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Reformulation of Elasticity Theory for Discontinuities and Long-Range Forces

S. A. Silling

Prepared by
Sandia National Laboratories
Albuquerque, New Mexico 87185 and Livermore, California 94550

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Reformulation of Elasticity Theory for Discontinuities and Long-Range Forces

S. A. Silling
Computational Physics and Mechanics Department
Sandia National Laboratories
P.O. Box 5800
Albuquerque, NM 87185-0820

Abstract

Some materials may naturally form discontinuities such as cracks as a result of deformation. As an aid to the modeling of such materials, a new framework for the basic equations of continuum mechanics, called the "peridynamic" formulation, is proposed. The propagation of linear stress waves in the new theory is discussed, and wave dispersion relations are derived. Material stability and its connection with wave propagation is investigated. It is demonstrated by an example that the reformulated approach permits the solution of fracture problems using the same equations either on or off the crack surface or crack tip. This is an advantage for modeling problems in which the location of a crack is not known in advance.

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1 Introduction

Many problems of fundamental importance in solid mechanics involve the spontaneous formation of discontinuities. Here, "spontaneous" means that a discontinuity forms where one was not present initially. The formation of a crack in a homogeneous solid is an example of such a problem.

The mathematical framework that has been developed for continuum mechanics is in some ways ill-suited to the modeling of such problems. The reason is that partial derivatives are used to represent the relative displacement and force between any two "neighboring" particles. By definition, the necessary partial derivatives with respect to the spatial coordinates are undefined along the discontinuities. Various remedies are employed to get around this difficulty, depending on the severity of the discontinuity. For example, phase changes involve a discontinuity in the first partial derivatives of displacement with respect to position. To study phenomena of this type, one may evaluate these first spatial derivatives on either side of the surface of discontinuity and use a weak solution of the underlying partial differential equations [1]. This technique fails when we attempt to study a more severe discontinuity, such as a crack, in which the displacement field is itself discontinuous. In this case, the only recourse is basically to redefine the body so that the crack lies on the boundary. Such a redefinition of the body has been an ingredient in essentially all of the work that has been done on the stress fields surrounding cracks (see [2] for a summary of this work).

Both these techniques, the use of weak solutions in the case of phase changes, and the redefinition of the body in the case of cracks, require us to know where the discontinuity is located. This limits the usefulness of these techniques in problems involving the spontaneous formation of discontinuities, in which we might not know their location in advance. This motivates, in part, the reformulation of the equations of continuum mechanics so that the same equations apply both on and off of a discontinuity. Another motivation is that it is simpler and more aesthetically pleasing to avoid using special techniques whenever a discontinuity happens to appear.

In this paper we propose a continuum model that does not distinguish between points in a body where a discontinuity in displacement or any of its spatial derivatives may be located. The essence of the model is that integration, rather than differentiation, is used to compute the force on a material particle. Since the spatial derivatives are not used, the equations

remain equally valid at points or surfaces of discontinuity. We propose the term *peridynamic* model for such a formulation, from the Greek roots for *near* and *force*.

The proposed method falls into the category of nonlocal models, because particles separated by a finite distance can interact with each other. Although there has been a considerable amount of research done on nonlocal elastic and thermoelastic models (see [3] for a general approach), the objective of eliminating the spatial derivatives appears not to have been pursued previously. Instead, most concepts of nonlocal modeling average the strains within some finite neighborhood and involve a stress tensor that must be differentiated in the equation of motion. The present approach is fundamentally different in that it avoids using these quantities.

2 Basic formulation

Suppose a body occupies a reference configuration in a region \mathcal{R} . We assume that each pair of particles interacts through a vector-valued function \mathbf{f} such that \mathbf{L} , the force per unit reference volume due to interaction with other particles, is a functional of the displacement field \mathbf{u} . At any point \mathbf{x} in the reference configuration, and at any time t , the value of \mathbf{L} is given by

$$\mathbf{L}_{\mathbf{u}}(\mathbf{x}, t) = \int_{\mathcal{R}} \mathbf{f}(\mathbf{u}(\mathbf{x}', t) - \mathbf{u}(\mathbf{x}, t), \mathbf{x}' - \mathbf{x}) dV_{\mathbf{x}'} \quad \forall \mathbf{x} \in \mathcal{R}, \quad t \geq 0. \quad (1)$$

More concisely,

$$\mathbf{L}_{\mathbf{u}}(\mathbf{x}) = \int_{\mathcal{R}} \mathbf{f}(\mathbf{u}' - \mathbf{u}, \mathbf{x}' - \mathbf{x}) dV' \quad \text{on } \mathcal{R}. \quad (2)$$

The *peridynamic equation of motion* is given by

$$\rho \ddot{\mathbf{u}} = \mathbf{L}_{\mathbf{u}} + \mathbf{b} \quad \text{on } \mathcal{R}, \quad t \geq 0, \quad (3)$$

and the *peridynamic equilibrium equation* is given by

$$\mathbf{L}_{\mathbf{u}} + \mathbf{b} = \mathbf{0} \quad \text{on } \mathcal{R}. \quad (4)$$

where \mathbf{b} is some prescribed *loading force density*, which represents external force per unit reference volume. The function \mathbf{f} will be called the *pairwise*

force function. Note that no spatial derivatives appear in (2). This is the feature promised in the Introduction.

Throughout this paper, all integrals refer to Riemann integration. It will be assumed that all functions are sufficiently well behaved to possess Riemann integrals.

The following notation will be used for relative displacement vectors and relative position vectors in the reference configuration:

$$\boldsymbol{\eta} = \mathbf{u}' - \mathbf{u}, \quad \boldsymbol{\xi} = \mathbf{x}' - \mathbf{x}. \quad (5)$$

This notational convenience will not be restated each time it is used. Note that $\boldsymbol{\xi} + \boldsymbol{\eta}$ is the relative position of the particles in the *deformed* configuration.

We call the reference configuration *equilibrated* if (4) is satisfied with $\mathbf{b} \equiv \mathbf{u} \equiv \mathbf{0}$. If $\mathbf{f}(\mathbf{0}, \boldsymbol{\xi}) = \mathbf{0}$ for all $\boldsymbol{\xi} \neq \mathbf{0}$, then the reference configuration will be called *pairwise equilibrated*. Note that pairwise equilibrated implies equilibrated. A third notion of equilibration of the reference configuration will be discussed in Section 9. This third notion, which will be called *unstressed*, allows for nonzero forces between pairs of particles even though there is no "stress" in the body in a sense to be defined later.

All constitutive information is contained in the function \mathbf{f} . There is no need to assume any particular degree of smoothness of this function with respect to either of its arguments.

The fact that the pairwise force function \mathbf{f} that appears in (2) does not contain history-dependent variables as arguments implies that the material described by this function does not have memory of its deformation history. We therefore call such a material, whose \mathbf{f} has the form $\mathbf{f}(\mathbf{u}' - \mathbf{u}, \mathbf{x}' - \mathbf{x})$, a *peridynamic material without memory*.

The form of \mathbf{L}_n shown in (2) is appropriate for homogeneous bodies. The form for nonhomogeneous bodies would have a more complicated integrand: $\mathbf{f}(\mathbf{u}' - \mathbf{u}, \mathbf{x}, \mathbf{x}')$. In this paper we will deal only with the homogeneous theory, for simplicity.

An important restriction on the form of \mathbf{f} is provided by Newton's Third Law: the force on particle 1 due to particle 2 equals minus the force on particle 2 due to particle 1. Thus,

$$\mathbf{f}(-\boldsymbol{\eta}, -\boldsymbol{\xi}) = -\mathbf{f}(\boldsymbol{\eta}, \boldsymbol{\xi}) \quad \forall \boldsymbol{\eta}, \boldsymbol{\xi}. \quad (6)$$

(6) will be called the *linear admissibility condition* on \mathbf{f} .

Another restriction on \mathbf{f} arises from conservation of angular momentum:

$$(\boldsymbol{\xi} + \boldsymbol{\eta}) \times \mathbf{f}(\boldsymbol{\eta}, \boldsymbol{\xi}) = \mathbf{0} \quad \forall \boldsymbol{\eta}, \boldsymbol{\xi}. \quad (7)$$

This says that the force vector between two particles is parallel to their relative current position vector. If this condition did not hold, we could choose a pair of particles, initially at rest, such that their combined angular momentum would change over time even in the absence of external forces.

(7) will be called the *angular admissibility condition* on \mathbf{f} .

An immediate conclusion from the restrictions (6) and (7) is that the most general form of \mathbf{f} is

$$\mathbf{f}(\boldsymbol{\eta}, \boldsymbol{\xi}) = F(\boldsymbol{\eta}, \boldsymbol{\xi})(\boldsymbol{\xi} + \boldsymbol{\eta}), \quad \forall \boldsymbol{\xi}, \boldsymbol{\eta}, \quad (8)$$

where F is a scalar-valued function such that

$$F(-\boldsymbol{\eta}, -\boldsymbol{\xi}) = F(\boldsymbol{\eta}, \boldsymbol{\xi}) \quad \forall \boldsymbol{\xi}, \boldsymbol{\eta}. \quad (9)$$

Conversely, any \mathbf{f} satisfying (8) and (9) also satisfies the requirements (6) and (7).

In the subsequent discussion, it will often be convenient to restrict attention to points in a body that are sufficiently far from its boundary that for constitutive modeling purposes, the point sees a surrounding body that is infinite in all directions. To make this more precise, suppose that for a given material there is some smallest positive number δ such that $\mathbf{f}(\boldsymbol{\eta}, \boldsymbol{\xi}) = \mathbf{0}$ for any $\boldsymbol{\eta}$ whenever $|\boldsymbol{\xi}| > \delta$. Such a number δ will be called the *horizon* for the material. If such a δ exists for a material, let \mathcal{R}^0 be the subset consisting of all points in \mathcal{R} that have a distance of at least δ from the nearest point on the boundary of \mathcal{R} :

$$\mathcal{R}^0 = \{\mathbf{x} \in \mathcal{R} : |\mathbf{x}' - \mathbf{x}| < \delta \Rightarrow \mathbf{x}' \in \mathcal{R}\} \quad (10)$$

The set \mathcal{R}^0 will be called the *internal subregion* of \mathcal{R} (Figure 1).

3 Isotropy

Let a peridynamic material without memory be given, and let its pairwise force function be \mathbf{f} . Suppose there is a set \mathcal{Z} of tensors such that

$$\mathbf{f}(\mathbf{Q}\boldsymbol{\eta}, \mathbf{Q}\boldsymbol{\xi}) = \mathbf{Q}\mathbf{f}(\boldsymbol{\eta}, \boldsymbol{\xi}) \quad \forall \boldsymbol{\eta}, \boldsymbol{\xi}, \forall \mathbf{Q} \in \mathcal{Z}. \quad (11)$$

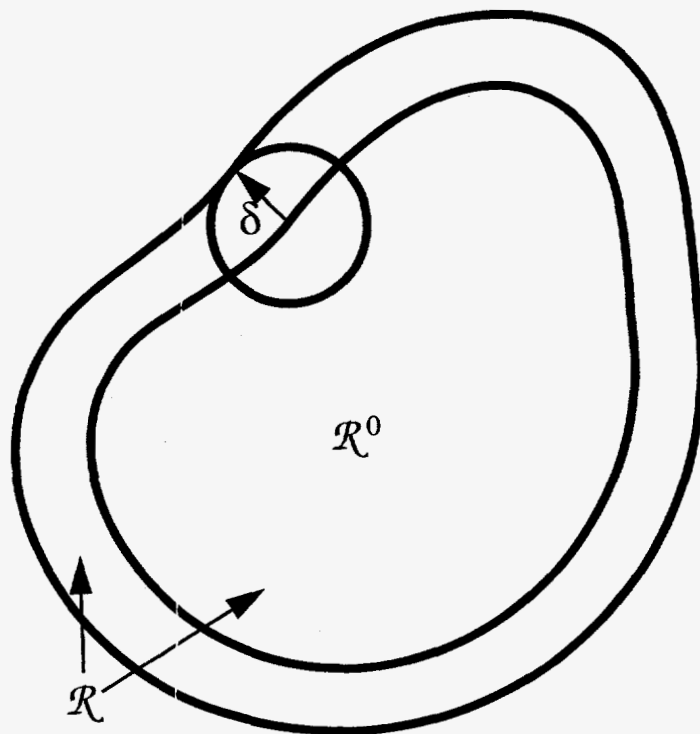


Figure 1. A body with an internal subregion.

Then \mathcal{Z} is a group under the tensor multiplication operator, and we say \mathcal{Z} is a *material symmetry group* of the material. This idea, of course, parallels the analogous concept in the conventional theory of elasticity.

