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Crack nucleation in a peridynamic solid

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Abstract A condition for the emergence of a
discontinuity in an elastic peridynamic body is pro-
posed, resulting in a material stability condition for
crack nucleation. The condition is derived by deter-
mining whether a small discontinuity in displace-
ment, superposed on a possibly large deformation,
grows over time. Stability is shown to be determined
by the sign of the eigenvalues of a tensor field that
depends only on the linearized material properties. This
condition for nucleation of a discontinuity in dis-
placement can be interpreted in terms of the dynamic
stability of plane waves with very short wavelength.
A numerical example illustrates that cracks in a peri-
dynamic body form spontaneously as the body is
loaded.

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1 Introduction

Common experience tells us that if a brittle solid body
is loaded sufficiently, eventually it fails due to crack-
ing. This paper addresses the following question: *How
does a crack appear spontaneously in a continuous
body?* For purposes of this discussion, this spontane-
ous appearance of such a discontinuity will be called
the "nucleation" of a crack.

The field of fracture mechanics is primarily
concerned with the evolution of pre-existing defects
within a body, rather than the nucleation of new defects.
It is frequently noted that real materials, now matter
how perfect they seem at the macroscale, invariably
contain many defects at the microscale. Therefore, it
could be claimed that the nucleation of a macroscale
crack never really occurs; instead the seemingly sudden
appearance of a discontinuity is merely the growth and
coalescence of a large number of pre-existing defects
at the smaller scale. However, as a practical matter,
an engineering model would require an impractically
detailed spatial resolution to capture such a distribu-
tion of tiny defects, even if the fundamental mechan-
ics of these defects were adequately understood. So,
it is desirable to have a practical mathematical model,
applicable at the macroscale, that reproduces the spon-
taneous emergence of discontinuities.

The classical theory of solid mechanics, because
of the requirements for smoothness of the deforma-
tion that are built into the fundamental assumptions
of the theory, cannot be considered an ideal tool for

the study of this problem. However, the peridynamic theory (Silling 2000; Silling et al. 2007) has been proposed as a reformulation of solid mechanics whose basic equations remain applicable regardless of the possible emergence of discontinuities in the deformation. In this paper, the nucleation of discontinuities is studied within the peridynamic theory from the point of view of material stability.

Material stability conditions have been investigated within the classical theory as possible criteria for nucleation of discontinuities. For hyperelastic materials in the classical theory, loss of ordinary ellipticity (Knowles and Sternberg 1975, 1978) provides a condition for the presence of static discontinuities in the first spatial derivatives of displacement in a homogeneous body. Material stability conditions with a structure similar to loss of ordinary ellipticity have also been considered as criteria for localization in elastic-plastic materials, particularly for shear bands (Hill 1962; Rudnicki and Rice 1975; Leroy and Ortiz 1989). Klein and Gao (1998) consider a criterion similar to loss of ordinary ellipticity as a condition for crack nucleation. Klein and Gao base this condition on the acoustic tensor corresponding to a material whose response is local but is derived from the response of a network of *virtual independent bonds* (VIB).

Bazant and Belytschko (1985) conclude that if loss of hyperbolicity (the analogue in the dynamic case of loss of ellipticity in the static case) occurs, then deformations can localize to a discontinuity. However, Belytschko et al. (2003), while adopting this condition as an indicator of crack growth, correctly include the following note of caution: "It must be stressed that these are empirical inferences and that little appears to be known about the morphology and evolution of such surfaces in multi-dimensions."

Although loss of ellipticity has been investigated by many authors as a localization criterion, the mechanical argument connecting it with nucleation of strong discontinuities such as cracks is indirect at best. The reason is that when a discontinuity in displacement forms spontaneously, it is difficult to argue that the fourth order elasticity tensor provides an adequate description of how material on one crack face interacts with material on the other face. This interaction is precisely what should, in a properly formulated mathematical model of a continuum, determine whether a discontinuity grows or does not grow. The ability to model this type of interaction explicitly is one feature that the peridynamic theory offers for purposes of modeling crack nucleation. In this paper, a material instability condition is derived that corresponds to the ability of a discontinuous perturbation in the deformation to grow in amplitude over time. The condition involves only the incremental material properties at each point.

Propagation, as opposed to nucleation, of cracks within the peridynamic model has been described elsewhere (Silling and Askari 2005) and has been applied to a number of problems involving complex patterns of fracture (Silling 2003; Silling and Bobaru 2005; Askari et al. 2006; Bobaru 2007; Xu et al. 2007; Colavito et al. 2007; Gerstle et al. 2007; Xu et al. 2008; Agwai et al. 2008a,b; Kilic and Madenci 2009; Kilic et al. 2009; Agwai et al. 2009). Crack growth occurs through the irreversible breakage of bonds as they stretch in the vicinity of a crack tip. The damage condition that governs bond breakage is treated as part of the constitutive model. As shown in Silling and Askari (2005), if bond breakage occurs at a prescribed value of bond stretch, then cracks advance according to the Griffith criterion, consuming a definite amount of energy per unit area. The nucleation and motion of phase boundaries, including material stability aspects, was investigated by Dayal and Bhattacharya (2006).

