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## An extended constitutive correspondence formulation of peridynamics based on nonlinear bond-strain measures

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#### Abstract

An extension of the constitutive correspondence framework of peridynamics is proposed. The main motivation is to address unphysical deformation modes which are shown to be permitted in the original constitutive formulation. The specific problem of matter interpenetration observed in numerical discretizations of peridynamics has usually been treated by adding short-range forces between neighboring particles in the discretization. Here, we propose a solution that is rooted directly within the nonlocal theory. The basic approach is to introduce generalized nonlocal peridynamic strain tensors based on corresponding bondlevel Seth-Hill strain measures which inherently avoid violations of the matter interpenetration constraint. Several analytic examples are used to show that the modified theory avoids issues of matter interpenetration in cases where the original theory fails. The resulting extended constitutive correspondence framework supports general classic constitutive laws as originally intended and is also shown to be ordinary.

Keywords: peridynamics, extended constitutive correspondence, nonlinear strain measures, matter interpenetration

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#### 1. Introduction

Peridynamics is a nonlocal continuum theory of solid mechanics based on integral equations, originally proposed to address elasticity problems involving discontinuities and long-range forces [1]. A key feature of peridynamics is the ability to naturally describe discontinuities such as cracks [2, 3, 4, 5, 6, 7] and phase transition boundaries [8] within a single continuum framework. This is in contrast to classical theories of continua which require additional constraints across surfaces of discontinuity. Peridynamics has been used in a variety of problems in continuum mechanics including: membrane and fiber models [2], phase transitions [8], inter-granular fracture [4], meso-scale modeling of material response [4], and heat transfer [9].

The most promising peridynamic theory appears to be the so-called statebased peridynamic formulation [10, 11], which makes it possible to incorporate very general material models. Within the state-based formulation, a distinction is made between ordinary and non-ordinary peridynamics constitutive models, where ordinary materials are defined by the restriction that bond forces always act in a direction parallel to the bond. Non-ordinary formulations allow for far more general constitutive responses [12]. In particular, the constitutive correspondence formulation t [10, 13] is a subset of non-ordinary formulations aimed at incorporating classical nonlinear constitutive models using the nonlocal approximation to the deformation gradient tensor  $\overline{F}$ . For example, state-based formulations of viscoplasticity models [13] and ductile damage models for metals [14, 15] have recently been proposed and effectively used in simulations based on particle discretizations. In principle, general constitutive laws can be formulated based on nonlocal versions of classical nonlinear tensor strain measures directly computed from this nonlocal  $\overline{F}$ . However, it will be shown below that the nonlocal deformation gradient allows for modes of deformation which are physically impossible and yet undetectable by the theory irrespective of the chosen strain measure.

The issue of unphysical deformation modes leading to matter interpenetration has been observed in numerical simulations of peridynamics based on particle discretizations, [3, 5]. In those references, matter interpenetration was effectively handled by the use of so-called short-range forces. From a theoretical point of view, short-range forces in peridynamics are justified in situations involving true short-range interactions (e.g. to describe contact mechanics). However, it can be argued that the addition of short range forces to avoid matter interpenetration constitutes a numerical artifact not easily justified in the theory of peridynamics, which is an essentially nonlocal theory predicated on the fundamental role of long-range interactions. In addition, it can be presumed that effective elimination of matter interpenetration in numerical simulations requires ad hoc tuning of the short-range force intensity to the specific problem at hand. It is therefore desirable to find a solution to the problem of matter interpenetration that is rooted directly within the nonlocal theory. It is this specific issue that this paper attempts to address.

Toward this end, we propose an extended constitutive correspondence formulation of peridynamics which addresses this fundamental issue and generalizes the constitutive framework to models expressed in terms of generalized strain tensors and their work-conjugate stresses. Towards this end, we introduce nonlinear measures of bond elongation which are inherently singular when the matter interpenetration constraint is violated and, thus, avoid unphysical deformations. The extended constitutive correspondence formulation is then expressed in terms of generalized nonlocal Seth-Hill strain tensors [16, 17] which are based on the bond-level strain measures and which are shown to be exact in the uniform infinitesimal limit. Importantly, it is also shown that the extended constitutive correspondence framework is ordinary and supports general inelastic and anisotropic materials models.