In the present discussion, we will be concerned with only one material symmetry group, the set of proper orthogonal tensors, \mathcal{O}^+ . A peridynamic material with this material symmetry group will be said to be *isotropic*. Thus, for an isotropic material,

$$\mathbf{f}(\mathbf{Q}\boldsymbol{\eta}, \mathbf{Q}\boldsymbol{\xi}) = \mathbf{Q}\mathbf{f}(\boldsymbol{\eta}, \boldsymbol{\xi}) \quad \forall \boldsymbol{\eta}, \boldsymbol{\xi}, \forall \mathbf{Q} \in \mathcal{O}^+. \quad (12)$$

This means that the response of the material is independent of the orientation of the material. In other words, the material has no special directions. Equivalently, isotropy holds if and only if

$$F(\mathbf{Q}\boldsymbol{\eta}, \mathbf{Q}\boldsymbol{\xi}) = F(\boldsymbol{\eta}, \boldsymbol{\xi}) \quad \forall \boldsymbol{\eta}, \boldsymbol{\xi}, \forall \mathbf{Q} \in \mathcal{O}^+. \quad (13)$$

We now seek further restrictions on F for isotropic materials. To do this, first note that by (13), in an isotropic material, we can rotate a given pair of vectors $\boldsymbol{\xi}$ and $\boldsymbol{\eta}$ arbitrarily without changing the value of F , provided the angle between the vectors is unchanged. This means that the value of F depends only on the geometry of the triangle with two sides of lengths $|\boldsymbol{\xi}|$ and $|\boldsymbol{\eta}|$, and the angle between these sides, $\cos^{-1} \boldsymbol{\xi} \cdot \boldsymbol{\eta} / (|\boldsymbol{\xi}| |\boldsymbol{\eta}|)$. (The case $\boldsymbol{\eta} = \mathbf{0}$ is easily treated as a special case.)

For reasons that will become clear in a later section, it is more convenient to deal with $|\boldsymbol{\xi} + \boldsymbol{\eta}|$ rather than $|\boldsymbol{\eta}|$, and it is completely equivalent to do so. Thus, the most general form of F for an isotropic material is

$$F(\boldsymbol{\eta}, \boldsymbol{\xi}) = I(p, q, r), \quad p = |\boldsymbol{\xi} + \boldsymbol{\eta}|, \quad q = \boldsymbol{\xi} \cdot \boldsymbol{\eta}, \quad r = |\boldsymbol{\xi}|, \quad \forall \boldsymbol{\xi}, \boldsymbol{\eta} \quad (14)$$

where I is a some scalar-valued function. Equivalently,

$$\mathbf{f}(\boldsymbol{\eta}, \boldsymbol{\xi}) = I(p, q, r)(\boldsymbol{\xi} + \boldsymbol{\eta}), \quad \forall \boldsymbol{\xi}, \boldsymbol{\eta}. \quad (15)$$

Since p , q , and r are invariant with respect to rigid rotations, any material described by (14) is necessarily isotropic according to (13).

4 Elasticity

A peridynamic material will be called *microelastic* if

$$\int_{\Gamma} \mathbf{f}(\boldsymbol{\eta}, \boldsymbol{\xi}) \cdot d\boldsymbol{\eta} = 0. \quad \forall \text{ closed curve } \Gamma, \forall \boldsymbol{\xi} \neq \mathbf{0}, \quad (16)$$

where $d\boldsymbol{\eta}$ represents differential vector path length along Γ . This means that the net work done on any material particle \mathbf{x}' due to interaction with another fixed particle \mathbf{x} as \mathbf{x}' moves along any closed path is zero.

If \mathbf{f} is continuously differentiable in $\boldsymbol{\eta}$, then by Stokes' Theorem, a necessary and sufficient condition for (16) to hold is that

$$\nabla_{\boldsymbol{\eta}} \times \mathbf{f}(\boldsymbol{\eta}, \boldsymbol{\xi}) = \mathbf{0} \quad \forall \boldsymbol{\xi} \neq \mathbf{0} \quad (17)$$

where the notation " $\nabla_{\boldsymbol{\eta}} \times$ " means the vector curl operator evaluated with respect to the coordinates of $\boldsymbol{\eta}$.

Another consequence of Stokes' Theorem is that a necessary and sufficient condition for a peridynamic material to be microelastic is the existence of a differentiable, scalar-valued function w , called the *pairwise potential function*, such that

$$\mathbf{f}(\boldsymbol{\eta}, \boldsymbol{\xi}) = \frac{\partial w}{\partial \boldsymbol{\eta}}(\boldsymbol{\eta}, \boldsymbol{\xi}). \quad (18)$$

To investigate the implications of the condition (17), we apply it to (8), assuming that F is continuously differentiable:

$$\mathbf{0} = \nabla_{\boldsymbol{\eta}} \times \left(\bar{F}(\boldsymbol{\eta}, \boldsymbol{\xi})(\boldsymbol{\xi} + \boldsymbol{\eta}) \right) = \frac{\partial F}{\partial \boldsymbol{\eta}}(\boldsymbol{\eta}, \boldsymbol{\xi}) \times (\boldsymbol{\xi} + \boldsymbol{\eta}) \quad \forall \boldsymbol{\xi} \neq \mathbf{0}. \quad (19)$$

This condition holds if and only if there exists a scalar-valued function A such that

$$\frac{\partial F}{\partial \boldsymbol{\eta}}(\boldsymbol{\eta}, \boldsymbol{\xi}) = A(\boldsymbol{\eta}, \boldsymbol{\xi})(\boldsymbol{\xi} + \boldsymbol{\eta}). \quad (20)$$

Integrating this, we find

$$F(\boldsymbol{\eta}, \boldsymbol{\xi}) = H(p, \boldsymbol{\xi}), \quad p = |\boldsymbol{\xi} + \boldsymbol{\eta}| \quad (21)$$

where H is another scalar-valued function, continuously differentiable in p . Equivalently, for a microelastic material we can write

$$\mathbf{f}(\boldsymbol{\eta}, \boldsymbol{\xi}) = H(p, \boldsymbol{\xi})(\boldsymbol{\xi} + \boldsymbol{\eta}), \quad p = |\boldsymbol{\xi} + \boldsymbol{\eta}| \quad \forall \boldsymbol{\xi}, \boldsymbol{\eta}. \quad (22)$$

Reversing the above steps shows that any material satisfying (21) is necessarily microelastic according to (17).

An interpretation of the result (22) is as follows: if a material is microelastic, every pair of points \mathbf{x} and \mathbf{x}' is connected by a (possibly nonlinear)

spring. The force in the spring depends only on the distance between the points in the deformed configuration. (Recall that $\boldsymbol{\xi} + \boldsymbol{\eta}$ is the relative deformed position vector, so p is the relative deformed distance between two particles whose original separation distance was $r = |\boldsymbol{\xi}|$.)

For a given microelastic material with a known H , the pairwise potential function is supplied by

$$w(\boldsymbol{\eta}, \boldsymbol{\xi}) = \int^{|\boldsymbol{\xi} + \boldsymbol{\eta}|} \bar{p} H(\bar{p}, \boldsymbol{\xi}) d\bar{p} + w_0, \quad \forall \boldsymbol{\xi}, \boldsymbol{\eta} \quad (23)$$

where w_0 is an arbitrary constant. This result may be confirmed by using the chain rule to evaluate $\partial w / \partial \boldsymbol{\eta}$ from (23). For such a material we write

$$w(\boldsymbol{\eta}, \boldsymbol{\xi}) = \tilde{w}(|\boldsymbol{\xi} + \boldsymbol{\eta}|, \boldsymbol{\xi}) \quad (24)$$

where \tilde{w} is a scalar-valued function.

If a material is isotropic as well as microelastic, then comparison of (21) with (14) shows that H can depend on its second argument, $\boldsymbol{\xi}$, only through $|\boldsymbol{\xi}|$. I cannot depend on its second argument, $q = \boldsymbol{\xi} \cdot \boldsymbol{\eta}$, at all. For a microelastic isotropic material, we can therefore write

$$w(\boldsymbol{\eta}, \boldsymbol{\xi}) = \check{w}(|\boldsymbol{\xi} + \boldsymbol{\eta}|, |\boldsymbol{\xi}|) \quad (25)$$

where \check{w} is a scalar-valued function.

Peridynamic materials without memory that are *not* microelastic are physically unreasonable, because in such a material we can always find a cyclical motion of two particles \mathbf{x} and \mathbf{x}' that produces energy. Therefore, the remaining discussion will concern only microelastic materials. However, there is still the possibility of physically reasonable peridynamic materials *with* memory that are not microelastic. Such materials will not be considered in this paper.

We now make the transition from microelasticity, a concept that concerns only the interaction between pairs of particles, to *macroelasticity*, which concerns bodies as a whole. Let a microelastic body be given, with pairwise potential function w . At any point \mathbf{x} in the body, define the *macroelastic energy density* functional $W_{\mathbf{u}}(\mathbf{x})$ by

$$W_{\mathbf{u}}(\mathbf{x}) = \frac{1}{2} \int_{\mathcal{R}} w(\mathbf{u}' - \mathbf{u}, \mathbf{x}' - \mathbf{x}) dV'. \quad (26)$$

Also define the *total macroelastic energy* functional Φ by

$$\Phi_{\mathbf{u}} = \int_{\mathcal{R}} W_{\mathbf{u}}(\mathbf{x}) dV, \quad (27)$$

provided conditions in a body are such that this integral exists. To demonstrate the significance of these quantities, we consider the motion of a microelastic body and the time derivative of its total macroelastic energy. (We allow \mathbf{u} to be time-dependent.)

$$\begin{aligned} \dot{\Phi}_{\mathbf{u}} &= \frac{1}{2} \frac{\partial}{\partial t} \int_{\mathcal{R}} \int_{\mathcal{R}} w(\mathbf{u}' - \mathbf{u}, \mathbf{x}' - \mathbf{x}) dV' dV \\ &= \frac{1}{2} \int_{\mathcal{R}} \int_{\mathcal{R}} \frac{\partial w}{\partial \boldsymbol{\eta}}(\mathbf{u}' - \mathbf{u}, \mathbf{x}' - \mathbf{x}) \cdot (\dot{\mathbf{u}}' - \dot{\mathbf{u}}) dV' dV. \end{aligned} \quad (28)$$

We can get rid of the term involving $\dot{\mathbf{u}}'$ by using the change of variables $\mathbf{x}' \leftrightarrow \mathbf{x}$ and applying (6). Then, using (18) and (3),

$$\begin{aligned} \dot{\Phi}_{\mathbf{u}} &= - \int_{\mathcal{R}} \int_{\mathcal{R}} \mathbf{f}(\mathbf{u}' - \mathbf{u}, \mathbf{x}' - \mathbf{x}) \cdot \dot{\mathbf{u}} dV' dV \\ &= - \int_{\mathcal{R}} [\rho \ddot{\mathbf{u}} - \mathbf{b}] \cdot \dot{\mathbf{u}} dV \\ &= - \int_{\mathcal{R}} \left[\frac{\partial}{\partial t} \left(\frac{\rho}{2} \dot{\mathbf{u}} \cdot \dot{\mathbf{u}} \right) - \mathbf{b} \cdot \dot{\mathbf{u}} \right] dV. \end{aligned} \quad (29)$$

So, we conclude

$$\dot{\Phi}_{\mathbf{u}} + \dot{T}_{\mathbf{u}} = \int_{\mathcal{R}} \mathbf{b} \cdot \dot{\mathbf{u}} dV \quad (30)$$

where $T_{\mathbf{u}}$ is the total kinetic energy of the body. This result states that work done by external forces on a microelastic body is converted either to kinetic energy or to macroelastic energy density, with no dissipation. This statement is identical to its well-known analogue in the conventional formulation of solid mechanics, provided we replace the macroelastic energy density with the conventional strain energy for an elastic solid. This analogy will allow us to compare in a meaningful way the constitutive behavior of elastic materials in the conventional and peridynamic theories. This will be discussed in a later section.

5 Structureless materials

A peridynamic material without memory will be called *structureless* if there is a vector-valued function \mathbf{f} of a single vector variable such that

$$\mathbf{f}(\boldsymbol{\eta}, \boldsymbol{\xi}) = \mathbf{g}(\boldsymbol{\eta} + \boldsymbol{\xi}) \quad \forall \boldsymbol{\xi}, \boldsymbol{\eta}. \quad (31)$$

The meaning of this definition is that in a structureless material, the pairwise force function \mathbf{f} depends only on the *current* (deformed) relative position of the two particles.

In a structureless material, deformations that merely “reshuffle” the particle positions without changing the local density of particles have no effect on the internal forces. Simple shear deformations fall into this category. In this respect, structureless materials are like compressible inviscid fluids.

For an *isotropic* structureless material, comparison of (31) with the form of the most general isotropic material (15) shows that there is a scalar-valued function G such that

$$F(\boldsymbol{\eta}, \boldsymbol{\xi}) = G(p), \quad p = |\boldsymbol{\xi} + \boldsymbol{\eta}| \quad \forall \boldsymbol{\xi}, \boldsymbol{\eta}. \quad (32)$$

Furthermore, comparison of (32) with (21) shows that any isotropic structureless material must be microelastic. Conversely, (15), (22), and (31) imply that any microelastic structureless material must be isotropic.

Suppose a structureless body undergoes an isotropic expansion of the form $\mathbf{x} + \mathbf{u} = \alpha \mathbf{x}$, where α is a constant. We compute the macroelastic energy density at a typical point \mathbf{x} in an internal subregion:

$$\begin{aligned} W(\mathbf{x}) &= \int_{\mathcal{R}} \check{w}(|\boldsymbol{\xi} + \boldsymbol{\eta}|) dV \\ &= 4\pi \int_0^\infty \check{w}(\alpha r) r^2 dr \\ &= \frac{4\pi}{\alpha^3} \int_0^\infty \check{w}(s) s^2 ds \end{aligned} \quad (33)$$

where the change of variables $s = \alpha r$ has been used. So, we have shown that $W \propto 1/(V\alpha^3)$, where $V\alpha^3$ is the total current volume of the body. Since W represents energy per unit reference volume, this means that energy per unit mass follows the same dependence.