In Sect. 2 of this paper, the fundamentals of the peridynamic theory are reviewed. In Sect. 3, the linearized equations are discussed that represent the superposition of a small displacement field on a large equilibrated deformation. In Sect. 4, the evolution of such a superposed displacement field containing a jump discontinuity is investigated, resulting in a material stability condition. The relationship between this condition and the wave speeds in the material is discussed in Sect. 5. A computational example illustrating the nucleation of a crack at a stress concentration in a plate is presented in Sect. 6.

2 Basic equations of peridynamics

In the peridynamic model, the strain energy density at a point $\mathbf{x}$ in an elastic body $\mathcal{B}$ is determined by the collective deformation of all the points within a predefined interaction distance of $\mathbf{x}$. This interaction distance is called the *horizon* and denoted δ. The relative position vector in the reference configuration from $\mathbf{x}$ to any point $\mathbf{q}$ within the horizon is called a *bond*, denoted $\boldsymbol{\xi} = \mathbf{q} - \mathbf{x}$.

The set of all bonds connected to **x** is called the *family* of **x** and denoted $\mathcal{H}$.

In the constitutive modeling of a peridynamic elastic material, the basic kinematical quantity that determines the strain energy density $W(\mathbf{x}, t)$ is called the *deformation state* at **x** and t, defined by

$$\underline{\mathbf{Y}}[\mathbf{x}, t]\langle \boldsymbol{\xi} \rangle = \mathbf{y}(\mathbf{x} + \boldsymbol{\xi}, t) - \mathbf{y}(\mathbf{x}, t) \qquad (1)$$

where **y** is the motion. The deformation state is a mapping that associates with any bond $\boldsymbol{\xi}$ its image under the motion. The bond that $\underline{\mathbf{Y}}$ operates on is written in angle brackets, $\langle \boldsymbol{\xi} \rangle$.

The deformation state is an example of a *vector state*, which is simply a mapping from bonds to vectors in $\mathbb{R}^3$. The *dot product* of two vector states $\underline{\mathbf{A}}$ and $\underline{\mathbf{B}}$ is defined by

$$\underline{\mathbf{A}} \bullet \underline{\mathbf{B}} = \int_{\mathcal{H}} \underline{\mathbf{A}}\langle \boldsymbol{\xi} \rangle \cdot \underline{\mathbf{B}}\langle \boldsymbol{\xi} \rangle \, dV_{\boldsymbol{\xi}}$$

where the integrand is the usual scalar product in $\mathbb{R}^3$ of the two vectors $\underline{\mathbf{A}}\langle \boldsymbol{\xi} \rangle$ and $\underline{\mathbf{B}}\langle \boldsymbol{\xi} \rangle$. The norm of a vector state is defined by

$$||\underline{\mathbf{A}}|| = \sqrt{\underline{\mathbf{A}} \bullet \underline{\mathbf{A}}}.$$

If Ψ is a scalar valued function of a vector state $\underline{\mathbf{A}}$, then its *Fréchet derivative* $\nabla \Psi(\underline{\mathbf{A}})$, if it exists, is defined by

$$\Psi(\underline{\mathbf{A}} + \underline{\mathbf{a}}) = \Psi(\underline{\mathbf{A}}) + \nabla \Psi(\underline{\mathbf{A}}) \bullet \underline{\mathbf{a}} + o(||\underline{\mathbf{a}}||)$$

for any vector state $\underline{\mathbf{a}}$.

A *double state* $\mathbb{D}$ is a mapping from pairs of bonds to second order tensors; thus the value of $\mathbb{D}\langle \boldsymbol{\xi}, \boldsymbol{\zeta} \rangle$ is a second order tensor. The *adjoint* of a double state is defined by

$$\mathbb{D}^{\dagger}\langle \boldsymbol{\xi}, \boldsymbol{\zeta} \rangle = \mathbb{D}^{T}\langle \boldsymbol{\zeta}, \boldsymbol{\xi} \rangle$$

for any bonds $\boldsymbol{\xi}$ and $\boldsymbol{\zeta}$, where the superscript T indicates the tensor transpose. The dot product of a double state $\mathbb{D}$ with a vector state $\underline{\mathbf{A}}$ is a vector state defined by

$$(\mathbb{D} \bullet \underline{\mathbf{A}})\langle \boldsymbol{\xi} \rangle = \int_{\mathcal{H}} \mathbb{D}\langle \boldsymbol{\xi}, \boldsymbol{\zeta} \rangle \, \underline{\mathbf{A}}\langle \boldsymbol{\zeta} \rangle \, dV_{\boldsymbol{\zeta}}$$

for any bond $\boldsymbol{\xi}$. If $\underline{\mathbf{S}}$ is a vector state valued function of a vector state, its Fréchet derivative $\nabla \underline{\mathbf{S}}(\underline{\mathbf{A}})$, if it exists, is defined by

$$\underline{\mathbf{S}}(\underline{\mathbf{A}} + \underline{\mathbf{a}}) = \underline{\mathbf{S}}(\underline{\mathbf{A}}) + \nabla \underline{\mathbf{S}}(\underline{\mathbf{A}}) \bullet \underline{\mathbf{a}} + o(||\underline{\mathbf{a}}||)$$

for any vector state $\underline{\mathbf{a}}$.

