl}(e)\, de = \int_{S^2} \Gamma_{\mathrm{mnop}}(Qe)\, de = \int_{S^2} \Gamma_{\mathrm{mnop}}(e)\, de. \tag{76}$$

Therefore we conclude that $\int_{S^2} \Gamma_{ijkl}(e)\, de$ is invariant under SO^3 and is therefore an isotropic symmetric fourth-order tensor and necessarily of the form

$$\int_{S^2} \Gamma_{ijkl}(e)\, de = a\left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}\right) + b\delta_{ij}\delta_{kl}. \tag{77}$$

So $\mathbb{M}$ can be written in the form

$$\mathbb{M}_{ijkl} = 2\mu \left(\frac{\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}}{2} \right) + \lambda \delta_{ij}\delta_{kl}, \tag{78}$$

with suitable choices of μ and λ. To evaluate μ and λ, we note the following relations between μ and λ for isotropic fourth-order tensors of the form above and their contractions

$$\mathbb{M}_{iijj} = 3(2\mu + 3\lambda), \tag{79}$$

$$\mathbb{M}_{ijij} = 3(4\mu + \lambda). \tag{80}$$

These relations can be readily verified by direct calculation.

On the other hand from the definition of $\mathbb{M}$ given by (68), we have

$$\mathbb{M}_{iijj} = \frac{\alpha f''(0)}{2V_1} \int_0^1 |\xi|^3 \omega(|\xi|)\, d|\xi| \int_{S^2} e_i^2 e_j^2\, de = \frac{4\pi\alpha f''(0)}{2V_1} \int_0^1 |\xi|^3 \omega(|\xi|)\, d|\xi|, \tag{81}$$

$$\mathbb{M}_{ijij} = \frac{\alpha f''(0)}{2V_1} \int_0^1 |\xi|^3 \omega(|\xi|)\, d|\xi| \int_{S^2} e_i^2 e_j^2\, de = \frac{4\pi\alpha f''(0)}{2V_1} \int_0^1 |\xi|^3 \omega(|\xi|)\, d|\xi|, \tag{82}$$

since $e_i^2 = \sum_i e_i^2 = 1$. Equation (72) now follows on recalling that $V_1 = \frac{4}{3}\pi$ and solving the system given by (79) and (80).

Focusing on the second term of (66) given by (69), we show that

$$\Lambda_{ij} = \frac{4\pi}{3} \int_0^1 |\xi|^3 \omega(|\xi|)\, d|\xi| \delta_{ij} \tag{83}$$

To see this we write

$$\Lambda_{ij}(e) = e_i e_j, \tag{84}$$

to observe that $\Lambda(e)$ is a totally symmetric tensor valued function defined for $e \in S^2$ with the property

$$\Lambda_{ij}(Qe) = Q_{im} e_m Q_{jn} e_n = Q_{im} Q_{jn} \Lambda_{mn}(e) \tag{85}$$

for every rotation Q in SO^3. As before repeated indices indicate summation. We consider

$$\int_{S^2} \Lambda_{ij}(e)\, de \tag{86}$$

to see that for every Q in SO^3

$$Q_{im} Q_{jn} \int_{S^2} \Lambda_{ij}(e)\, de = \int_{S^2} \Lambda_{mn}(Qe)\, de = \int_{S^2} \Lambda_{mn}(e)\, de. \tag{87}$$

Therefore we conclude that $\int_{S^2} \Lambda_{ij}(e)\,de$ is an isotropic symmetric second-order tensor and of the form

$$\int_{S^2} \Lambda_{ij}(e)\,de = a\delta_{ij}, \tag{88}$$

i.e., a multiple of the identity. So from (70) Λ is of the form

$$\Lambda_{ij} = \gamma\delta_{ij}. \tag{89}$$

To evaluate γ we take the trace of (70) and (83) as follows.

Now the second term is given by

$$\frac{\beta g''(0)}{2V_1^2}\left(\frac{4\pi}{3}\right)^2\left(\int_0^1 |\xi|^3\omega(|\xi|)d|\xi|\right)^2\sum_{ijkl}\delta_{ij}\delta_{kl}F_{ij}F_{kl} =$$

$$= \beta g''(0)\frac{1}{2}\left(\int_0^1 |\xi|^3\omega(|\xi|)d|\xi|\right)^2\sum_{ijkl}\delta_{ij}\delta_{kl}F_{ij}F_{kl} = \mathbb{K}_{ijkl}F_{ij}F_{kl} \tag{90}$$