Therefore, regardless of the details of G , specific energy is inversely proportional to volume in homogeneous deformations. This means that structureless materials cannot be used to accurately model most real fluids. The reason for this restriction is that in real fluids, degrees of freedom corresponding to thermal motion of the molecules, including vibrational and rotational modes, play a key role in determining the internal energy density. These degrees of freedom are not captured in the present theory, although the theory could perhaps be modified to do so.

Alternatively, an enhanced version of the theory is presented in Section 15 that permits a significant generalization of the response of structureless materials under isotropic expansion.

6 Harmonic materials

Consider an isotropic, microelastic material for which F is independent of η , so that we can write

$$F(\eta, \xi) = K(|\xi|) \quad \text{or} \quad \mathbf{f}(\eta, \xi) = K(|\xi|)(\xi + \eta) \quad \forall \xi, \eta \quad (34)$$

for some function K . For such a material, (2) becomes

$$\mathbf{L}_{\mathbf{u}}(\mathbf{x}) = \int_{\mathcal{R}} K(|\mathbf{x}' - \mathbf{x}|) ((\mathbf{u}' - \mathbf{u}) + (\mathbf{x}' - \mathbf{x})) \, dV'. \quad (35)$$

In this case, \mathbf{L} is linear, so the principle of superposition can be applied as in conventional linear elasticity.

Then if \mathcal{R} contains an internal subregion \mathcal{R}^0 , and if $\mathbf{b} \equiv \mathbf{0}$, the equilibrium equation (4) simplifies to

$$\int_{\mathcal{R}} K(|\mathbf{x}' - \mathbf{x}|) (\mathbf{u}' - \mathbf{u}) \, dV' = \mathbf{0} \quad \forall \mathbf{x} \in \mathcal{R}^0. \quad (36)$$

Any displacement field that satisfies Laplace's equation, $\nabla^2 \mathbf{u} = 0$ on \mathcal{R} , also satisfies (36) on \mathcal{R}^0 . To see this, let \mathbf{u} be any displacement field that satisfies Laplace's equation on \mathcal{R} . Let \mathcal{S}_r be the spherical shell of radius r centered at any given \mathbf{x} in the interior of \mathcal{R} . If \mathcal{S}_r is contained in \mathcal{R} , we have

$$\int_{\mathcal{S}_r} (\mathbf{u}(\mathbf{x}') - \mathbf{u}(\mathbf{x})) \, dA_{\mathbf{x}'} = \mathbf{0}. \quad (37)$$

This is the famous averaging property of solutions to Laplace's equation. It is readily confirmed by writing out the Taylor series for $\mathbf{u}(\mathbf{x}')$ centered at \mathbf{x} and applying the differential equation to the derivatives that appear in the coefficients in the series. The fact that such a displacement field satisfies (36) now follows because from (37),

$$\int_0^\delta K(r) \left[\int_{S_r} (\mathbf{u}' - \mathbf{u}) dA' \right] dr = \mathbf{0}, \quad r = |\mathbf{x}' - \mathbf{x}|, \quad \forall \mathbf{x} \in \mathcal{R}^0. \quad (38)$$

Because of this property, isotropic microelastic materials of the form (34) will be called *harmonic materials*.

Note that for harmonic materials, the relation to Laplace's equation established above holds regardless of the particular choice of K . The corresponding statement when there is time dependence is *not* true: it will be shown in Section 12 that wave speeds depend on the details of K . Also, the results of Section 10 show that the form of K affects material stability.

7 Relation to the conventional theory

Because of its importance in relation to measurable quantities, we now discuss a notion of "force per unit area." Imagine a homogeneous, microelastic body that has undergone a homogeneous deformation. Suppose a plane \mathcal{P} divides the body into two subregions \mathcal{R}^+ and \mathcal{R}^- . Then \mathcal{R}^+ exerts some force on \mathcal{R}^- . This force is applied not just on the surface of \mathcal{R}^- , but through "action at a distance" to particles below the surface as well. If this force is divided by the area of $\mathcal{P} \cap \mathcal{R}$, we have a notion of force per unit area.

To make this concept more precise and general, we now define $\boldsymbol{\tau}(\mathbf{x}, \mathbf{n})$, the *areal force density*, at a point \mathbf{x} in \mathcal{R} in the direction of unit vector \mathbf{n} . Let \mathbf{x} and \mathbf{n} be given, and let

$$\mathcal{R}^+ = \{\mathbf{x}' \in \mathcal{R} : (\mathbf{x}' - \mathbf{x}) \cdot \mathbf{n} \geq 0\}, \quad \mathcal{R}^- = \{\mathbf{x}' \in \mathcal{R} : (\mathbf{x}' - \mathbf{x}) \cdot \mathbf{n} \leq 0\}. \quad (39)$$

Let \mathcal{L} be the following set of colinear points:

$$\mathcal{L} = \{\hat{\mathbf{x}} \in \mathcal{R}^- : \hat{\mathbf{x}} = \mathbf{x} - s\mathbf{n}, \quad 0 \leq s < \infty\}. \quad (40)$$

Now define

$$\boldsymbol{\tau}(\mathbf{x}, \mathbf{n}) = \int_{\mathcal{L}} \int_{\mathcal{R}^+} \mathbf{f}(\mathbf{u}' - \hat{\mathbf{u}}, \mathbf{x}' - \hat{\mathbf{x}}) dV_{\mathbf{x}'} d\hat{\ell} \quad (41)$$

where $d\hat{\ell}$ represents differential path length over \mathcal{L} . This quantity is about as close as one can come to the concept of traction, which plays a central role in the conventional theory.

A configuration is said to be *unstressed* if

$$\boldsymbol{\tau}(\mathbf{x}, \mathbf{n}) = \mathbf{0} \quad \forall \mathbf{x} \in \mathcal{R}, \quad \forall \mathbf{n}. \quad (42)$$

In general, an unstressed configuration cannot be found for a given body. For example, a body composed of the gas-like structureless, microelastic material with $G(p) = 1/p^2$ has no unstressed configuration. However, materials that behave more like solids can have unstressed configurations. An example is the isotropic, microelastic material with $I(p, q, r) = (p - r)^2$. This material is pairwise equilibrated in the reference configuration, so the reference configuration is necessarily unstressed (see Section 2).

The foregoing definition of $\boldsymbol{\tau}$ is most useful in the case of a homogeneous deformation of a body with an internal subregion \mathcal{R}^0 . In this case, for $\mathbf{x} \in \mathcal{R}^0$, $\boldsymbol{\tau}(\mathbf{x}, \mathbf{n})$ equals the force per unit area in the intuitive sense, *i.e.*, in the sense of the first paragraph of this section. For such a homogeneous deformation, we can repeat Cauchy's proof of the linear dependence of $\boldsymbol{\tau}$ on \mathbf{n} . Therefore, we can meaningfully speak of a stress tensor $\boldsymbol{\sigma}$, independent of \mathbf{x} , such that

$$\boldsymbol{\tau}(\mathbf{x}, \mathbf{n}) = \boldsymbol{\sigma} \mathbf{n} \quad \forall \mathbf{x} \in \mathcal{R}^0, \quad \forall \mathbf{n}. \quad (43)$$

This stress tensor is really a Piola-Kirchhoff stress tensor, because $\boldsymbol{\tau}$ represents force per unit area in the *reference* configuration.

For a microelastic material, it was established in the discussion leading up to (30) that there is a connection between the macroelastic energy density W defined in (26) and the strain energy density of conventional elasticity theory, which we will call \hat{W} . The connection is that they both represent stored energy accumulated through deformation, and this energy is recoverable by reversing the deformation. In the case of homogeneous deformation, these two quantities must therefore be identical in \mathcal{R}^0 . This also establishes that the $\boldsymbol{\sigma}$ defined in (43) is identical with the stress tensor in the conventional theory, $\partial \hat{W} / \partial \mathbf{F}$, where \mathbf{F} is the deformation gradient tensor.

We now turn to the issue of how \hat{W} can be computed from a given pairwise potential function w . To do this, we use (26) noting that $\mathbf{u}' - \mathbf{u} = (\mathbf{F} - \mathbf{1})(\mathbf{x}' - \mathbf{x})$:

$$\hat{W}(\mathbf{F}) = \frac{1}{2} \int_{\mathcal{R}} w((\mathbf{F} - \mathbf{1})\boldsymbol{\xi}, \boldsymbol{\xi}) dV_{\boldsymbol{\xi}} \quad \forall \mathbf{F}. \quad (44)$$

Using (24), (44) becomes

$$\hat{W}(\mathbf{F}) = \frac{1}{2} \int_{\mathcal{R}} \tilde{w}(\sqrt{\boldsymbol{\xi} \cdot (\mathbf{F}^T \mathbf{F}) \boldsymbol{\xi}}, \boldsymbol{\xi}) dV_{\boldsymbol{\xi}} \quad \forall \mathbf{F}. \quad (45)$$

This shows that the \hat{W} defined in this way represents a legitimate hyperelastic material in the conventional theory, because its only dependence on \mathbf{F} is through $\mathbf{F}^T \mathbf{F}$, *i.e.*, the right Cauchy-Green tensor.

If the material is also isotropic, then we can use (25) and the fact that the eigenvalues of $\mathbf{F}^T \mathbf{F}$ are the squares of the principal stretches, $\lambda_1, \lambda_2, \lambda_3$. Thus, using components in a principal basis for $\mathbf{F}^T \mathbf{F}$,

$$\hat{W}(\mathbf{F}) = \frac{1}{2} \int_{\mathcal{R}} \tilde{w}(\sqrt{\lambda_1^2 \xi_1^2 + \lambda_2^2 \xi_2^2 + \lambda_3^2 \xi_3^2}, |\boldsymbol{\xi}|) dV_{\boldsymbol{\xi}} \quad \forall \mathbf{F}. \quad (46)$$

This shows immediately that for such a material we can write

$$\hat{W}(\mathbf{F}) = \Omega(\lambda_1, \lambda_2, \lambda_3) \quad (47)$$

where Ω is a function that possesses the necessary symmetries for an isotropic material:

$$\Omega(\lambda_1, \lambda_2, \lambda_3) = \Omega(\lambda_2, \lambda_1, \lambda_3) = \dots \quad (48)$$

As an example, consider the isotropic microelastic peridynamic material with the following pairwise potential function:

$$\tilde{w}(|\boldsymbol{\xi} + \boldsymbol{\eta}|, |\boldsymbol{\xi}|) = \gamma(|\boldsymbol{\xi}|) (|\boldsymbol{\xi} + \boldsymbol{\eta}|^2 - |\boldsymbol{\xi}|^2)^2 \quad (49)$$

where γ is a scalar-valued *shielding function* that describes the way that the strength of interaction between particles drops off as a function of their separation in the reference configuration. Using components in a principal basis for $\mathbf{F}^T \mathbf{F}$, we have $\xi_i + \eta_i = \lambda_i \xi_i$ (no sum). Carrying out the integration indicated in (46) for this material, we find, after simplification,

$$\hat{W}(\mathbf{F}) = \frac{2\pi}{15} [(I_1 - 3)(3I_1 - 1) - 4(I_2 - 3)] \int_0^\infty \gamma(r) r^6 dr \quad (50)$$

where the fundamental scalar invariants of $\mathbf{F}^T \mathbf{F}$ are

$$\begin{aligned} I_1 &= \text{Tr } \mathbf{F}^T \mathbf{F} = \lambda_1^2 + \lambda_2^2 + \lambda_3^2, \\ I_2 &= \frac{1}{2} [I_1^2 - \text{Tr } (\mathbf{F}^T \mathbf{F})^2] = \lambda_1^2 \lambda_2^2 + \lambda_2^2 \lambda_3^2 + \lambda_3^2 \lambda_1^2 \\ I_3 &= \det \mathbf{F}^T \mathbf{F} = \lambda_1^2 \lambda_2^2 \lambda_3^2. \end{aligned} \quad (51)$$

The conventional hyperelastic material described by (50) is a reasonably behaved compressible material, provided $\int_0^\infty \gamma(r)r^6 dr > 0$. This example illustrates that many different peridynamic materials can have the same “large scale” response as a given hyperelastic material in the conventional theory of elasticity. To see this, note that if we choose two functions $\gamma^{(1)}$ and $\gamma^{(2)}$ such that

$$\int_0^\infty \gamma^{(1)}(r)r^6 dr = \int_0^\infty \gamma^{(2)}(r)r^6 dr, \quad (52)$$

then these materials have the same \hat{W} according to (50). Yet they may have very different “small scale” properties in the peridynamic theory, as discussed in Section 12.

In summary, for any microelastic material, we have found the corresponding conventional elastic material (in the sense of homogeneous deformations). Now we briefly consider the converse: for a given function \hat{W} in the conventional theory of elasticity, can we find a pairwise potential function that generates it in the peridynamic theory? The answer is in general no. As a demonstration of this, it will be shown in Section 11 that the linear elastic moduli that can be generated from peridynamic materials are quite restricted.