In the constitutive modeling of an elastic material, the strain energy density $W(\mathbf{x}, t)$ is, in general, determined by the collective deformation of all the bonds
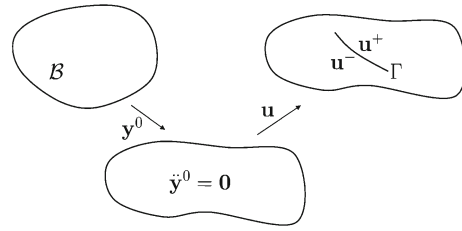

Fig. 1 An incremental displacement field **u** containing a jump across the surface Γ is superposed on an equilibrated, possibly large deformation $\mathbf{y}^0$

connected to **x**, not merely by the individual bonds independently of each other. It is this collective dependence that leads to the need for W to be considered a function of $\underline{\mathbf{Y}}$. Thus, the constitutive model for an elastic material is written

$$W(\mathbf{x}, t) = \hat{W}(\underline{\mathbf{Y}}[\mathbf{x}, t], \mathbf{x}),$$

in which the explicit dependence of $\hat{W}$ on **x** reflects possible heterogeneity. The functional for total potential energy of a bounded body $\mathcal{B}$ in terms of the motion **y** is given by

$$\Phi_{\mathbf{y}} = \int_{\mathcal{B}} (\hat{W}(\underline{\mathbf{Y}}[\mathbf{x}], \mathbf{x}) - \mathbf{b} \cdot \mathbf{y}) \, dV_{\mathbf{x}},$$

where **b** is a prescribed body force density field. Deriving the Euler-Lagrange equation associated with stationary values of $\Phi_{\mathbf{y}}$, and applying d'Alembert's principle, leads to the peridynamic equation of motion:

$$\rho(\mathbf{x})\ddot{\mathbf{y}}(\mathbf{x}, t) = \int_{\mathcal{B}} \{ \underline{\mathbf{T}}[\mathbf{x}, t]\langle \mathbf{q} - \mathbf{x} \rangle - \underline{\mathbf{T}}[\mathbf{q}, t]$$
$$\langle \mathbf{x} - \mathbf{q} \rangle \} \, dV_{\mathbf{q}} + \mathbf{b}(\mathbf{x}, t) \qquad (2)$$

where $\underline{\mathbf{T}}$ is the *force state*, a vector state defined by

$$\underline{\mathbf{T}}[\mathbf{x}, t] = \underline{\hat{\mathbf{T}}}(\underline{\mathbf{Y}}[\mathbf{x}, t], \mathbf{x}) = \nabla \hat{W}(\underline{\mathbf{Y}}[\mathbf{x}, t], \mathbf{x}), \qquad (3)$$

in which ∇ denotes the Fréchet derivative with respect to $\underline{\mathbf{Y}}$. $\underline{\hat{\mathbf{T}}}$ is the constitutive model that gives the force state as a function of the deformation state. The force state is the work conjugate of the deformation state:

$$\hat{W}(\underline{\mathbf{Y}} + d\underline{\mathbf{Y}}) - \hat{W}(\underline{\mathbf{Y}}) = \underline{\mathbf{T}} \bullet d\underline{\mathbf{Y}}.$$

3 Linearized form of peridynamics

Consider an equilibrated, continuous deformation $\mathbf{y}^0$ corresponding to time-independent external body force

density field $\mathbf{b}$. Let $\mathbf{u}$ be a small variation in the deformation (Fig. 1). Linearizing the function $\underline{\hat{\mathbf{T}}}$ near $\mathbf{y}^0$ leads to

$$\underline{\mathbf{T}} = \underline{\mathbf{T}}^0 + \mathbb{K} \bullet \underline{\mathbf{U}} + o(||\underline{\mathbf{U}}||) \qquad (4)$$

where

$$\underline{\mathbf{T}}^0[\mathbf{x}] = \underline{\hat{\mathbf{T}}}(\underline{\mathbf{Y}}^0[\mathbf{x}], \mathbf{x}), \quad \underline{\mathbf{U}}[\mathbf{x}]\langle \mathbf{p} - \mathbf{x}\rangle = \mathbf{u}(\mathbf{p}) - \mathbf{u}(\mathbf{x}) \qquad (5)$$

for all points $\mathbf{x}$ and $\mathbf{p}$ in $\mathcal{B}$. $\mathbb{K}$ is a double state called the *modulus state* defined, through the second Fréchet derivative of the strain energy density function, by

$$\mathbb{K}[\mathbf{x}] = \nabla\nabla\hat{W}(\underline{\mathbf{Y}}^0[\mathbf{x}], \mathbf{x}). \qquad (6)$$

The modulus state is analogous to the fourth order elasticity tensor in the standard theory, because it contains the material properties that give the internal forces within a body in terms of small changes in the deformation. From the properties of Fréchet derivatives, and from (6), it can be shown that $\mathbb{K}$ is self-adjoint (Silling 2010):

$$\mathbb{K}^\dagger = \mathbb{K}. \qquad (7)$$

Using (4), and neglecting terms of higher order than $||\underline{\mathbf{U}}||$, the equation of motion (2) becomes

$$\rho(\mathbf{x})\ddot{\mathbf{u}}(\mathbf{x}, t) = \int_{\mathcal{B}} \left\{ (\mathbb{K}[\mathbf{x}] \bullet \underline{\mathbf{U}}[\mathbf{x}])\langle \mathbf{p} - \mathbf{x}\rangle \right. \\ \left. - (\mathbb{K}[\mathbf{p}] \bullet \underline{\mathbf{U}}[\mathbf{p}])\langle \mathbf{x} - \mathbf{p}\rangle \right\} dV_{\mathbf{p}} + \mathbf{b}(\mathbf{x}, t).$$