Collecting results we see that the leading order of the energy is given by

$$E^\delta = \sum_{ijkl}(\mathbb{M}_{ijkl} + \mathbb{K}_{ijkl})F_{ij}F_{kl} = \sum_{ijkl}\left(2\overline{\mu}\frac{\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}}{2} + \overline{\lambda}\delta_{ij}\delta_{kl}\right)F_{ij}F_{kl} \tag{91}$$

where the shear modulus is given by

$$\overline{\mu} = \frac{\alpha f''(0)}{10}\int_0^1 |\xi|^3\omega(|\xi|)\,d|\xi|, \tag{92}$$

and the Lame constant is given by

$$\overline{\lambda} = \frac{\alpha f''(0)}{10}\int_0^1 |\xi|^3\omega(|\xi|)\,d|\xi| + \frac{\beta g''(0)}{2}\left(\int_0^1 |\xi|^3\omega(|\xi|)d|\xi|\right)^2. \tag{93}$$

One is free to choose α and β provided that the resulting elastic tensor satisfies the constraints of ellipticity. Here one is no longer restricted to Poisson ratios of $1/4$ as in the bond-based formulation.

An identical calculation shows that for two-dimensional problems the elastic constants are given by

$$\overline{\mu} = \frac{\alpha f''(0)}{8}\int_0^1 |\xi|^2\omega(|\xi|)\,d|\xi|, \tag{94}$$

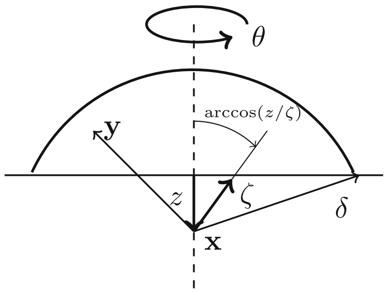

Fig. 4 Evaluation of energy release rate $\mathcal{G}_s$. For each point x along the dashed line, $0 \leq z \leq \delta$, the work required to break the interaction between x and y in the spherical cap is summed up in (96) using spherical coordinates centered at x

and

$$\overline{\lambda} = \frac{\alpha f''(0)}{8} \int_0^1 |\xi|^2 \omega(|\xi|)\, d|\xi| + \frac{\beta g''(0)}{2} \left(\int_0^1 |\xi|^2 \omega(|\xi|) d|\xi| \right)^2, \tag{95}$$

and one is no longer restricted to Poisson ratio $1/3$ materials.

We note here that the two-dimensional moduli $\bar{\mu}$ and $\bar{\lambda}$ are directly related to the well-known moduli appearing in the plane strain or plane stress solutions for isotropic materials. This relationship is now well known and can be found in Jasiuk et al. (1994) and also Milton (2002).

Calibrating Energy Release Rate

In regions of large strain, the same force potentials (3) and (4) are used to calculate the amount of energy consumed by a crack per unit area of growth, i.e., the energy release rate. The energy release rate equals the work necessary to eliminate force interaction on either side of a fracture surface per unit fracture area. In this model the energy release rate has two components: one associated with the force potential for tensile strain (3) and the other associated with the force potential for hydrostatic strain (4). The critical energy release rate $\mathcal{G}s$ associated with fracture under tensile forces is found to be the same for all choices of horizon δ. However the critical energy release rate for hydrostatic fracture $\mathcal{G}_h$ increases with decreasing horizon and becomes infinite as $\delta \to 0$ at the rate $1/\delta$.

For tensile forces we use (3) and calculate the work required to eliminate interaction between two points x and y; this is given by $\mathcal{W}^\delta(\infty) = \lim_{S\to\infty} \mathcal{W}^\delta(S)$ where $\mathcal{W}^\delta(\infty) = \omega^\delta(|y-x|) f_\infty/\delta$. We suppose x gives the center of the peridynamic neighborhood located a distance z away from the planar interface separating upper and lower half spaces. We suppose x lies in the lower half space, and the points y lie in the upper half space inside the peridynamic neighborhood of x (see Fig. 4). The critical energy release rate $\mathcal{G}_s$ associated with tensile forces equals the work necessary to eliminate force interaction on either side of a fracture surface per unit fracture area. It is given in three dimensions by integration of $\mathcal{W}^\delta(\infty)$ over the intersection of the neighborhood of x and the upper half space given by the spherical cap (see Fig. 4),