Therefore, the peridynamic theory is simultaneously more general and less general than the conventional theory of elasticity. Not all conventional elastic materials can be modeled with the peridynamic approach. But for those that can be, there may be an infinite number of peridynamic materials corresponding to the same conventional material, as demonstrated in the last example.

8 Linearization

Now we return to the general peridynamic material (8) and assume that $|\eta| \ll 1$. Assuming that the required partial derivatives exist (these are not the spatial derivatives discussed in the Introduction), we linearize the function $\mathbf{f}(\cdot, \boldsymbol{\xi})$ while holding $\boldsymbol{\xi}$ fixed:

$$\mathbf{f}(\boldsymbol{\eta}, \boldsymbol{\xi}) = \mathbf{C}(\boldsymbol{\xi})\boldsymbol{\eta} + \mathbf{f}(\mathbf{0}, \boldsymbol{\xi}) \quad \forall \boldsymbol{\xi}, \boldsymbol{\eta} \quad (53)$$

where \mathbf{C} is the second-order *micromodulus* tensor given by

$$\mathbf{C}(\boldsymbol{\xi}) = \frac{\partial \mathbf{f}}{\partial \boldsymbol{\eta}}(\mathbf{0}, \boldsymbol{\xi}). \quad (54)$$

Error terms of order $O(|\boldsymbol{\eta}|^2)$ have been omitted from (53). Thus, for a linear peridynamic material, (2) and (53) lead to

$$\mathbf{L}\mathbf{u} = \int_{\mathcal{R}} [\mathbf{C}(\mathbf{x}' - \mathbf{x})(\mathbf{u}' - \mathbf{u}) + \mathbf{f}(\mathbf{0}, \mathbf{x}' - \mathbf{x})] dV' \quad \forall \mathbf{x} \in \mathcal{R} \quad (55)$$

where the notation $\mathbf{L}\mathbf{u} = \mathbf{L}_{\mathbf{u}}$ is used since \mathbf{L} is now a linear operator. If the body possesses an internal subregion \mathcal{R}^0 , then in view of (6), (55) simplifies to

$$\mathbf{L}\mathbf{u} = \int_{\mathcal{R}} \mathbf{C}(\mathbf{x}' - \mathbf{x})(\mathbf{u}' - \mathbf{u}) dV' \quad \forall \mathbf{x} \in \mathcal{R}^0. \quad (56)$$

\mathbf{C} inherits the following property from \mathbf{f} according to (6) and (54):

$$\mathbf{C}(-\boldsymbol{\xi}) = \mathbf{C}(\boldsymbol{\xi}) \quad \forall \boldsymbol{\xi}. \quad (57)$$

Differentiation of (8) with respect to $\boldsymbol{\eta}$ yields

$$\mathbf{C}(\boldsymbol{\xi}) = \boldsymbol{\xi} \otimes \frac{\partial F}{\partial \boldsymbol{\eta}}(\mathbf{0}, \boldsymbol{\xi}) + F(\mathbf{0}, \boldsymbol{\xi})\mathbf{1} \quad \forall \boldsymbol{\xi}. \quad (58)$$

If a linear material is microelastic, (17) applied to (54) shows that

$$\mathbf{C}(\boldsymbol{\xi}) = \mathbf{C}^T(\boldsymbol{\xi}) \quad \forall \boldsymbol{\xi}. \quad (59)$$

This condition is also sufficient for the linear material derived from (58) to be microelastic. Comparing (59) with (58), evidently not all linear materials are microelastic, since in general the \mathbf{C} derived from (58) is not symmetric. A necessary and sufficient condition for it to be symmetric is that there be a scalar-valued function λ such that

$$\boldsymbol{\xi} \otimes \frac{\partial F}{\partial \boldsymbol{\eta}}(\mathbf{0}, \boldsymbol{\xi}) = \lambda(\boldsymbol{\xi})\boldsymbol{\xi} \otimes \boldsymbol{\xi} \quad \forall \boldsymbol{\xi}, \quad (60)$$

in other words $\partial F / \partial \boldsymbol{\eta}(\mathbf{0}, \boldsymbol{\xi})$ must be parallel to $\boldsymbol{\xi}$. If this is the case, we write

$$\mathbf{C}(\boldsymbol{\xi}) = \lambda(\boldsymbol{\xi})\boldsymbol{\xi} \otimes \boldsymbol{\xi} + F_0(\boldsymbol{\xi})\mathbf{1} \quad \forall \boldsymbol{\xi} \quad (61)$$

where λ and F_0 are given by

$$\lambda(\boldsymbol{\xi}) = \frac{1}{|\boldsymbol{\xi}|^2} \boldsymbol{\xi} \cdot \frac{\partial F}{\partial \boldsymbol{\eta}}(\mathbf{0}, \boldsymbol{\xi}), \quad F_0(\boldsymbol{\xi}) = F(\mathbf{0}, \boldsymbol{\xi}) \quad \forall \boldsymbol{\xi}. \quad (62)$$

Note that because of (57) and (61), λ and F_0 satisfy

$$\lambda(-\boldsymbol{\xi}) = \lambda(\boldsymbol{\xi}), \quad F_0(-\boldsymbol{\xi}) = F_0(\boldsymbol{\xi}), \quad \forall \boldsymbol{\xi}. \quad (63)$$

Also note that $F_0 \equiv 0$ if the reference configuration is pairwise equilibrated. In this case $\mathbf{f}(\mathbf{0}, \cdot) \equiv \mathbf{0}$ in (53). On the other hand, there is no reason to assume that this condition would exist in real materials. (See Section 9).

For a microelastic material, using (21):

$$\lambda(\boldsymbol{\xi}) = \frac{1}{|\boldsymbol{\xi}|} \frac{\partial H}{\partial p}(|\boldsymbol{\xi}|, \boldsymbol{\xi}), \quad F_0(\boldsymbol{\xi}) = H(|\boldsymbol{\xi}|, \boldsymbol{\xi}) \quad \forall \boldsymbol{\xi}. \quad (64)$$

For an isotropic material, using (14):

$$\lambda(\boldsymbol{\xi}) = \frac{1}{|\boldsymbol{\xi}|} \frac{\partial I}{\partial p}(|\boldsymbol{\xi}|, 0, |\boldsymbol{\xi}|) + \frac{\partial I}{\partial q}(|\boldsymbol{\xi}|, 0, |\boldsymbol{\xi}|), \quad F_0(\boldsymbol{\xi}) = I(|\boldsymbol{\xi}|, 0, |\boldsymbol{\xi}|) \quad \forall \boldsymbol{\xi}. \quad (65)$$

Note that in a linear isotropic material, λ and F_0 depend on $\boldsymbol{\xi}$ only through $|\boldsymbol{\xi}|$. We will use the same symbols $\lambda(|\boldsymbol{\xi}|) = \lambda(\boldsymbol{\xi})$ and $F_0(|\boldsymbol{\xi}|) = F_0(\boldsymbol{\xi})$ in this case to avoid a proliferation of notation. Also note from the discussion following (24) that if the material is microelastic as well as isotropic, then the term $\partial I / \partial q$ vanishes in (65).

For an isotropic structureless material, using (32):

$$\lambda(\boldsymbol{\xi}) = \frac{1}{|\boldsymbol{\xi}|} \frac{dG}{dp}(|\boldsymbol{\xi}|), \quad F_0(\boldsymbol{\xi}) = G(|\boldsymbol{\xi}|) \quad \forall \boldsymbol{\xi}. \quad (66)$$

9 Unstressed configurations

As discussed in Section 7, a body is in an unstressed configuration if $\boldsymbol{\tau}(\mathbf{x}, \mathbf{n}) = \mathbf{0}$ at all points \mathbf{x} in the body for all directions \mathbf{n} . Consider an isotropic, microelastic body \mathcal{R} with an internal subregion \mathcal{R}^0 . Let an orthonormal basis $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ be given. From (8), (41) and (42), an unstressed *reference* configuration has

$$0 = \tau_1(\mathbf{0}, \mathbf{e}_1) = \int_0^\infty \int_{\mathcal{R}^+} F(\mathbf{0}, \mathbf{x}' + s\mathbf{e}_1)(\mathbf{x}' + s\mathbf{e}_1) dV_{\mathbf{x}'} ds. \quad (67)$$

Setting $\boldsymbol{\xi} = \mathbf{x}' + s\mathbf{e}_1$ and using a spherical coordinate system with

$$\xi_1 = r \cos \theta, \quad \xi_2 = r \sin \theta \cos \phi, \quad \xi_3 = r \sin \theta \sin \phi, \quad (68)$$

the integral in (67) becomes

$$\int_0^\infty \int_0^r \int_0^{\cos^{-1}(s/r)} \int_0^{2\pi} F_0(r)(r \cos \theta)r^2 \sin \theta \, d\phi \, d\theta \, ds \, dr = \Psi \quad (69)$$

where

$$\Psi = \frac{2\pi}{3} \int_0^\infty F_0(r)r^4 \, dr \quad (70)$$

and F_0 is defined in (62). (See Figures 2(a) and 2(b) for an illustration of the change of variables.) So, for an unstressed reference configuration, we have

$$\Psi = 0. \quad (71)$$

This result places a restriction on F if the reference configuration is to be unstressed. It is of importance because in modeling real materials, it is too restrictive to assume pairwise equilibration, which requires that the force between any two particles vanish (see Section 2). On the contrary, it is to be expected that there may be significant forces between particles even when no loading is applied. Equation (71) implies that this distribution of forces between particles, if it is nonzero, be repulsive (negative) for some values of interparticle distance and attractive (positive) for others.

10 Material stability

Suppose that for a bounded body \mathcal{R} composed of a microelastic material, a displacement field \mathbf{u} satisfies the equilibrium equation (4) for some specified \mathbf{b} field. Define the *potential energy* functional Π by

$$\Pi_{\mathbf{u}} = \Phi_{\mathbf{u}} - \int_{\mathcal{R}} \mathbf{b} \cdot \mathbf{u} \, dV \quad (72)$$

where Φ is the total macroelastic energy defined in (27). If ε is a scalar and \mathbf{v} is a vector field on \mathcal{R} , define a functional $\hat{\Pi}$ by

$$\hat{\Pi}_{\mathbf{v}}(\varepsilon) = \Pi_{\mathbf{u}+\varepsilon\mathbf{v}}. \quad (73)$$

From (73), (27), and (26),

$$\hat{\Pi}_{\mathbf{v}}(\varepsilon) = \frac{1}{2} \int_{\mathcal{R}} \int_{\mathcal{R}} w((\mathbf{u}' - \mathbf{u}) + \varepsilon(\mathbf{v}' - \mathbf{v}), \mathbf{x}' - \mathbf{x}) \, dV' \, dV - \int_{\mathcal{R}} \mathbf{b} \cdot (\mathbf{u} + \varepsilon\mathbf{v}) \, dV. \quad (74)$$

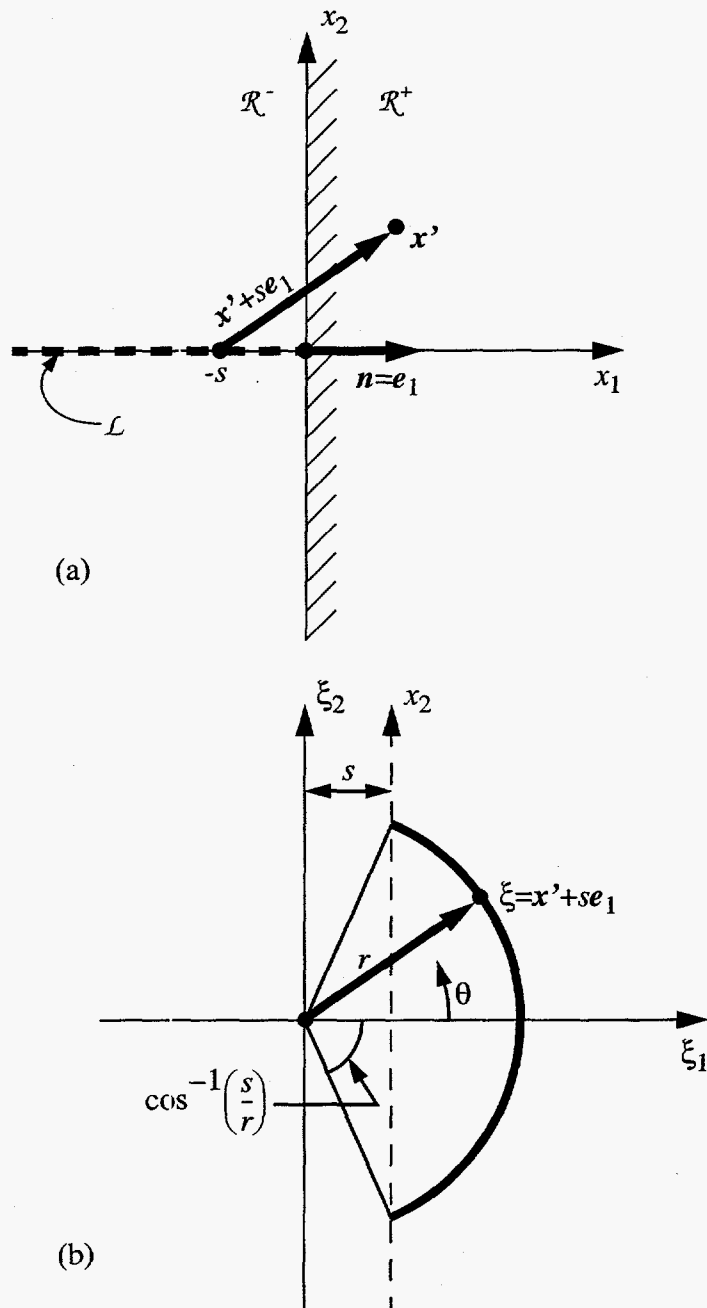


Figure 2(a) Computation of τ , and (b) Change of variables.