Writing this out in terms of the displacements using (5) yields

$$\rho(\mathbf{x})\ddot{\mathbf{u}}(\mathbf{x}, t) \\ = \int_{\mathcal{B}} \mathbf{C}_0(\mathbf{x}, \mathbf{q})\mathbf{u}(\mathbf{q}, t) \, dV_{\mathbf{q}} - \mathbf{P}_0(\mathbf{x})\mathbf{u}(\mathbf{x}, t) \qquad (8)$$

where $\mathbf{C}_0$ is the tensor valued function defined by

$$\mathbf{C}_0(\mathbf{x}, \mathbf{q}) \\ = \int_{\mathcal{B}} \left(\mathbb{K}[\mathbf{x}]\langle \mathbf{p} - \mathbf{x}, \mathbf{q} - \mathbf{x}\rangle - \mathbb{K}[\mathbf{p}]\langle \mathbf{x} - \mathbf{p}, \mathbf{q} - \mathbf{p}\rangle \right. \\ \left. + \mathbb{K}[\mathbf{q}]\langle \mathbf{x} - \mathbf{q}, \mathbf{p} - \mathbf{q}\rangle \right) \, dV_{\mathbf{p}} \qquad (9)$$

and where $\mathbf{P}_0$ is the tensor field defined by

$$\mathbf{P}_0(\mathbf{x}) = \int_{\mathcal{B}} \int_{\mathcal{B}} \mathbb{K}[\mathbf{x}]\langle \mathbf{p} - \mathbf{x}, \mathbf{q} - \mathbf{x}\rangle \, dV_{\mathbf{q}} \, dV_{\mathbf{p}}. \qquad (10)$$

By integrating (9) with respect to $\mathbf{q}$, it follows that

$$\mathbf{P}_0(\mathbf{x}) = \int_{\mathcal{B}} \mathbf{C}_0(\mathbf{x}, \mathbf{q}) \, dV_{\mathbf{q}}.$$

In practice, the expressions for $\mathbf{C}_0$ in many materials of interest contain Dirac delta functions centered at $\mathbf{x}$.

It is convenient to move this term outside the integral in the equation of motion (8) by rewriting it as

$$\rho(\mathbf{x})\ddot{\mathbf{u}}(\mathbf{x}, t) = \int_{\mathcal{B}} \mathbf{C}(\mathbf{x}, \mathbf{q})\mathbf{u}(\mathbf{q}, t) \, dV_{\mathbf{q}} - \mathbf{P}(\mathbf{x})\mathbf{u}(\mathbf{x}, t) \\ + \mathbf{b}(\mathbf{x}, t), \qquad (11)$$

for all $\mathbf{x}$ and t, where

$$\mathbf{C}(\mathbf{x}, \mathbf{q}) = \mathbf{C}_0(\mathbf{x}, \mathbf{q}) + \lambda(\mathbf{x})\Delta(\mathbf{q} - \mathbf{x}), \qquad (12)$$

$$\mathbf{P}(\mathbf{x}) = \mathbf{P}_0(\mathbf{x}) + \lambda(\mathbf{x}) = \int_{\mathcal{B}} \mathbf{C}(\mathbf{x}, \mathbf{q}) \, dV_{\mathbf{q}}, \qquad (13)$$

$$\lambda(\mathbf{x}) = -\lim_{\epsilon \to 0} \int_{\mathcal{S}_\epsilon} \mathbf{C}_0(\mathbf{x}, \mathbf{q}) \, dV_{\mathbf{q}}, \qquad (14)$$

where $\mathcal{S}_\epsilon$ is the interior of a sphere of radius ϵ centered at $\mathbf{x}$, and Δ is the Dirac delta function in $\mathbb{R}^3$. For an elastic material, it can be shown (Silling 2010) that $\mathbf{C}$ and $\mathbf{P}$ have the following symmetries:

$$\mathbf{C}^T(\mathbf{x}, \mathbf{q}) = \mathbf{C}(\mathbf{q}, \mathbf{x}), \quad \mathbf{P}^T(\mathbf{x}) = \mathbf{P}(\mathbf{x}).$$

As discussed in Silling (2010), the condition for linearization of the peridynamic equations is

$$\min_{\mathbf{q} \in \mathcal{H}} |\mathbf{u}(\mathbf{q}) - \mathbf{u}(\mathbf{x})| << \delta \quad \forall \mathbf{x} \in \mathcal{B}.$$

This is a weaker condition than the corresponding requirement in the *classical* linear theory of elasticity,

$$|\text{grad } \mathbf{u}(\mathbf{x})| << 1 \quad \forall \mathbf{x} \in \mathcal{B}.$$

The weaker requirement in the linear peridynamic theory permits us to consider perturbations containing jump discontinuities in $\mathbf{u}$, a property that is used in the next section. The linearized equation of motion (11) is essentially the same as the fundamental equation of motion in Kunin's nonlocal theory (Kunin 1983), but with the additional constitutive structure of the peridynamic model.