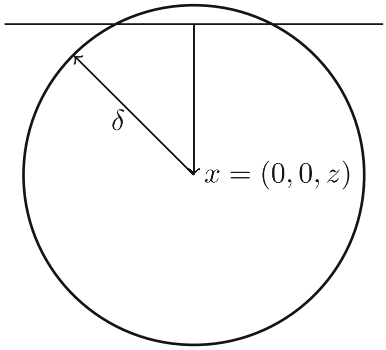

Fig. 5 Hydrostatic energy release rate $\mathcal{G}_h$

$$\mathcal{G}_s = \frac{4\pi}{V_\delta} \int_0^\delta \int_z^\delta \int_0^{\cos^{-1}(z/\zeta)} \mathcal{W}^\delta(\infty, \zeta)\zeta^2 \sin\phi \, d\phi \, d\zeta \, dz \tag{96}$$

where $\zeta = |y - x|$. This integral is calculated and for d dimensions $d = 1, 2, 3$, the result is

$$\mathcal{G}_s = M \frac{2\omega_{d-1}}{\omega_d} f_\infty \,, \tag{97}$$

where $M = \int_0^1 r^d \omega(r) dr$ and ω_d is the volume of the d dimensional unit ball, $\omega_1 = 2, \omega_2 = \pi, \omega_3 = 4\pi/3$. We see from this calculation that the critical energy release rate is independent of δ.

For hydrostatic forces we use (4) and calculate the work required to eliminate interaction between x and the upper half plane. As before we suppose x gives the center of the peridynamic neighborhood located a distance z away from the planar interface separating upper and lower half spaces. We suppose x lies in the lower half space, and the peridynamic neighborhood of x intersects the upper half space (see Fig. 5).

The critical energy release rate $\mathcal{G}_h$ associated with hydrostatic forces equals the work necessary to eliminate force interaction on either side of a fracture surface per unit fracture area. The work per unit volume needed to eliminate hydrostatic interaction between a point x and its neighbors is

$$\mathcal{V}^\delta(\infty)(x) = \lim_{\theta \to \infty} \frac{\beta g(\theta)}{\delta^2} = \frac{\beta g_\infty}{\delta^2}. \tag{98}$$

For points $x = (0, 0, z)$, with $0 < |z| < \delta$ above and below the $z = 0$ plane, the work per unit area to eliminate hydrostatic interaction between the lower half space $z < 0$ and upper half space $z > 0$ is

$$\mathcal{G}_h = 2 \int_0^\delta \frac{\beta g_\infty}{\delta^2} \, dz = \frac{2\beta g_\infty}{\delta}. \tag{99}$$

For d dimensions $d = 1, 2, 3$, the result is the same and

$$\mathcal{G}_s = \frac{2\beta g_\infty}{\delta}. \tag{100}$$

We see from this calculation that the energy release rate for hydrostatic fracture is increasing at the rate $1/\delta$.

Linear Elastic Operators in the Limit of Vanishing Horizon

In this section we consider smooth evolutions u in space and show that away from fracture set the operators $\mathcal{L}^T + \mathcal{L}^D$ acting on u converge to the operator of linear elasticity in the limit of vanishing nonlocality. We denote the fracture set by $\tilde{D}$ and consider any open un-fractured set D' interior to D with its boundary a finite distance away from the boundary of D and the fracture set $\tilde{D}$. In what follows we suppose that the nonlocal horizon δ is smaller than the distance separating the boundary of D' from the boundaries of D and $\tilde{D}$.

Theorem 4. *Convergence to linear elastic operators. Suppose that* $u(x,t) \in C^2([0,T_0], C^3(D,\mathbb{R}^3))$ *and for every* $x \in D' \subset D \setminus \tilde{D}$*, then there is a constant* $C > 0$ *independent of nonlocal horizon* δ *such that, for every* (x,t) *in* $D' \times [0,T_0]$*, one has*

$$|\mathcal{L}^T(u(t)) + \mathcal{L}^D(u(t)) - \nabla \cdot \mathbb{C}\,\mathcal{E}(u(t))| < C\delta, \tag{101}$$

where the elastic strain is $\mathcal{E}(u) = (\nabla u + (\nabla u)^T)/2$ *and the elastic tensor is isotropic and given by*

$$\mathbb{C}_{ijkl} = 2\bar{\mu}\left(\frac{\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}}{2}\right) + \bar{\lambda}\delta_{ij}\delta_{kl}, \tag{102}$$

with shear modulus $\bar{\mu}$ *and Lamé coefficient* $\bar{\lambda}$ *given by* (92) *and* (93)*. The numbers* α *and* β *can be chosen independently and can be any pair of real numbers such that* $\mathbb{C}$ *is positive definite.*