To find a field \mathbf{u} that makes Π stationary, we set $d\hat{\Pi}_{\mathbf{v}}/d\varepsilon(0) = 0$:

$$\frac{1}{2} \int_{\mathcal{R}} \int_{\mathcal{R}} \mathbf{f}(\mathbf{u}' - \mathbf{u}, \mathbf{x}' - \mathbf{x}) \cdot (\mathbf{v}' - \mathbf{v}) dV' dV - \int_{\mathcal{R}} \mathbf{b} \cdot \mathbf{v} dV = 0 \quad (75)$$

where (18) has been used. To obtain the Euler-Lagrange equation corresponding to Π , we take

$$\mathbf{v}(\mathbf{x}) = \mathbf{a}\Delta(\mathbf{x} - \mathbf{X}) \quad \forall \mathbf{x} \in \mathcal{R} \quad (76)$$

where \mathbf{a} is an arbitrary non-null vector, \mathbf{X} is an arbitrary point in \mathcal{R} , and Δ is the delta function for a vector variable. Applying this to (75) and using the properties of the delta function to evaluate one of the double integrals leads to

$$\mathbf{L}_{\mathbf{u}} + \mathbf{b} = \mathbf{0} \quad \text{on } \mathcal{R} \quad (77)$$

where the linear admissibility condition (6) has been used. Thus the equilibrium equation is the Euler-Lagrange equation for Π . This result is of course the well-known principle of stationary potential energy applied to peridynamic materials.

Now we go a step further and investigate the conditions required for Π to reach a *minimum* at \mathbf{u} in addition to merely being stationary there. To do this, we define

$$\chi_{\mathbf{v}}(\varepsilon) = \frac{d^2 \hat{\Pi}_{\mathbf{v}}}{d\varepsilon^2}(\varepsilon) \quad (78)$$

and require $\chi_{\mathbf{v}}(0) > 0$ for all choices of \mathbf{v} . Differentiating (74) again,

$$\int_{\mathcal{R}} \int_{\mathcal{R}} (\mathbf{v}' - \mathbf{v}) \cdot \left(\frac{\partial \mathbf{f}}{\partial \boldsymbol{\eta}}(\mathbf{u}' - \mathbf{u}, \mathbf{x}' - \mathbf{x}) \right) (\mathbf{v}' - \mathbf{v}) dV' dV > 0. \quad (79)$$

This condition would apply to a large displacement field \mathbf{u} as well as a small one. However, since we have worked out the linear theory in Section 8 only for linearization about the reference configuration, we will now assume that displacements are small. Then, by (54) and (79), we have

$$\chi_{\mathbf{v}}(0) = \int_{\mathcal{R}} \int_{\mathcal{R}} (\mathbf{v}' - \mathbf{v}) \cdot (\mathbf{C}(\mathbf{x}' - \mathbf{x})(\mathbf{v}' - \mathbf{v})) dV' dV > 0 \quad (80)$$

or, in component form,

$$\chi_{\mathbf{v}}(0) = \int_{\mathcal{R}} \int_{\mathcal{R}} C_{ij}(\mathbf{x}' - \mathbf{x})(v'_i - v_i)(v'_j - v_j) dV' dV > 0. \quad (81)$$

A sufficient condition for this to hold for all choices of the field \mathbf{v} is that $\mathbf{C}(\boldsymbol{\xi})$ be positive definite for all $\boldsymbol{\xi}$, *i.e.*,

$$\boldsymbol{\eta} \cdot \mathbf{C}(\boldsymbol{\xi})\boldsymbol{\eta} > 0 \quad \text{or} \quad C_{ij}(\boldsymbol{\xi})\eta_i\eta_j > 0 \quad \forall \boldsymbol{\xi}, \boldsymbol{\eta} \neq \mathbf{0}. \quad (82)$$

Taking the specific case of a linear isotropic material, we see from (61) that the eigenvalues of $\mathbf{C}(\boldsymbol{\xi})$ are

$$\lambda(r)r^2 + F_0(r) \quad \text{and} \quad F_0(r), \quad r = |\boldsymbol{\xi}|. \quad (83)$$

Both these eigenvalues need to be positive if $\mathbf{C}(\boldsymbol{\xi})$ is to be positive definite. So this implies $F_0(r) > 0$ for all $r > 0$. But it was shown in Section 9 that if F_0 is positive over some interval and the reference configuration is unstressed, F_0 must also be negative over some other interval. Therefore it is not possible for $\mathbf{C}(\boldsymbol{\xi})$ to be positive definite for all $\boldsymbol{\xi}$ in an unstressed configuration.

In particular, if $F_0 \equiv 0$, \mathbf{C} cannot be positive definite regardless of λ . Consider a material with $F_0 = 0$ and $\lambda > 0$ within some horizon. Physically, the material is a complex network of linear springs with positive spring constants. In the reference configuration, there is zero force in each spring. Surely this material is expected to be stable by any reasonable criterion for material stability. (One hardly expects such a system to undergo unbounded deformation in response to an infinitesimal load.) So we must seek a more useful condition than (82), which is sufficient for an equilibrated deformation to be a minimizer of Π , but is not physically reasonable.

To do this, we search for a non-null field \mathbf{v} that makes $\chi_{\mathbf{v}}(0)$ a minimum. If the value of $\chi_{\mathbf{v}}(0)$ at this minimum turns out to be positive, then (80) must be satisfied for all \mathbf{v} . Since we are only interested in the "direction" of \mathbf{v} (in the sense of infinite dimensional vector spaces), it is necessary to normalize χ by defining

$$\bar{\chi}_{\mathbf{v}} = \frac{\chi_{\mathbf{v}}}{\int_{\mathcal{R}} \mathbf{v} \cdot \mathbf{v} \, dV}. \quad (84)$$

Now we seek an extremum for $\bar{\chi}$ by deriving its Euler-Lagrange equation. Carrying out calculations similar to those leading up to (77), we find that the Euler-Lagrange equation for $\bar{\chi}_{\mathbf{v}}$ is

$$\mathbf{L}\mathbf{v} = -\beta\mathbf{v} \quad \text{on } \mathcal{R}, \quad \beta = \frac{\chi_{\mathbf{v}}(0)}{2}. \quad (85)$$

This is an eigenvalue equation for \mathbf{v} , since β is a scalar. So if all eigenvalues β are positive, then (80) must be satisfied for all \mathbf{v} . The interpretation of

this eigenvalue equation is as follows: if $\bar{\chi}$ reaches an extremum at \mathbf{v} , then the instantaneous acceleration field that would result from applying this \mathbf{v} to the body and then suddenly releasing it would be

$$\rho\ddot{\mathbf{v}} = -\beta\mathbf{v} \quad \text{on } \mathcal{R}. \quad (86)$$

Since the system is linear, if (86) holds for some particular time, *i.e.*, the time at which it is released, it must hold for all times after this. Therefore, (86) describes a system of standing waves of frequency $\sqrt{\beta/\rho}$. Such a system is equivalent to the superposition of some combination of propagating plane waves. The conclusion is that we can get the entire material stability picture by studying plane waves: if the wave speeds are real for all waves, then the material must be stable in the sense of potential energy minimization. In Section 12 it will be shown in detail how to translate this requirement for wave transmission into specific conditions on λ and F_0 for an isotropic material.

A particular choice of \mathbf{v} in (80) leads to an interesting necessary condition for material stability that will come up again later. We choose

$$\mathbf{v}(\mathbf{x}) = \mathbf{a}\sqrt{\Delta(\mathbf{x})} \quad \forall \mathbf{x} \in \mathcal{R} \quad (87)$$

where \mathbf{a} is an arbitrary non-null vector. Applying this to (80) leads to

$$\mathbf{a} \cdot \mathbf{P}\mathbf{a} > 0 \quad \forall \mathbf{a} \neq \mathbf{0}, \quad \mathbf{P} = \int_{\mathcal{R}} \mathbf{C}(\boldsymbol{\xi}) dV_{\boldsymbol{\xi}}. \quad (88)$$

Since \mathbf{C} is symmetric, the condition (88) means \mathbf{P} is positive definite. It is interesting to look at the implications of (88) for λ and F_0 in a microelastic, isotropic, linear material. Using (61), we find

$$\mathbf{P} = \int_{\mathcal{R}} (\lambda(|\boldsymbol{\xi}|)\boldsymbol{\xi} \otimes \boldsymbol{\xi} + F_0(|\boldsymbol{\xi}|)\mathbf{1}) dV_{\boldsymbol{\xi}}. \quad (89)$$

The integral may be evaluated with the help of the spherical coordinate system defined in (68). The result is

$$\mathbf{P} = 4\pi\mathbf{1} \int_0^\infty \left[\frac{\lambda(r)r^4}{3} + F_0(r)r^2 \right] dr. \quad (90)$$

If (88) holds for all points in a body, the material will be said to possess *single-point stability*. Its interpretation is that if we displace a single point while holding all the others fixed, that point will experience a force that opposes its displacement. Single-point stability is a necessary but not sufficient condition for potential energy minimization.

11 Homogeneous deformations in the linear theory

In this section we compute the elastic moduli, in the sense of the conventional theory of linear elasticity, corresponding to a given isotropic microelastic peridynamic material. We assume the material is unstressed in the reference configuration. The micromodulus tensor is given by $\mathbf{C}(\boldsymbol{\xi})$, which we decompose according to (61). Let an orthonormal basis $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ be given. Let \mathcal{R} be a body having an internal subregion \mathcal{R}^0 , and let \mathcal{R} undergo the homogeneous deformation given by $u_1 = \epsilon_{11}x_1$, $u_2 \equiv u_3 \equiv 0$, where ϵ_{11} is a constant, $|\epsilon_{11}| \ll 1$. Hence $\eta_1 = \epsilon_{11}\xi_1$, $\eta_2 \equiv \eta_3 \equiv 0$. Then, by (61), we have

$$\begin{aligned} f_1 &= \epsilon_{11}[\lambda(r)\xi_1^3 + F_0(r)\xi_1], \\ f_2 &= \epsilon_{11}\lambda(r)\xi_1^2\xi_2, \\ f_3 &= \epsilon_{11}\lambda(r)\xi_1^2\xi_3 \end{aligned} \quad (91)$$

where the notation $r = |\boldsymbol{\xi}|$ is used. We now compute the "stress" component $\sigma_{11} = \tau_1(\mathbf{e}_1)$ where $\boldsymbol{\tau}$ is defined in (41). Using the spherical coordinate system (68), we find

$$\begin{aligned} \tau_1(\mathbf{e}_1) &= \epsilon_{11} \int_0^\infty \int_0^r \int_0^{\cos^{-1}(s/r)} \int_0^{2\pi} \\ &\quad [\lambda(r)(r \cos \theta)^3 + F_0(r)(r \cos \theta)] r^2 \sin \theta \, d\phi \, d\theta \, ds \, dr \\ &= (\Lambda + \Psi)\epsilon_{11}, \end{aligned} \quad (92)$$

where

$$\Lambda = \frac{2\pi}{5} \int_0^\infty \lambda(r)r^6 dr \quad (93)$$

and Ψ was defined in (70). Recall from (71) that $\Psi = 0$ in an unstressed reference configuration. Carrying out similar computations for the tractions in the other directions, and comparing the result with the stress corresponding to this deformation in the conventional theory of elasticity, we find

$$[\boldsymbol{\sigma}] = \epsilon_{11} \begin{bmatrix} \Lambda & 0 & 0 \\ 0 & \Lambda/3 & 0 \\ 0 & 0 & \Lambda/3 \end{bmatrix} = \epsilon_{11} \begin{bmatrix} \ell + 2\mu & 0 & 0 \\ 0 & \ell & 0 \\ 0 & 0 & \ell \end{bmatrix} \quad (94)$$

where ℓ is the Lamé modulus and μ is the shear modulus. From this and the standard relations among the elastic moduli, we conclude that

$$\ell = \mu = \frac{\Lambda}{3}, \quad \nu = \frac{1}{4}, \quad E = \frac{5\Lambda}{6}, \quad k = \frac{5\Lambda}{9} \quad (95)$$

where ν is Poisson's ratio, E is Young's modulus, and k is bulk modulus. Not surprisingly, this value for ν is identical to Cauchy's result for a solid composed of a lattice of points that interact only through a central force potential [4]. It will be shown in Section 15 how materials with other Poisson's ratios can be modeled in the peridynamic approach, but this requires fundamental changes to the functional L . For the present, we will pursue the more restricted approach.