4 Perturbation by a jump

Now consider a piecewise-continuous variation $\mathbf{u}$ that contains a small step discontinuity across a surface Γ. Assume that Γ divides $\mathcal{B}$ into two open sets $\mathcal{R}^+$ and $\mathcal{R}^-$. Let $\mathbf{C}$ be continuous on $\mathcal{B} \times \mathcal{B}$. Let the jumps in displacement and acceleration at some $\mathbf{x} \in \Gamma$ be denoted

$$[[\mathbf{u}]] = \mathbf{u}(\mathbf{x}^+) - \mathbf{u}(\mathbf{x}^-), \quad [[\ddot{\mathbf{u}}]] = \ddot{\mathbf{u}}(\mathbf{x}^+) - \ddot{\mathbf{u}}(\mathbf{x}^-)$$

where $\mathbf{x}^- \in \mathcal{R}^-$ and $\mathbf{x}^+ \in \mathcal{R}^+$ represent points arbitrarily close to $\mathbf{x}$. Then from (11),

$$\rho(\mathbf{x})[[\ddot{\mathbf{u}}]] = \int_{\mathcal{B}} [[\mathbf{C}(\mathbf{x}, \mathbf{q})]]\mathbf{u}(\mathbf{q}) \, dV_{\mathbf{q}} - [[\mathbf{Pu}]].$$

Since $\mathbf{C}$, and therefore $\mathbf{P}$, are continuous, it follows that

$$[[\mathbf{C}]] = \mathbf{0} \quad \text{and} \quad [[\mathbf{P}]] = \mathbf{0},$$

therefore

$$\rho(\mathbf{x})[[\ddot{\mathbf{u}}]] = -\mathbf{P}(\mathbf{x})[[\mathbf{u}]]. \tag{15}$$

The small discontinuity at $\mathbf{x} \in \Gamma$ introduced by the variation is considered unstable if it gets larger with time. This means it is unstable if

$$[[\ddot{\mathbf{u}}]] \cdot [[\mathbf{u}]] > 0. \tag{16}$$

Taking the scalar product of $[[\mathbf{u}]]$ with both sides of (15), and using (16), the conclusion is that instability occurs if

$$(\mathbf{P}(\mathbf{x})[[\mathbf{u}]]) \cdot [[\mathbf{u}]] < 0. \tag{17}$$

If there is some $[[\mathbf{u}]]$ such that (17) holds at some $\mathbf{x}$, then the material is unstable with respect to amplification of a discontinuity.[1] Since $\mathbf{P}(\mathbf{x})$ is symmetric, it has three real eigenvalues, which will be denoted $\{P_1, P_2, P_3\}$. (17) implies that if $\mathbf{P}(\mathbf{x})$ has a negative eigenvalue, then the material is unstable with respect to amplification of the jump. The condition for crack nucleation is then

$$Z(\mathbf{x}) < 0, \tag{18}$$

where

$$Z(\mathbf{x}) = \min \{P_1, P_2, P_3\}. \tag{19}$$

$Z(\mathbf{x})$ is called the *stability index*.

If $\mathbf{P}$ is positive definite on $\mathcal{B}$, then in the terminology of Silling (2000), *single-point stability* holds. In this case, then clearly (18) cannot hold, since $\mathbf{P}$ has no negative eigenvalues. In Silling (2000), it is shown that single-point stability is a necessary but not sufficient condition for local minimization of potential energy. Therefore, it follows that if the nucleation condition (18) is met, then the configuration cannot be a local minimizer of potential energy.

A result closely related to (18) was also obtained in Weckner and Abeyaratne (2005) in a more restrictive setting. In this reference, it was shown that in a homogeneous, bond-based, linear microelastic bar, jumps in an initial displacement field grow exponentially over time if

$$\int\limits_{-\infty}^{\infty} C(\xi) \, d\xi < 0$$

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[1] The word "amplification" is used instead of "growth" here to avoid confusion with advance of a crack tip.

where C is the micromodulus function. This integral is the specialization of $\mathbf{P}$ in (13) to a linear, homogeneous bar.

To interpret $\mathbf{P}$ mechanically, note that from (11), it follows that $-\mathbf{P}(\mathbf{x})\mathbf{e}$ is the restoring force density experienced by $\mathbf{x}$ if it is displaced by a vector $\mathbf{e}$, holding all other points in $\mathcal{B}$ fixed. In the next section, a connection between $\mathbf{P}$ and the stable propagation of certain types of plane waves is demonstrated.