We start by reviewing the state-based formulation of peridynamics, and the constitutive frameworks for ordinary peridynamic materials and constitutive correspondence in Section 2. In Section 3 we show by way of example the kinematic deficiency present in the original correspondence formulation. Section 4 is devoted to the new peridynamic bond-strain measures, the corresponding family of nonlocal strain tensors and their properties, including a demonstration that the new formulation fixes the violation of the matter interpenetration constraint in cases where the original version fails. In Section 5, the extended constitutive correspondence formulation is then stated and shown to be ordinary. We conclude the presentation with a brief summary in Section 6.

#### 2. Review of state-based peridynamics

For completeness, we briefly review the state-based peridynamics formulation, primarily following the notation and approach in [10, 11]. State-based peridynamics is a nonlocal continuum theory which describes the dynamics of a continuum body which occupies the region  $\mathcal{B}_0 \subset \mathbb{R}^3$  in the reference configuration at time  $t = 0$  and the region  $\mathcal{B}_t \subset \mathbb{R}^3$  at time t.

Consider material points in the reference configuration  $\mathbf{x}, \mathbf{x}' \in \mathcal{B}_0$ . From the perspective of point  $x$ , the bond to  $x'$  is the vector

$$
\pmb{\xi}:=\mathbf{x}'-\mathbf{x}.
$$

Under the deformation mapping  $\varphi : \mathcal{B}_0 \to \mathcal{B}_t$ , points x and x' map to  $y = \varphi(x)$ and  $\mathbf{y}' = \boldsymbol{\varphi}(\mathbf{x}')$  respectively. Following the definition from [11], a family H at



Figure 1: Schematic representation of a body  $\mathcal{B}_0$  and the family  $\mathcal{H}(\mathbf{x})$  under the mapping  $\varphi$ .

x is given by

$$
\mathcal{H}(\mathbf{x}) := \left\{ \boldsymbol{\xi} \in \mathbb{R}^3 \mid (\boldsymbol{\xi} + \mathbf{x}) \in \mathcal{B}_0, \ |\boldsymbol{\xi}| < \delta \right\},
$$

where  $\delta$  provides an intrinsic length scale in the formulation. A schematic of a peridynamic body and the family at x is depicted in Figure 1.

The state-based theory of peridynamics is formulated in terms of mathematical objects called peridynamics states which are used to express peridynamic constitutive relations and peridynamic equations of motion in a compact notation. In peridynamic theories they play a role which is analogous to tensors in classical continuum theories [11]. A peridynamic vector-state  $\mathbf{A}[\mathbf{x}] \in \mathcal{V}^3(\mathbf{x})$  at a point  $\mathbf{x} \in \mathcal{B}_0$  is a function

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

where  $\mathcal{V}^3(\mathbf{x}) := \mathcal{H}(\mathbf{x}) \times \mathbb{R}^3$  is the space of vector-states at **x**. Similarly, a peridynamic scalar-state  $\underline{a}[\mathbf{x}] \in \mathcal{V}^1(\mathbf{x})$  is a function

$$
\underline{a}[\mathbf{x}] \langle \cdot \rangle : \mathcal{H}(\mathbf{x}) \to \mathbb{R},
$$

where  $V^1(\mathbf{x}) := \mathcal{H}(\mathbf{x}) \times \mathbb{R}$  is the space of scalar-states. Peridynamic vectorstates are denoted in this paper using bold type-faced capital letters with an underscore, while scalar-states are denoted using lowercase letters with an underscore.