There is nothing to prevent us from carrying out the above computations for σ in the case of a reference configuration that is *not* unstressed, in which case Ψ may be nonzero. However, the definitions of the elastic moduli become ambiguous if the reference configuration is not unstressed, so to avoid confusion, this approach is not pursued here.

The result in (95) is significant in applying the theory to real materials because it relates a function that is not directly measurable, λ , to easily measurable quantities, ν and E , based on experimental data. It will be shown in the next section that we can make further progress in constraining λ .

12 Plane waves in a linear material

In an internal subregion of a homogeneous body composed of a linear microelastic peridynamic material, we investigate the existence of plane waves of the form

$$\mathbf{u}(\mathbf{x}, t) = \mathbf{a}e^{i(\kappa\mathbf{N}\cdot\mathbf{x}-\omega t)} \quad (96)$$

where \mathbf{a} is the constant *amplitude vector*, $i = \sqrt{-1}$, κ is the constant positive wavenumber, \mathbf{N} is a constant unit vector that gives the direction of propagation, and ω is the constant angular frequency. The following relations hold from the elementary kinematics of waves: $\kappa = 2\pi/\text{wavelength}$, $\omega = 2\pi/\text{period}$, and $c = \omega/\kappa$, where c is the wave speed. The components of \mathbf{a} may be complex, but only the real part of the right hand side of (96) represents a physical displacement.

We assume that the material has an unstressed reference configuration. We do not at the moment assume isotropy. Applying the equation of motion (3) together with (56) to (96), we find that any wave of the assumed form must be a solution to the following eigenvalue problem:

$$\rho\omega^2\mathbf{a} = \mathbf{M}(\mathbf{N}, \kappa)\mathbf{a} \quad (97)$$

where $\mathbf{M}(\mathbf{N}, \kappa)$ is a tensor given by

$$\mathbf{M}(\mathbf{N}, \kappa) = \int_{\mathcal{R}} \mathbf{C}(\boldsymbol{\xi}) \left(1 - e^{2\kappa\mathbf{N}\cdot\boldsymbol{\xi}}\right) dV_{\boldsymbol{\xi}}. \quad (98)$$

Since the material is assumed to be microelastic, the symmetry of \mathbf{M} follows from the symmetry of \mathbf{C} (see (59)). Also, the components of \mathbf{M} must be real-valued because \mathbf{C} is an even function, as shown in (57), so the imaginary part of the exponential integrates to zero. This allows us to rewrite (98) in the form

$$\mathbf{M}(\mathbf{N}, \kappa) = \int_{\mathcal{R}} \mathbf{C}(\boldsymbol{\xi})(1 - \cos \kappa\mathbf{N}\cdot\boldsymbol{\xi})dV_{\boldsymbol{\xi}}. \quad (99)$$

We now further restrict the material to being isotropic. In this case, (65) shows that λ and F_0 depend on $|\boldsymbol{\xi}|$ only, and (98) becomes

$$M_{ij}(\mathbf{N}, \kappa) = \int_{\mathcal{R}} (\lambda(|\boldsymbol{\xi}|)\xi_i\xi_j + F_0(|\boldsymbol{\xi}|)\delta_{ij})(1 - \cos(\kappa\mathbf{N}\cdot\boldsymbol{\xi}))dV_{\boldsymbol{\xi}}. \quad (100)$$

For fixed \mathbf{N} , define an orthonormal basis $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ such that $\mathbf{e}_1 = \mathbf{N}$. Once again using the spherical coordinate system specified in (68), we carry out the integration in (100) as follows:

$$\begin{aligned} M_{11}(\mathbf{e}_1, \kappa) &= \int_0^\infty \int_0^\pi \int_0^{2\pi} [\lambda(r)(r \cos \theta)^2 + F_0(r)] \\ &\quad \cdot (1 - \cos(\kappa r \cos \theta))r^2 \sin \theta \, d\phi \, d\theta \, dr, \\ M_{22}(\mathbf{e}_1, \kappa) &= \int_0^\infty \int_0^\pi \int_0^{2\pi} [\lambda(r)(r \sin \theta \cos \phi)^2 + F_0(r)] \\ &\quad \cdot (1 - \cos(\kappa r \cos \theta))r^2 \sin \theta \, d\phi \, d\theta \, dr, \\ &\vdots \end{aligned} \quad (101)$$

The result is

$$\begin{aligned} M_{11}(\mathbf{e}_1, \kappa) &= 4\pi \int_0^\infty [\lambda(r)r^4 A_1(\kappa r) + F_0(r)r^2 B(\kappa r)] \, dr, \\ M_{22}(\mathbf{e}_1, \kappa) &= 4\pi \int_0^\infty [\lambda(r)r^4 A_2(\kappa r) + F_0(r)r^2 B(\kappa r)] \, dr, \\ M_{33} = M_{22}, \quad M_{12} = M_{21} = M_{23} = M_{32} = M_{31} = M_{13} &= 0 \end{aligned} \quad (102)$$

where

$$\begin{aligned}
A_1(\kappa r) &= \frac{1}{3} - \frac{\sin(\kappa r)}{\kappa r} - \frac{2 \cos(\kappa r)}{(\kappa r)^2} + \frac{2 \sin(\kappa r)}{(\kappa r)^3} \\
A_2(\kappa r) &= \frac{1}{3} + \frac{\cos(\kappa r)}{(\kappa r)^2} - \frac{\sin(\kappa r)}{(\kappa r)^3} \\
B(\kappa r) &= 1 - \frac{\sin(\kappa r)}{\kappa r}.
\end{aligned} \tag{103}$$

The functions A_1 , A_2 , and B are bounded as $r \rightarrow 0$ in spite of the fact that they contain terms that individually are unbounded. In the limit of long wavelengths (small κ), we can further simplify these integrals by using the first three terms of the Taylor series for sin and cos:

$$\sin z = z - \frac{z^3}{3!} + \frac{z^5}{5!} - \dots \quad \cos z = 1 - \frac{z^2}{2!} + \frac{z^4}{4!} - \dots \tag{104}$$

which yield

$$M_{11}(\mathbf{e}_1, \kappa) = (\Lambda + \Psi)\kappa^2, \quad M_{22}(\mathbf{e}_1, \kappa) = M_{33}(\mathbf{e}_1, \kappa) = (\Lambda/3 + \Psi)\kappa^2 \tag{105}$$

where Λ is defined in (93) and Ψ in (70). Using the elementary relation $c = \omega/\kappa$, and the fact that the $\rho\omega^2$ are the eigenvalues of \mathbf{M} according to (97), the wave speeds for long dilatational and shear waves are given by

$$c_d^2 = \frac{M_{11}}{\rho\kappa^2} = \frac{\Lambda + \Psi}{\rho}, \quad c_s^2 = \frac{M_{22}}{\rho\kappa^2} = \frac{\Lambda/3 + \Psi}{\rho}. \tag{106}$$

In the case of an unstressed reference configuration ($\Psi = 0$), these results are consistent with the conventional formulation of solid mechanics for a linear isotropic elastic solid with elastic moduli given by (95).

However, differences between the conventional formulation and the peridynamic theory occur for shorter wavelengths (higher κ). In the present formulation, unlike the conventional theory, the wave speeds depend on wavelength. For example, in the limit of very short waves, (102) and (103) show that the diagonal components of \mathbf{M} become equal and independent of κ as $\kappa \rightarrow \infty$:

$$M_{11}(\mathbf{e}_1, \kappa) = M_{22}(\mathbf{e}_1, \kappa) = M_{33}(\mathbf{e}_1, \kappa) = 4\pi \int_0^\infty \left[\frac{\lambda(r)r^4}{3} + F_0(r)r^2 \right] dr \tag{107}$$

hence the wave speeds become inversely proportional to κ :

$$c_d^2 = c_s^2 = \frac{4\pi}{\rho\kappa^2} \int_0^\infty \left[\frac{\lambda(r)r^4}{3} + F_0(r)r^2 \right] dr. \quad (108)$$

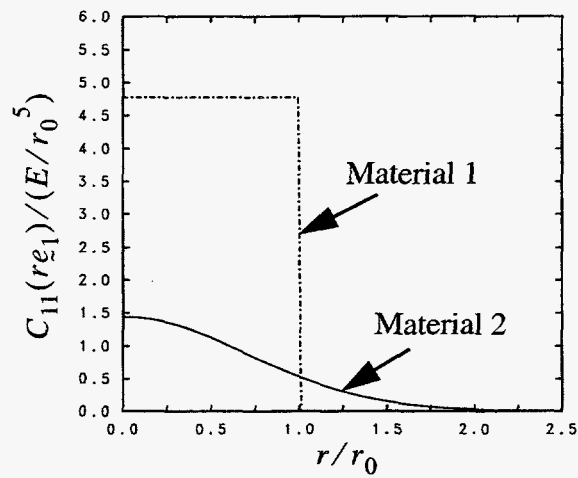
The reduction in wave speed at small wavelengths is suggestive of the inability of real materials to sustain waves of arbitrarily small wavelength. The explicit relation that has been developed above in (102) between the eigenvalues of \mathbf{M} and the form of λ suggests a way of fitting λ and F_0 to experimental wave dispersion curves for a given material, *i.e.*, frequency measurements as a function of wavenumber. As an illustration of how this process might work, we compare the predicted dispersion curves for two materials:

$$\begin{aligned} \text{Material 1: } F_0 &\equiv 0, & \lambda(r) &= \begin{cases} 15E/\pi r_0^5 r^2, & r < r_0 \\ 0, & r \geq r_0 \end{cases} \\ \text{Material 2: } F_0 &\equiv 0, & \lambda(r) &= (8E/5\pi^{3/2} r_0^5 r^2) \exp(-r^2/r_0^2), \end{aligned} \quad (109)$$

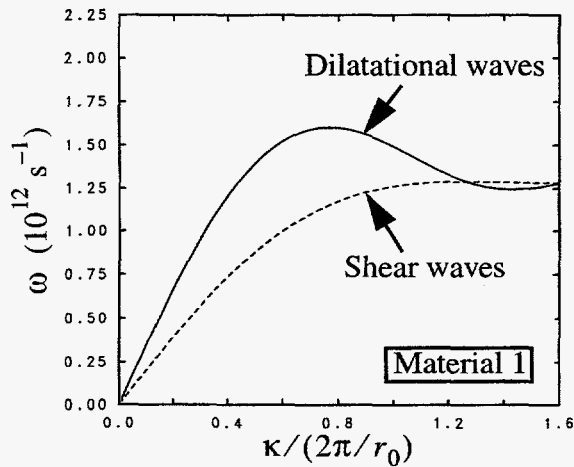
where $r_0 = 10^{-8}$ m and $E = 200$ GPa. The density for both materials is $\rho = 8000$ kg-m⁻³. Both these materials have the same Young's modulus E , which may be confirmed using (95). The micromodulus component C_{11} is plotted for both these materials in Figure 3(a). Material 1 has a sharp cutoff at $r = r_0$ for interaction between particles, while material 2 has a more gradual reduction. Figures 3(b) and (c) show the dispersion curves for dilatational and shear waves in both materials. The wave speeds for long waves are given by the slope of the dispersion curves near $\kappa = 0$. These long wave speeds are identical between the two materials, as predicted by (106), since the materials have the same Young's modulus. Both materials have dispersion curves that level off as wavenumber is increased past some value that is on the order of $2\pi/r_0$. This feature is characteristic of real materials. Yet the details of the predicted dispersion curves depend on the details of the shapes of the λ (and F_0) curves. This dependence provides a basis for evaluating these functions, approximately, from dispersion data for a real material [5]. (Other nonlocal models also predict nonlinear dispersion curves, because they introduce a length scale for constitutive behavior [6].)

Recall from Section 10 that there is a close connection between real wave speeds and material stability in linear materials. For long waves, (106) leads to the material stability requirements

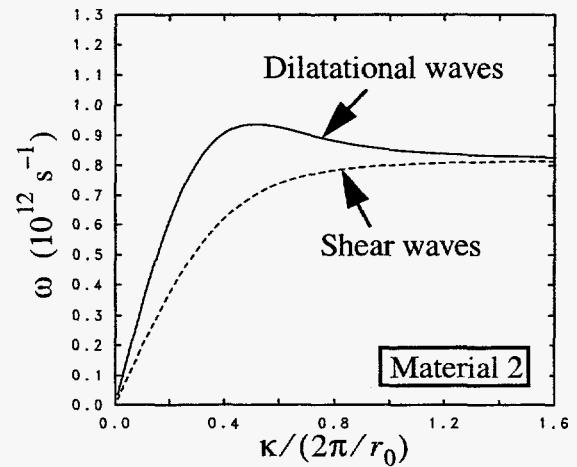
$$\Lambda + \Psi > 0, \quad \text{and} \quad \Lambda/3 + \Psi > 0. \quad (110)$$



(a)



(b)



(c)

Figure 3. Effect of changing λ on predicted dispersion curves. (a) Microelastic modulus as a function of particle separation distance for the materials used in computing the example dispersion curves. (b) Dispersion curves for Material 1. (c) Dispersion curves for Material 3.