5 Relation to wave speeds

An alternate interpretation of (18) may be obtained by considering plane waves in the interior of a large, homogeneous, homogeneously deformed body. In this case, $\mathbf{P}$ is independent of position. Since $\mathbf{C}$ is also independent of position, we write $\mathbf{C}(\boldsymbol{\xi})$. The condition for propagation of a plane wave may be obtained by substituting the assumed form of the displacement field

$$\mathbf{u}(\mathbf{x}, t) = \mathbf{a} \, e^{i(\kappa \mathbf{x} \cdot \mathbf{n} - \omega t)}$$

into (11), where $i = \sqrt{-1}$, $\mathbf{a}$ is a unit vector in the direction of particle motion, $\mathbf{n}$ is the unit vector in the direction of propagation of the wave, κ is the wave number, and ω is the angular frequency. The result is that waves can exist if there exist $\mathbf{a}$, $\mathbf{n}$, κ, and $\omega(\kappa, \mathbf{n})$ such that

$$\rho\omega^2(\kappa, \mathbf{n})\mathbf{a} = \left(\mathbf{P} - \int_{\mathcal{H}} \mathbf{C}(\boldsymbol{\xi}) \cos(\kappa\boldsymbol{\xi} \cdot \mathbf{n}) \, dV_{\boldsymbol{\xi}}\right) \mathbf{a}. \tag{20}$$

The quantity in parentheses is a tensor. The dispersion relation for the waves is obtained by evaluating the eigenvalue ω of this tensor for a given κ and $\mathbf{n}$. The eigenvectors $\mathbf{a}$ give the direction of particle motion.

Now consider the limit $\kappa \to \infty$ in (20). Because $\mathbf{C}$ is bounded and continuous, the integral vanishes in this limit, for any choice of $\mathbf{n}$. Therefore, the eigenvalue equation (20) can be written as

$$\rho\omega^2(\infty, \mathbf{n})\mathbf{a} = \mathbf{P}\mathbf{a}.$$

Taking the scalar product of both sides of this equation with the unit vector $\mathbf{a}$,

$$\rho\omega^2(\infty, \mathbf{n}) = \mathbf{a} \cdot \mathbf{P}\mathbf{a}. \tag{21}$$

Comparing this result with (17) and (18), it follows that the condition for nucleation of discontinuities is met if and only if the frequency of plane waves in the limit of zero wavelength is imaginary.

Note that it is possible for waves with finite wave number to be unstable even if this limiting frequency is real. In other words, long waves might be unstable while short waves are stable. This is in contrast to the standard theory, in which the stability of plane waves is independent of the wavelength.

The interpretation of the crack nucleation condition (18) given in this section in terms of imaginary frequencies of very short waves should not be taken too literally, because this interpretation assumes a homogeneously deformed, homogeneous body. In contrast, (18) makes no such assumptions, and is therefore more general.

6 Example

This computational example illustrates the nucleation of a crack at a point at which the condition (18) is first met as the body is loaded. The body is a nonlinearly elastic plate containing a hole and stretched from the ends. The constitutive model is a nonlinear peridynamic elastic model of the following form:

$$\underline{\mathbf{T}}\langle\boldsymbol{\xi}\rangle = \frac{1}{2}f(\eta,\xi)\mathbf{M}, \quad \mathbf{M} = \frac{\underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle}{|\underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle|}, \qquad (22)$$

for any bond $\boldsymbol{\xi}$, where f is a function and the bond extension η and bond length ξ are given by

$$\eta = |\underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle| - |\boldsymbol{\xi}|, \quad \xi = |\boldsymbol{\xi}|.$$

The unit vector $\mathbf{M}$ is in the direction of the deformed bond. The scalar valued function f is the bond force density, which has dimensions of force/volume^2. The direction of the force state $\underline{\mathbf{T}}\langle\boldsymbol{\xi}\rangle$ is parallel to the deformed bond vector $\underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle$. For the particular material in this example, f is given by

$$f(\eta,\xi)$$
$$= \begin{cases} cs & \text{if } 0 \le s \le s_1 \\ cs_1 - c'(s - s_1) & \text{if } s_1 \le s < s_0 \quad s = \frac{\eta}{\xi} \quad (23) \\ 0 & \text{if } s_0 < s, \end{cases}$$

where c, c', s_1, and s_0 are constants related by

$$c' = \frac{cs_1}{s_0 - s_1}, \quad 0 < s_1 < s_0, \quad c > 0.$$

(See Fig. 2). The scalar s is the bond strain, i.e., change in bond length divided by reference bond length. Evaluating the Fréchet derivative of (22), one easily finds that

$$\mathbb{K}\langle\boldsymbol{\xi},\boldsymbol{\zeta}\rangle$$
$$= \frac{1}{2}\left(\frac{\mathbf{1} - \mathbf{M}\otimes\mathbf{M}}{|\underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle|}f + (\mathbf{M}\otimes\mathbf{M})\frac{\partial f}{\partial\eta}\right)\Delta(\boldsymbol{\xi} - \boldsymbol{\zeta})$$
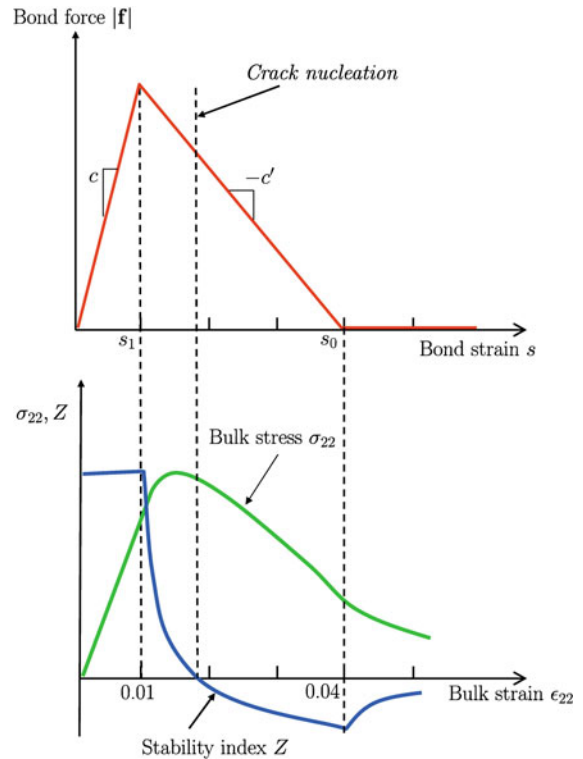