Following the standard peridynamic conventions [10, 11], we use square brackets to indicate the field dependence over space  $x$  and time  $t$ , angle brackets to express dependence on the bonds  $\xi \in \mathcal{H}(\mathbf{x})$ , and parentheses to express dependence on other variables and vector-states. We will often suppress the field dependence on  $x$  and  $t$  to simplify notation when there are no ambiguities. For a functional

$$
f(\mathbf{\underline{A}}): \mathcal{V}^d \to \mathbb{R},
$$

with  $d = 1$  or 3, we denote its Frechét derivative with respect to the vector-state  $\underline{\mathbf{A}}$  by  $f_{, \underline{\mathbf{A}}}$ . We refer the reader to [11] for a definition of the Frechét derivative used in this context, noting that our notation differs slightly in that we add a comma before the sub-scripted vector-state to avoid potential ambiguities. Note that the Frechét derivative of a functional of a vector-state is itself a vector-state [11].

An important example of a vector-state is the deformation vector-state  $\underline{\mathbf{Y}}[\mathbf{x}] \in \mathcal{V}^3(\mathbf{x})$ , which is defined as

$$
\underline{\mathbf{Y}}\left[\mathbf{x}\right]\langle \boldsymbol{\xi}\rangle := \mathbf{y}' - \mathbf{y} = \boldsymbol{\varphi}(\mathbf{x} + \boldsymbol{\xi}) - \boldsymbol{\varphi}(\mathbf{x}), \quad \forall \boldsymbol{\xi} \in \mathcal{H}(\mathbf{x}).
$$

The deformation vector-state assigns every bond to its deformed image (see Figure 1) and is the primary deformation measure in peridynamics. A critical, physically motivated, kinematic constraint in continuum mechanics is that distinct material points in the reference configuration remain distinct in the deformed configuration, or, in other words, the deformation mapping must be one-to-one. In classical continuum mechanics, a necessary condition for this constraint is

$$
\det(\mathbf{F}) > 0,\tag{1}
$$

which ensures that the material density remains positive and finite, and, in turn, that the material can not fully collapse or invert to obtain negative volume. In peridynamics the one-to-one condition can be expressed directly in terms of the deformation vector-state [10, 11]:

$$
\underline{\mathbf{Y}}\left[\mathbf{x}\right]\langle\xi\rangle \neq \mathbf{0}, \ \ \forall \xi \neq \mathbf{0} \in \mathcal{H}(\mathbf{x}), \ \ \forall \mathbf{x} \in \mathcal{B}_0. \tag{2}
$$

The peridynamic equations of motion are written in terms of the force vectorstate  $\underline{\mathbf{T}}$ , where  $\underline{\mathbf{T}}\langle \xi \rangle$  is a bond-force with units of force per unit volume-squared acting between nearby materials points. In peridynamics, the force vector-state plays an analogous role to the stress tensor in classical continuum theories. The peridynamic equations of motion [10] are

$$
\rho_0(\mathbf{x})\ddot{\mathbf{y}}(\mathbf{x}) = \int_{\mathcal{H}(\mathbf{x})} \underline{\mathbf{T}}\langle \boldsymbol{\xi} \rangle - \underline{\mathbf{T}}'\langle \boldsymbol{\xi}' \rangle \, d\boldsymbol{\xi} + \mathbf{b}(\mathbf{x}), \quad \forall \mathbf{x} \in \mathcal{B}_0,\tag{3}
$$

where  $\mathbf{T}'\langle \xi' \rangle := \mathbf{T}[\mathbf{x}'] \langle -\xi \rangle$ , **b** is an externally applied body force, and  $\rho_0$  is the reference material density. This equation expresses conservation of linear momentum. Angular momentum is conserved provided that the material is non-polar and the following constitutive condition holds [10]:

$$
\int_{\mathcal{H}(\mathbf{x})} \underline{\mathbf{T}}\langle \xi \rangle \times \underline{\mathbf{Y}}\langle \xi \rangle \, d\xi = \mathbf{0}, \quad \forall \mathbf{x} \in \mathcal{B}_0.
$$
\n(4)

When formulating new concepts in peridynamics, it is often helpful to focus on the similarities with classical continuum mechanics. Table 2 shows some



of the analogies between the two theories, where  $\hat{\psi}(\mathbf{F})$  is the classical elastic energy density function,  $\nabla$  is the standard gradient operator, and  $\bar{\psi}(\underline{Y})$  is the peridynamic elastic energy density functional.