If the reference configuration is unstressed, then $\Psi = 0$, so in this case (110) and (95) state that the bulk modulus and shear modulus of conventional elasticity theory must be positive. These are familiar requirements for material stability in the conventional theory. For short waves, (108) and (90) show that the requirement of real wave speeds is equivalent to single-point stability, (88). The requirements for short and long waves, (110) and (88), are necessary but not sufficient for material stability.

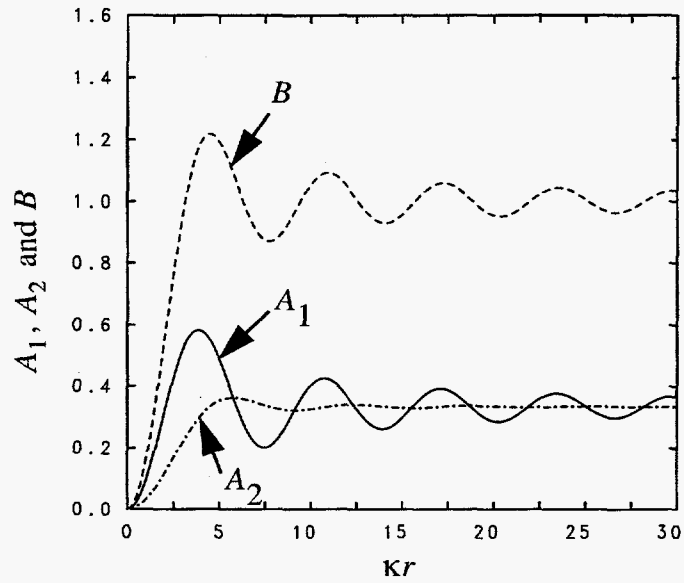
For sufficiency, the condition is that wave speeds be real at *any* wavelength. This means that the integrals in (102) must be positive for all κ . To see what this implies for λ and F_0 , we examine the functions A_1 , A_2 , and F_0 in more detail. These functions are plotted in Figure 4(a). They are positive for $\kappa r > 0$. The ratios A_1/B and A_2/B are plotted as functions of κr in Figure 4(b). Note that $A_1/B > 1/5$ and $A_2/B > 1/5$ for $\kappa r > 0$. Therefore, the integrals in (102) will be positive if

$$\lambda(r) \geq 0 \quad \text{and} \quad \frac{\lambda(r)r^2}{5} + F_0(r) > 0, \quad 0 < r < \delta \quad (111)$$

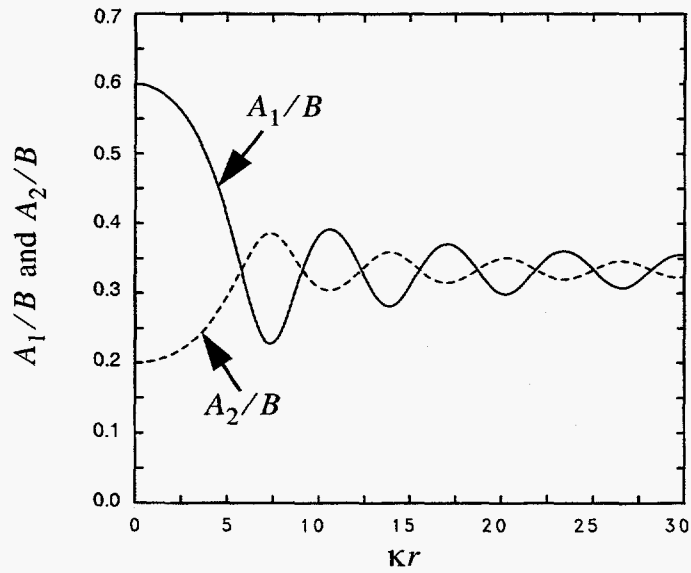
where δ is a horizon for the material. The first of (111) is a reasonable requirement physically; by (64) it means that the spring constants must be nonnegative. The second of (111) is also reasonable. It shows that we can tolerate negative values of F_0 (repulsive forces in the reference configuration) if the springs are sufficiently stiff to compensate for it. Note that this is a stronger condition than single-point stability. But it is a weaker condition than positive-definiteness of \mathbf{C} , which, as discussed in Section 10, implies the physically unreasonable requirement that F_0 be positive everywhere.

13 Loading conditions

So far nothing has been said about any boundary conditions that might be required to solve practical problems using the peridynamic approach. In the conventional theory of continuum mechanics, boundary conditions must be supplied to make the partial differential equations yield specific solutions in equilibrium problems. The boundaries of a body play a special role in the conventional theory because the differential equations model forces between particles that are in "direct contact" with each other. So, in the interior of a body in the conventional theory, the differential equations form a complete



(a)



(b)

Figure 4(a). Graphs of the functions A_1 , A_2 , and B . (b) Ratios of these functions.

description of how a given particle interacts with the system as a whole. On the other hand, at boundaries, a particle is not surrounded by neighbors and therefore additional conditions, namely boundary conditions, are required to provide a complete description. Mathematically, the significance of boundary conditions emerges when the Euler-Lagrange equations are evaluated from the potential energy functional, in which case "natural boundary conditions" appear automatically when one enforces the requirement that the functional reach a stationary value.

The situation is very different in the peridynamic theory. In the derivation of the equilibrium equation from the potential energy functional discussed previously (see (77)), no natural boundary condition emerged. Also, there is no traction vector that plays any natural role in the mechanics of a problem (although we artificially introduced such a concept in Section 7 as a way of making comparisons of constitutive models between the present formulation and the conventional theory). Hence the concept of a traction boundary condition, which appears naturally in the conventional theory, does not apply in the present approach. Instead, external forces must be supplied through the loading force density \mathbf{b} . These can be made nonzero in some layer near the boundary if one wishes to model loading on the surface. Such a condition, together with any external fields such as gravity that are modeled in a problem, will be called *force loading conditions*.

Displacement boundary conditions do have an analogue in the present theory. We continue to let \mathcal{R} be the region in which the equilibrium equation (4) or equation of motion (3) hold. We further imagine that in the complement of \mathcal{R} there is another set of points \mathcal{R}^* containing material in which we specify the displacements. Call the specified displacement field \mathbf{u}^* , a vector field defined on \mathcal{R}^* . Points in \mathcal{R} interact with points in \mathcal{R}^* through the pairwise force function \mathbf{f} . Therefore, if displacement loading conditions are present, we modify the functional \mathbf{L} as follows:

$$\mathbf{L}_{\mathbf{u}}(\mathbf{x}) = \int_{\mathcal{R}} \mathbf{f}(\mathbf{u}' - \mathbf{u}, \mathbf{x}' - \mathbf{x}) dV' + \int_{\mathcal{R}^*} \mathbf{f}(\mathbf{u}^* - \mathbf{u}, \mathbf{x}^* - \mathbf{x}) dV^* \quad (112)$$

where the shorthand $\mathbf{u}^* =: \mathbf{u}^*(\mathbf{x}^*)$, $dV^* = dV_{\mathbf{x}^*}$ has been used. This analogue to displacement boundary conditions will be called a *displacement loading condition*, and the new term in \mathbf{L} will be called the *displacement load*. Because the specified displacements interact with the points of \mathcal{R} only through \mathbf{f} , the displacement load acts something like an elastic boundary condition

in the conventional theory.

Note that assuming \mathbf{u}^* is bounded, \mathcal{R}^* must contain a nonzero volume in order for the displacement loading term to have any effect; otherwise it would simply integrate to zero. (The requirements for \mathcal{R}^* can be made more precise using the concept of measure, but there appears to be little to be gained in doing this.) Therefore, it does not suffice merely to specify \mathbf{u}^* on the boundary of \mathcal{R} .

A nice feature of the present theory is that we no longer need to talk about a displacement field satisfying the equilibrium equation *and the boundary conditions*, as we would in the conventional theory. The loading conditions are incorporated into the equations of equilibrium and motion and do not represent something that must be applied separately.

14 Example of fracture

In this section we illustrate some capabilities of the peridynamic approach in modeling fracture. For simplicity, we consider this in the setting of anti-plane shear. Assume that the body \mathcal{R} is infinitely long in the x_3 -direction. All quantities are assumed to be independent of x_3 , and we write $u(x_1, x_2) = u_3(\mathbf{x})$ and

$$f(\eta, \xi_1, \xi_2) = \int_{-\infty}^{\infty} f_3(\eta \mathbf{e}_3, \xi_1 \mathbf{e}_1 + \xi_2 \mathbf{e}_2 + \xi_3 \mathbf{e}_3) d\xi_3 \quad \forall \eta, \xi_1, \xi_2. \quad (113)$$

where $\eta = \eta_3$. Thus, the equation of equilibrium (4) becomes

$$\int_{\bar{\mathcal{R}}} \int_{\bar{\mathcal{R}}} f(u' - u, x'_1 - x_1, x'_2 - x_2) dx'_2 dx'_1 + b = 0 \quad \forall (x_1, x_2) \in \bar{\mathcal{R}} \quad (114)$$

where $b = b_3$ and $\bar{\mathcal{R}}$ is the cross-section of \mathcal{R} in the x_1 - x_2 plane. Consider the following (three-dimensional) microelastic, isotropic, peridynamic material:

$$\mathbf{f}(\boldsymbol{\eta}, \boldsymbol{\xi}) = \begin{cases} \mu(p - r)(\boldsymbol{\xi} + \boldsymbol{\eta})/p, & \text{if } |p - r| \leq u_* \text{ and } r \leq \delta \\ \mathbf{0}, & \text{otherwise} \end{cases} \quad (115)$$

where μ , δ , and u_* are positive constants and, as before,

$$p = |\boldsymbol{\xi} + \boldsymbol{\eta}|, \quad r = |\boldsymbol{\xi}|. \quad (116)$$

Thus, the spring connecting any two particles is linear for small relative displacements, but it breaks when the change in distance between the particles exceeds u_* . Only particles within a distance δ from each other in the reference configuration interact. To simplify the algebra, assume that $|\eta| \ll \bar{r}$. Evaluating f from (113) and (115) for this material, we find

$$f(\eta, \xi_1, \xi_2) = 2\mu\eta \left(z - \bar{r} \tan^{-1} \frac{z}{\bar{r}} \right) \quad (117)$$

where

$$\bar{r} = \sqrt{\xi_1^2 + \xi_2^2}, \quad z = \min \left\{ \frac{\bar{r}u_*}{\sqrt{\eta^2 - u_*^2}}, \sqrt{\delta^2 - \bar{r}^2} \right\}. \quad (118)$$

Figure 5(a) shows the behavior of the three-dimensional interparticle force function defined in (115). Figure 5(b) shows the anti-plane shear force function f that was derived from this material in (117) for a few values of \bar{r} . Oddly, the material described by (117) is harmonic (see Section 6) in the sense of scalar-valued functions of two coordinates, although the underlying three-dimensional material (115) from which it was derived is not harmonic.

A computer program was written to solve anti-plane shear problems in equilibrium. The numerical method uses a relaxation method with a brute-force integration scheme, *i.e.*, the double integral in (114) is evaluated in each integration step by summing over every node in the mesh. This program was applied to the material described by (117) with displacement loading conditions derived from the asymptotic mode-III crack tip field in the conventional theory of linear elasticity. The same equations are applied regardless of whether a node is on a discontinuity or not. (This is the feature promised in the Introduction.)

Figure 6(a) shows the resulting numerical solution near the crack tip for the peridynamic model. The figure shows the shape into which a sheet of material initially in the x_1 - x_2 plane is deformed. The vertical surface represents a crack surface.

An interesting feature of the numerical solution is the cusp-like shape of the crack surfaces. This differs from the analogous result in the conventional theory of elasticity, which is parabolic in shape near a crack tip (Figure 6(b)). To sustain this parabolic shape requires unbounded stresses near the tip (the well-known $r^{-1/2}$ singularity of linear fracture mechanics). Since real materials cannot sustain infinite stresses, it is necessary to introduce additional

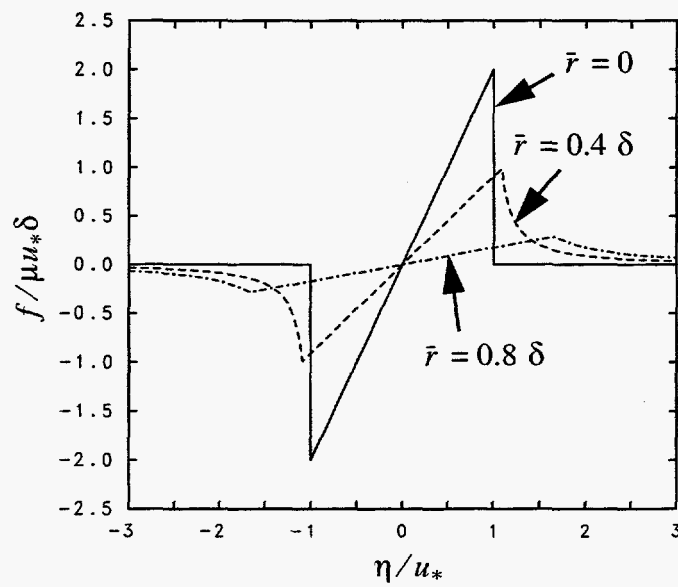
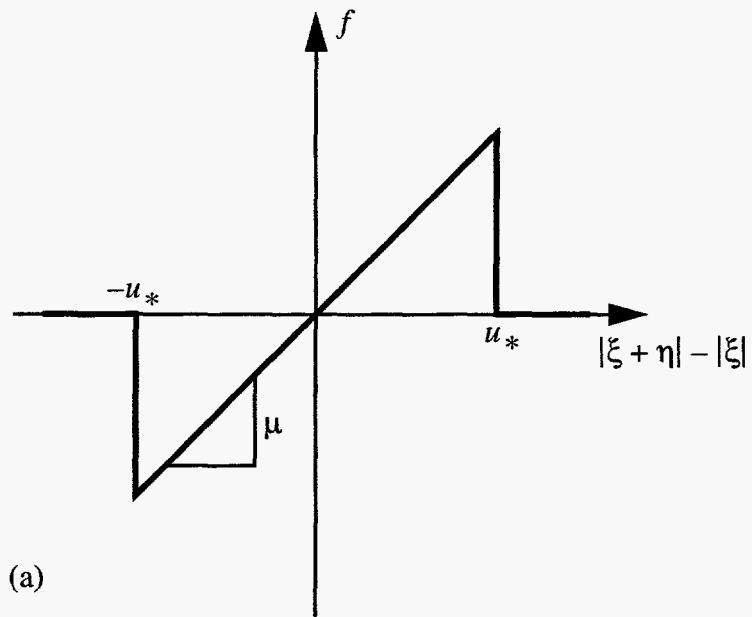


Figure 5. Example of material behavior in anti-plane shear. (a) Pairwise force function (three-dimensional). (b) Anti-plane shear force function derived from (a).