Fig. 2 Properties of a plate composed of the material in the example problem under uniaxial strain. *Top*: bond force as a function of bond strain. *Bottom*: stress-strain curves in a plate under homogeneous, uniaxial strain. The peak stress occurs before the crack nucleation condition is met

where Δ denotes the Dirac delta function in three dimensions.

The top curve in Fig. 2 shows the bond force as a function of bond strain for the material. Also shown are the normal stress in the vertical direction and the stability index Z as a function of bulk strain, both assuming homogeneous deformation of a homogeneous plate. The stability index starts dropping when some bonds pass the peak in the curve of bond force vs. bond strain. As the plate is stretched more, the stability index eventually becomes negative, thus satisfying the condition (18) for nucleation of a discontinuity. (This condition occurs at a strain greater than the peak in the bulk stress-strain curve.)

The geometry of the plate is shown in Fig. 3. Figure 4 shows contours of u_2 and Z near the stress concentration for three values of global strain, defined by $\varepsilon = \Delta\ell/\ell$. The displacement field is computed with the Emu peridynamic computer code (Silling and Askari 2005). A small crack appears at a global strain
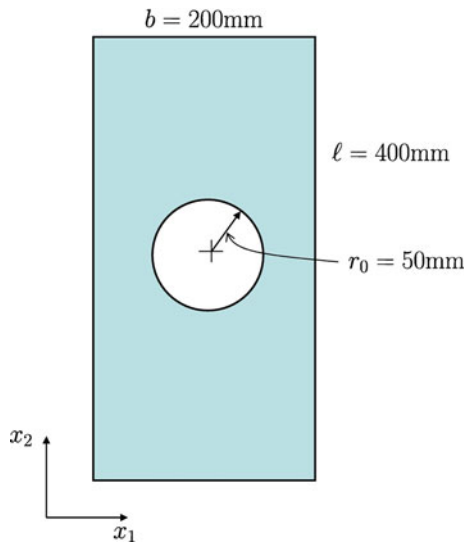
Fig. 3 Geometry of the plate in Example 1

of approximately $\varepsilon = 0.0049$, by which time Z has become small at the stress concentration. The crack immediately grows dynamically toward the outer free edges. The contours in the plot on the lower right show that Z becomes strongly negative ahead of a dynamically growing crack tip. Figure 5 shows the values of Z at the point $\mathbf{x}_0$, which is located 54 mm from the center

of the hole as a function of global strain. The figure also shows the crack tip position a as a function of global strain. The crack first appears at $a \approx 54$ mm, at the time when Z at that location first becomes negative. As soon as the crack nucleates, Z at this location becomes positive again, because the material is no longer unstable there.

7 Discussion

Even though the peridynamic theory is a nonlocal theory, the crack nucleation condition (18) is a local condition, because it involves only the value of the tensor field $\mathbf{P}$ at $\mathbf{x}$. This $\mathbf{P}(\mathbf{x})$ can be evaluated anywhere in the body in terms of the incremental properties of the constitutive model evaluated following the large equilibrated deformation $\mathbf{y}$.

The crack nucleation condition (18) is not related to the maximum of any bulk stress-strain curve for a homogeneous body or to any tangent modulus. To see this, consider the form of (19) for a one-dimensional homogeneous bar:

$$Z = \int_{-\delta}^{\delta} C(\xi) \, d\xi. \tag{24}$$

Fig. 4 Contours of vertical displacement u_2 (*left column*) and stability index Z (*right column*) at three times. The global stretch of the plate $\varepsilon = \Delta\ell/\ell$ at these times takes on the values 0.0047, 0.0049, and 0.0061. Crack nucleation occurs at approximately $\varepsilon = 0.0049$. The stability index first becomes negative near this time and becomes more strongly negative in front of the growing crack tip
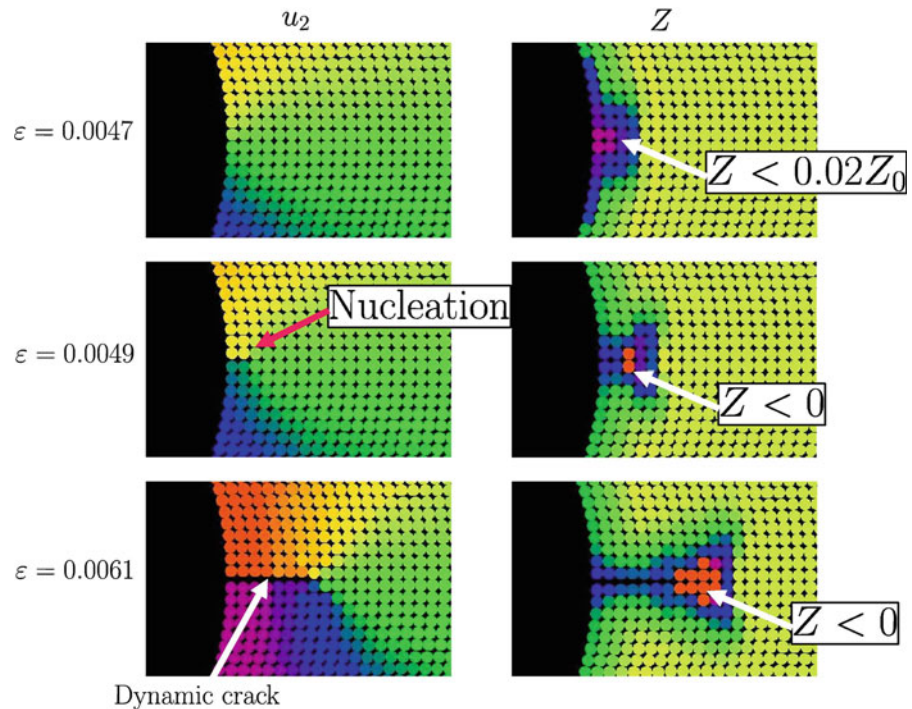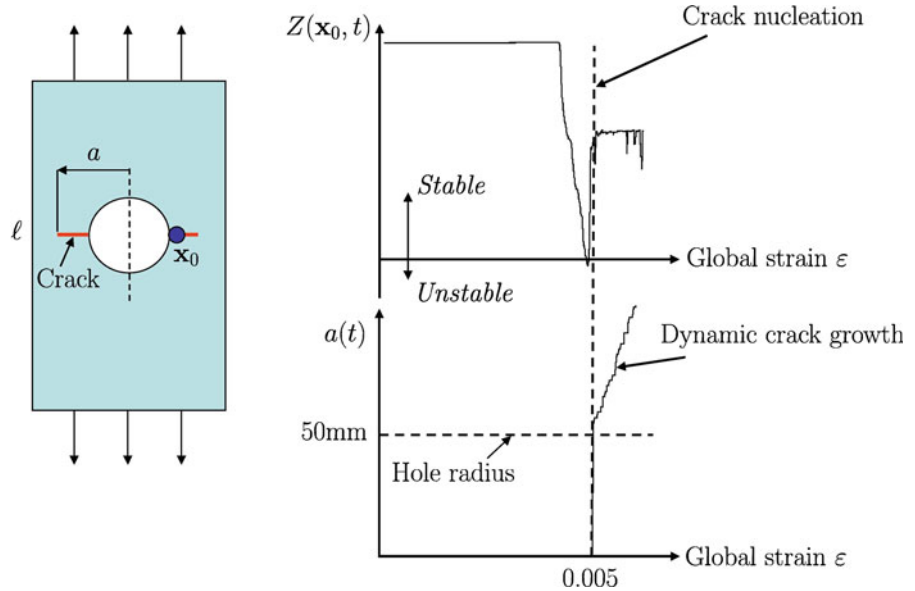
Fig. 5 Time histories of
stability index Z (*top*) and
crack tip position a (*bottom*)
at the point $\mathbf{x}_0$, located at
radius $r_0 = 0.054$ mm.
Nucleation occurs at near
this point as Z becomes
negative

On the other hand, the tangent modulus (Weckner and Abeyaratne 2005) is given by

$$E = \int\limits_0^\delta \xi^2 C(\xi)\, d\xi.$$

Evidently $E < 0$ is neither a necessary or sufficient condition for $Z < 0$. Therefore, the tangent modulus is unrelated to the crack nucleation condition.

Another observation from (24) is that in one dimension, there must be *some* bonds that are softening if the crack nucleation condition is met. In other words, in one dimension, $Z < 0$ implies $C(\xi) < 0$ for some bonds ξ. This is not true in two or three dimensions, since geometrical nonlinearities due to a large deformation $\mathbf{y}^0$ could reduce the eigenvalues of $\mathbf{P}$.

For the material considered in the example problem in Sect. 6, it was noted that under the assumption of homogeneous deformation of a homogeneous plate, the crack nucleation condition occurs *after* the maximum in the bulk stress-strain curve (Fig. 2) as the plate is extended in uniaxial strain. Under these conditions, one would expect some sort of instability to occur as soon as the stress-strain curve starts to decline. Why does such an instability not appear in the example problem? The reason is that in the example problem, the deformation is not homogeneous. On the contrary, the strain concentration creates a small region where strains are high enough for the crack nucleation criterion to be met.

The eigenvector of $\mathbf{P}(\mathbf{x})$ that first becomes negative as the body is deformed, resulting in the condition (18) first being met, gives the direction of the displacement jump [[$\mathbf{u}$]]. However, we have not been able to obtain any information about the orientation of a crack that is nucleated. Another currently unresolved issue is the status of bodies in which $Z = 0$. It is not known whether this condition, as opposed to $Z < 0$, represents a type of neutral stability with respect to the formation of discontinuities, or whether closer examination would reveal a different condition for nucleation in this case.

As demonstrated computationally in the example in Sect. 6, there is a subregion ahead of a dynamically growing crack within which Z is strongly negative. It seems possible that future investigation will establish a link between the values of Z ahead of such a crack, the crack growth velocity, and [[$\ddot{\mathbf{u}}$]] near the crack tip.

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