A standard constitutive assumption of state-based peridynamics is that the force vector-state is given by a constitutive law  $\overline{\mathbf{T}}$  of the form:

$$
\underline{\mathbf{T}}=\underline{\bar{\mathbf{T}}}\left(\underline{\mathbf{Y}},\dot{\underline{\mathbf{Y}}},\underline{\mathbf{q}},\mathbf{q}\right),
$$

where  ${\bf q}$  are internal field variables such as temperature or damage, and  ${\bf \underline q}$  are internal vector-state field variables. We proceed with a brief review of the two primary constitutive modeling frameworks for state-based peridynamics, namely ordinary peridynamic materials and constitutive correspondence.

#### 2.1. Ordinary peridynamic materials

A peridynamic model  $\bar{\mathbf{T}}$  is said to be *ordinary* [10] if, for all  $\underline{\mathbf{Y}} \in \mathcal{V}^3$ ,

$$
\bar{\underline{\mathbf{T}}}\langle \xi \rangle \times \underline{\mathbf{Y}}\langle \xi \rangle = 0, \, \forall \, \xi \in \mathcal{H}.
$$

This condition simply states that the force vector-state must be parallel to the deformation vector-state, automatically ensuring that the angular momentum constraint (4) is satisfied. For elastic materials, this condition is equivalent to requiring the elastic energy to depend only on the magnitude of the relative deformation between neighboring materials points (not on angles between deformed material points, for example). While this imposes an added restriction on possible constitutive models, ordinary peridynamic materials have been shown to be capable of modeling nonlocal isotropic elasticity [10], as well as nonlocal isotropic plasticity [18].

#### 2.2. Constitutive correspondence

The other general approach for formulating material models in state-based peridynamics is based on the so-called constitutive correspondence concept. A peridynamic material model is said to correspond to a classical material model when the strain energy density of both the classical and peridynamic material are equal under affine deformations. For this purpose an approximate nonlocal deformation gradient  $\bar{\mathbf{F}} \in \mathbb{R}^3 \times \mathbb{R}^3$  was introduced [10]:

$$
\bar{\mathbf{F}}\left(\underline{\mathbf{Y}}\right) := \left[ \int_{\mathcal{H}} \underline{\omega} \langle \xi \rangle \left( \underline{\mathbf{Y}} \langle \xi \rangle \otimes \xi \right) d\xi \right] \bar{\mathbf{K}}^{-1},\tag{5}
$$

where  $\underline{\omega}$  is a positive influence scalar-state which for simplicity will be assumed spherical throughout the paper, i.e.

$$
\underline{\omega}\langle \xi \rangle = \omega(|\xi|) > 0, \quad \forall \xi \in \mathcal{H},\tag{6}
$$

for a scalar influence function  $\omega$ , and the nonlocal shape tensor  $\bar{\mathbf{K}} \in \mathbb{R}^3 \times \mathbb{R}^3$  is

$$
\bar{\mathbf{K}}:=\int_{\mathcal{H}}\underline{\omega}\langle\xi\rangle\left(\boldsymbol{\xi}\otimes\boldsymbol{\xi}\right)d\boldsymbol{\xi}.
$$

It has been shown that the nonlocal deformation gradient obtained in this way is identical to the classical deformation gradient (i.e., the continuous gradient of the deformation mapping,  $\bf{F}$ ) for affine deformations [10]. It can be seen from equation (5) that the constitutive correspondence form of  $\overline{F}$  provides a description of deformation near a point x which is based on a weighted average of the deformation of all the neighboring bonds.