Proof. We start by showing

$$|\mathcal{L}^T(u(t)) - \frac{f''(0)}{2\omega_3}\int_{B_1(0)} e|\xi|J(|\xi|)e_i e_j e_k \, d\xi \partial^2_{jk} u_i(x)| < C\delta, \tag{103}$$

where $\omega_3 = 4\pi/3$ and $e = e_{y-x}$ are unit vectors on the sphere; here repeated indices indicate summation. To see this recall the formula for $\mathcal{L}^T(u)$ and write $\partial_S f(\sqrt{|y-x|}S) = f'(\sqrt{|y-x|}S)\sqrt{|y-x|}$. Now Taylor expand

$f'(\sqrt{|y-x|}S)$ in $\sqrt{|y-x|}S$ and Taylor expand $u(y)$ about x, denoting e_{y-x} by e to find that all odd terms in e integrate to zero and

$$|\mathcal{L}^T(u(t))_l - \frac{2}{V_\delta}\int_{B_\delta(x)} \frac{J^\delta(|y-x|)}{\delta|y-x|}\frac{f''(0)}{4}|y-x|^2\partial^2_{jk}u_i(x)e_ie_je_ke_l, dy| \\ < C\delta, l = 1,2,3. \tag{104}$$

On changing variables $\xi = (y-x)/\delta$, we recover (103). Now we show

$$|\mathcal{L}^D(u(t))_k - \frac{1}{\omega_3}\int_{B_1(0)} |\xi|\omega(|\xi|)e_ie_j\,d\xi\frac{\beta g''(0)}{2\omega_3}\int_{B_1(0)} |\xi|\omega(|\xi|)e_ke_l\,d\xi\partial^2_{lj}u_i(x)| \\ < C\delta, k = 1,2,3. \tag{105}$$

We note for $x \in D'$ that $D \cap B_\delta(x) = B_\delta(x)$ and the integrand in the second term of (14) is odd and the integral vanishes. For the first term in (14), we Taylor expand $\partial_\theta g(\theta)$ about $\theta = 0$ and Taylor expand $u(z)$ about y inside $\theta(y,t)$ noting that terms odd in $e = e_{z-y}$ integrate to zero to get

$$|\partial_\theta g(\theta(y,t)) - g''(0)\frac{1}{V_\delta}\int_{B_\delta(y)} \omega^\delta(|z-y|)|z-y|\partial_j u_i(y)e_ie_j\,dz| < C\delta^3. \tag{106}$$

Now substitution for the approximation to $\partial_\theta g(\theta(y,t))$ in the definition of $\mathcal{L}^D$ gives

$$\Big|\mathcal{L}^D(u)\frac{1}{V_\delta}\int_{B_\delta(x)} \frac{\omega^\delta(|y-x|)}{\delta^2}e_{y-x}\frac{1}{2V_\delta}\int_{B_\delta(y)} \omega^\delta(|z-y|)|z-y| \\ \beta g''(0)\partial_j u_i(y)e_ie_j\,dz\,dy\Big| < C\delta. \tag{107}$$

We Taylor expand $\partial_j u_i(y)$ about x; note that odd terms involving tensor products of e_{y-x} vanish when integrated with respect to y in $B_\delta(x)$, and we obtain (105).

We now calculate as in (Lipton 2016 equation (6.64)) or in section "Calibrating the Peridynamic Energy to Elastic Properties" to find that

$$\frac{f''(0)}{2\omega_3}\int_{B_1(0)} |\xi|J(|\xi|)e_ie_je_ke_l\,d\xi\partial^2_{jk}u_i(x) \\ = \left(2\mu_1\left(\frac{\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk}}{2}\right)+\lambda_1\delta_{ij}\delta_{kl}\right)\partial^2_{jk}u_i(x), \tag{108}$$

where

$$\mu_1 = \lambda_1 = \frac{f''(0)}{10}\int_0^1 r^3\omega(r)\,dr. \tag{109}$$

Next observe that a straightforward calculation gives

$$\frac{1}{\omega_3}\int_{B_1(0)}|\xi|\omega(|\xi|)e_ie_j\,d\xi=\delta_{ij}\int_0^1 r^3\omega(r)\,dr, \tag{110}$$

and we deduce that

$$\begin{aligned}&\frac{1}{\omega_3}\int_{B_1(0)}|\xi|\omega(|\xi|)e_ie_j\,d\xi\frac{\beta g''(0)}{2\omega_3}\int_{B_1(0)}|\xi|\omega(|\xi|)e_ke_l\,d\xi\partial^2_{lj}u_i(x)\\&=\frac{\beta g''(0)}{2}\left(\int_0^1 r^3\omega(r)\,dr\right)^2\delta_{ij}\delta_{kl}\partial^2_{lj}u_i(x).\end{aligned} \tag{111}$$