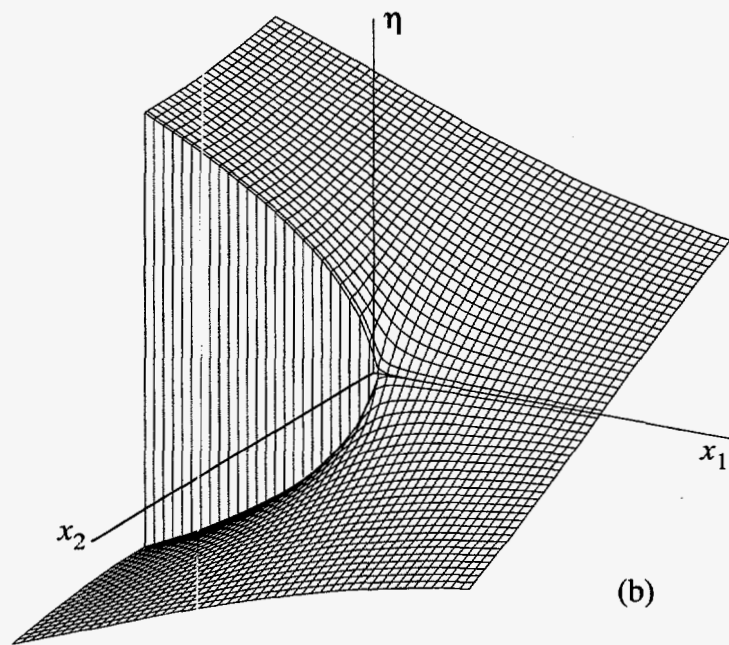
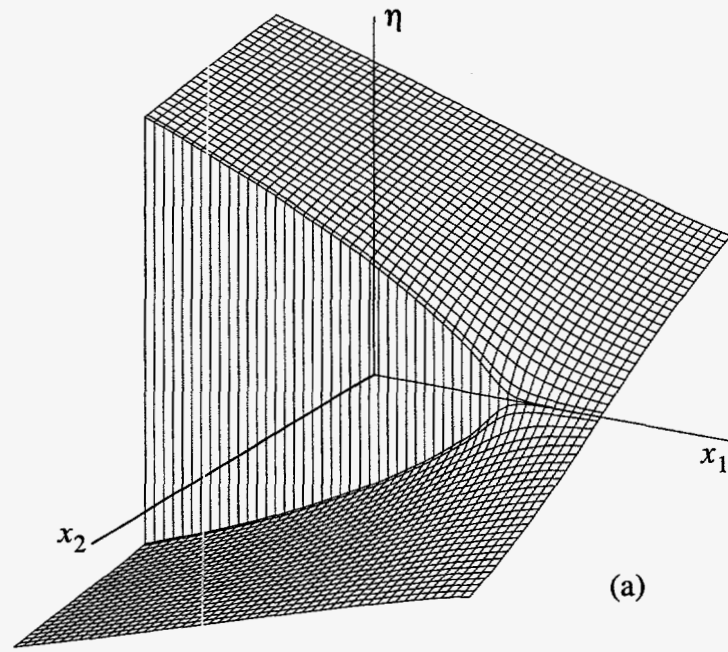


Figure 6. Mode-III crack tip behavior predicted by (a) the peridynamic and (b) the conventional theories.

ad hoc assumptions into the conventional theory, such as the models of Griffith and Barenblatt, to get physically reasonable crack-tip fields [7]. After modifying the conventional theory in this way, the result is a cusp-like deformation like the one predicted by the peridynamic theory. The fact that the peridynamic approach predicts this crack-tip shape without any additional mechanisms is an encouraging result. Other approaches to nonlocal elasticity can also have the property of avoiding the unbounded stresses near crack tips [8]. However, because they use partial derivatives in space, they still require special treatment of a crack surface or tip.

15 Generalization

It was shown in Section 11 that in the theory that has been developed so far, the Poisson's ratio obtained for homogeneous deformations of a linear isotropic material is $1/4$. Also, in Section (5), it was shown that structureless materials, although essentially fluids, have a severely limited range of energy-volume relations that they can represent. To provide a generalization, we must alter the form of \mathbf{L} assumed in (2) in a fundamental way. A brief sketch of one way to do this will now be given.

First, we modify the macroelastic energy density so that

$$\bar{W}(\mathbf{x}) = W(\mathbf{x}) + e(\vartheta(\mathbf{x})), \quad (119)$$

where

$$\vartheta(\mathbf{x}) = \int_{\mathcal{R}} j(|\boldsymbol{\xi}|) |\boldsymbol{\xi} + \boldsymbol{\eta}| dV', \quad (120)$$

and where W is defined in (26), and e and j are scalar-valued functions. The quantity ϑ is a weighted average of the extension of all the springs connecting \mathbf{x} with all the other particles in the body. It may be thought of as essentially giving the volume of a deformed sphere that was centered at \mathbf{x} in the reference configuration. The function e therefore represents, in effect, a volume-dependent strain energy term. For convenience, we assume that j is normalized so that $\boldsymbol{\eta} \equiv \mathbf{0}$ implies $\vartheta = 1$.

Note the fundamental way that the energy density has been altered here. It is no longer merely the sum of the spring energies, although these energies are still included through W . Instead, it includes a new term that depends on how the particles deform *together*. This type of energy dependence is

motivated by the behavior of real materials. In metals, for example, the electrons are so mobile that they are often regarded as a "cloud." In spite of this mobility, the cloud as a whole is tied to the lattice. So, as the crystal expands, the electron cloud also expands, and the resulting change in energy of the cloud must be considered in computing the energy of the crystal at a given deformation.

It is not obvious how the force density \mathbf{L} should be modified for such a material. To figure this out, we can use Hamilton's principle in the following form: we seek stationary values of the functional

$$\Upsilon_{\mathbf{u}} = \int_0^\infty \left[\int_{\mathcal{R}} \bar{W} dV - \int_{\mathcal{R}} \frac{\rho \dot{\mathbf{u}} \cdot \dot{\mathbf{u}}}{2} dV - \int_{\mathcal{R}} \mathbf{b} \cdot \mathbf{u} dV \right] dt. \quad (121)$$

Upon evaluation of the Euler-Lagrange equation associated with this functional, we find that the force density $\bar{\mathbf{L}}$ that gives the resulting acceleration field is

$$\bar{\mathbf{L}}_{\mathbf{u}}(\mathbf{x}) = \mathbf{L}_{\mathbf{u}}(\mathbf{x}) - \int_{\mathcal{R}} (P(\mathbf{x}') + P(\mathbf{x})) j(|\boldsymbol{\xi}|) \frac{\boldsymbol{\xi} + \boldsymbol{\eta}}{|\boldsymbol{\xi} + \boldsymbol{\eta}|} dV' \quad \forall \mathbf{x} \in \mathcal{R}. \quad (122)$$

where

$$P(\mathbf{x}) = -\frac{de}{d\vartheta}(\vartheta(\mathbf{x})) \quad \forall \mathbf{x} \in \mathcal{R}. \quad (123)$$

Here, P is something like the hydrostatic pressure in the conventional theory, and the integral in (122) is something like the gradient of hydrostatic pressure. It is easily shown that the admissibility conditions (6) and (7) are satisfied by the force density $\bar{\mathbf{L}}_{\mathbf{u}}$ defined in (122).

Linearization about an unstressed reference configuration alters (120), (123), and (122) as follows. If \mathbf{x} is any point in \mathcal{R} sufficiently far from the boundary,

$$\vartheta(\mathbf{x}) = \int_{\mathcal{R}} j(|\boldsymbol{\xi}|) \frac{\boldsymbol{\xi} \cdot \boldsymbol{\eta}}{|\boldsymbol{\xi}|} dV' + 1, \quad (124)$$

$$P(\mathbf{x}) = \zeta(\vartheta(\mathbf{x}) - 1), \quad \zeta = \frac{dP}{d\vartheta}(1) \quad (125)$$

$$\bar{\mathbf{L}}_{\mathbf{u}}(\mathbf{x}) = \mathbf{L}_{\mathbf{u}}(\mathbf{x}) - \int_{\mathcal{R}} (P(\mathbf{x}') + P(\mathbf{x})) j(|\boldsymbol{\xi}|) \frac{\boldsymbol{\xi}}{|\boldsymbol{\xi}|} dV'. \quad (126)$$

The form of (124) shows that $\vartheta = 1$ in simple shear. By computing the areal force density on any plane in a body undergoing isotropic expansion, using a

method similar to that leading up to (95), the bulk and shear moduli in the generalized system are found to be

$$\bar{k} = \frac{5\Lambda + \zeta}{9}, \quad \bar{\mu} = \frac{\Lambda}{3}. \quad (127)$$

So \bar{k} can take on any value in the generalized system of equations, while $\bar{\mu}$ is unchanged by the generalization. The modified Poisson's ratio, making use of the standard relations between the elastic moduli, is

$$\bar{\nu} = \frac{1}{2} \left(\frac{3\bar{k} - 2\bar{\mu}}{3\bar{k} + \bar{\mu}} \right) = \frac{1}{4} \left(\frac{\Lambda + \zeta/3}{\Lambda + \zeta/6} \right). \quad (128)$$

where Λ is given by (93). From (128), evidently $\Lambda = 0 \Rightarrow \nu = 1/2$. Suitable choices of Λ and ζ can be found that yield an arbitrary value of ν using (128). Presumably, material stability considerations would limit the admissible range of ζ and possibly place restrictions on j , but this has not been pursued.

So, the generalization has retained the property of not using partial derivatives in space, but the some of the simplicity of the pairwise force method has been lost.

16 Summary

We have shown that the peridynamic approach allows discontinuities of various types to be modeled without the use of special mathematical techniques at the points where the discontinuities occur. This has a potential advantage for solving practical problems in which these discontinuities form spontaneously or grow along trajectories not known in advance.

It was shown that this theory makes contact with the conventional theory of elasticity in the following ways. First, a legitimate strain energy density for purposes of the conventional theory of elasticity may be derived from a known pairwise potential function in the peridynamic theory. Second, upon linearization, the peridynamic approach yields "large scale" behavior consistent with that predicted by the conventional linear theory. Third, linear elastic waves with large wavelengths are identical between the peridynamic and conventional theories.

On the other hand, the peridynamic theory predicts different "small scale" behavior than the conventional theory. This is shown by the nonlinearities in the predicted dispersion curves. In contrast, the conventional linear theory of elasticity predicts linear dispersion curves regardless of wavelength. The nonlinear dispersion curves are similar to those found in real materials and provide a possible means of evaluating, or at least approximating, the constitutive function F . A given material in the conventional theory may have multiple peridynamic materials that agree with it in the large-scale limit but differ from each other in small-scale behavior. These differences may include different material stability properties. This suggests that a properly formulated function F in the peridynamic theory may contain "more information" about material behavior than can be expressed in conventional constitutive models.

Long-range forces, which are thought to be important in thin film mechanics and many other applications can be included in a natural way in the peridynamic approach. The generalization discussed in the previous section provides a way to get around the restriction $\nu = 1/4$, although there appear to be many interesting phenomena that can be modeled without this enhancement.

There is a parallel between the present theory and molecular dynamics (MD) computations, since in both approaches, the motion of any particle is found by a process of summation of forces due to neighboring particles. However, there are important differences as well. First, the peridynamic approach is a continuum theory. This means that individual atoms need not be modeled, and that a true, physically correct, interatomic potential need not be known. Second, in MD, interaction between particles is analogous to the structureless interactions described in Section 5, because particles in MD have no memory of their position in any reference configuration. There is no analogue in MD to materials that are not structureless.

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