Theorem 4 follows on adding (108) and (111) □

Conclusions

We have introduced a regularized model for free fracture propagation based on nonlocal potentials. At each instant of the evolution, we identify the softening zone where strains lie above the strength of the material. We have shown that discontinuities associated with flaws larger than the length scale of nonlocality δ can become unstable and grow. An explicit inequality is found that shows that the volume of the softening zone goes to zero linearly with the length scale of nonlocal interaction. This scaling is consistent with the notion that a softening zone of width proportional to δ converges to a sharp fracture as the length scale of nonlocal interaction goes to zero. Inside quiescent regions with no cracks, the nonlocal operator converges to the local elastic operator at a rate proportional to the radius of nonlocal interaction. We show that the model can be calibrated to measured values of critical energy release rate, shear modulus, and bulk modulus of material samples. The double-well state-based potential developed here no longer has Poisson ratio constrained to be $1/4$. For this model we can choose the potentials so that the small strain behavior is specified by the isotropic elasticity tensor for any material with prescribed shear and Lamé moduli.

The energy release rate necessary for tensile forces to create fractures is constant in δ, whereas the forces necessary to create a fracture using hydrostatic forces grows as $1/\delta$. Thus creation of fracture surfaces by hydrostatic forces will not be seen when

$$\delta<\frac{2\beta g_\infty}{G_s}. \tag{112}$$

On the other hand, the elastic properties for small strains can be made to correspond to any positive definite isotropic elastic tensor.

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References

A. Agwai, I. Guven, E. Madenci, Predicting crack propagation with peridynamics: a comparative study. Int. J. Fract. **171**, 65–78 (2011)

F. Bobaru, W. Hu, The meaning, selection, and use of the peridynamic horizon and its relation to crack branching in brittle materials. Int. J. Fract. **176**, 215–222 (2012)

F. Bobaru, J.T. Foster, P.H. Geubelle, S.A. Silling, *Handbook of Peridynamic Modeling* (CRC Press, Boca Raton, 2016)

K. Dayal, K. Bhattacharya, Kinetics of phase transformations in the peridynamic formulation of continuum mechanics. J. Mech. Phys. Solids **54**, 1811–1842 (2006)

P. Diehl, R. Lipton, M.A. Schweitzer, Numerical verification of a bond-based softening peridynamic model for small displacements: deducing material parameters from classical linear theory. Institut für Numerische Simulation Preprint No. 1630 (2016)

B.K. Driver, *Analysis Tools with Applications*. E-book (Springer, Berlin, 2003)

Q. Du, M. Gunzburger, R. Lehoucq, K. Zhou, Analysis of the volume-constrained peridynamic Navier equation of linear elasticity. J. Elast. **113**, 193–217 (2013)

J.T. Foster, S.A. Silling, W. Chen, An energy based failure criterion for use with peridynamic states. Int. J. Multiscale Comput. Eng. **9**, 675–688 (2011)

W. Gerstle, N. Sau, S. Silling, Peridynamic modeling of concrete structures. Nucl. Eng. Des. **237**, 1250–1258 (2007)

Y.D. Ha, F. Bobaru, Studies of dynamic crack propagation and crack branching with peridynamics. Int. J. Fract. **162**, 229–244 (2010)

I. Jasiuk, J. Chen, M.F. Thorpe, Elastic moduli of two dimensional materials with polygonal and elliptical holes. Appl. Mech. Rev. **47**, S18–S28 (1994)

R. Lipton, Dynamic brittle fracture as a small horizon limit of peridynamics. J. Elast. **117**, 21–50 (2014)

R. Lipton, Cohesive dynamics and brittle fracture. J. Elast. **124**(2), 143–191 (2016)

R. Lipton, S. Silling, R. Lehoucq, Complex fracture nucleation and evolution with nonlocal elastodynamics. arXiv preprint arXiv:1602.00247 (2016)

G.W. Milton, *The Theory of Composites* (Cambridge University Press, Cambridge, 2002)

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

S.A. Silling, E. Askari, A meshfree method based on the peridynamic model of solid mechanics. Comput. Struct **83**, 1526–1535 (2005)

S.A. Silling, F. Bobaru, Peridynamic modeling of membranes and fibers. Int. J. Nonlinear Mech. **40**, 395–409 (2005)

S.A. Silling, R.B. Lehoucq, Convergence of peridynamics to classical elasticity theory. J. Elast. **93**, 13–37 (2008)

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

S. Silling, O. Weckner, E. Askari, F. Bobaru, Crack nucleation in a peridynamic solid. Int. J. Fract. **162**, 219–227 (2010)

O. Weckner, R. Abeyaratne, The effect of long-range forces on the dynamics of a bar. J. Mech. Phys. Solids **53**, 705–728 (2005)