The resulting force vector-state for constitutive correspondence is

$$
\underline{\mathbf{T}}\langle \pmb{\xi}\rangle=\underline{\omega}\langle \pmb{\xi}\rangle\,\bar{\mathbf{P}}\bar{\mathbf{K}}^{-1}\pmb{\xi},
$$

where  $\bar{\mathbf{P}} = \hat{\mathbf{P}}(\bar{\mathbf{F}})$  is the first Piola-Kirchhoff stress tensor obtained from a classical constitutive law  $\hat{\mathbf{P}}$  as a function of the nonlocal deformation gradient. This form of the force vector-state leads to a peridynamic formulation which conserves angular momentum provided that the classical constitutive model used is one which ensures conservation of angular momentum and is non-polar. This is the case if the resulting Cauchy stress  $\bar{\sigma}$  is symmetric, i.e.,

$$
\bar{\boldsymbol{\sigma}} = \bar{J}^{-1} \bar{\mathbf{P}} \bar{\mathbf{F}}^T = \bar{\boldsymbol{\sigma}}^T, \quad \bar{J} = \det \bar{\mathbf{F}}.
$$

#### 3. Limitation in the kinematics of constitutive correspondence

In this section we investigate a basic fundamental limitation of the kinematic assumption of the constitutive correspondence formulation. Specifically, we demonstrate using several examples how unphysical deformation modes may be undetectable by the nonlocal deformation gradient  $\overline{\mathbf{F}}$ .

1. Sub-horizon material collapse: Consider the extreme situation depicted in Figure 2 where a small volume of material  $\mathcal{G} \subset \mathcal{B}_0$  collapses to a single point  $z \in \mathcal{B}_t$ . The peridynamic deformation vector-state in this

case is  $Y[\mathbf{x}]\langle \xi \rangle = 0$  for  $\mathbf{x}, \mathbf{x}' \in \mathcal{G}$ , where  $\mathbf{x}' = \mathbf{x} + \xi$ . This deformation is clearly unphysical as it violates the matter interpenetration constraint (2).



Figure 2: Schematic showing a region  $\mathcal{G} \subset \mathcal{B}_0$  collapsing to a single point  $\mathbf{z} \in \mathcal{B}_t$ .

However, it is easy to see that the nonlocal deformation gradient  $F(x)$ remains positive-definite at a point **x** whose horizon  $\mathcal{H}(\mathbf{x})$  contains the collapsed region G, i.e.  $\mathcal{G} \subset \mathcal{H}(\mathbf{x})$ . In other words,  $\overline{\mathbf{F}}$  is unable to detect this localized unphysical deformation, because violating the kinematic constraint (2) on the bond-level does not imply that the resulting nonlocal deformation gradient violates the tensor-level kinematic constraint (1).

2. Jump discontinuities in 1D: Another example consists of a displacement jump discontinuity with a displacement field of  $y(x) = a + x$  for  $x > 0$  and  $y(x) = x$  for  $x < 0$ . A schematic showing the nature of this discontinuity for the 2D case<sup>1</sup> is shown in Figure 3 for  $a > 0$  on the left (which is physically acceptable), and  $a < 0$  on the right (which is physically impossible). For the opening displacement case,  $a > 0$ , the nonlocal scalar deformation gradient  $\overline{F}(x)$  obtained from the 1D version of equa-

<sup>&</sup>lt;sup>1</sup>Even though the analysis here is conducted in 1D, we depict the 2D case in Figure 3 as it is more visually illustrative of the physical issues involved.



Figure 3: Schematic of surface discontinuities, with both an opening deformation discontinuity (left) and an interpenetrating deformation discontinuity (right).

tion (5) satisfies the classical kinematic constraint (1), with  $\bar{F}(x) > 1$  for  $|x| < \delta$ . This means opening jump displacements are kinematically admissible deformation modes for the constitutive correspondence formulation, as desired.

However, a value of  $a < 0$  which corresponds to unphysical interpenetration (and violates the peridynamic kinematic constraint (2)) results in  $\bar{F} > 0$  for  $|a| \ll \delta$ . In other words, the constitutive correspondence formulation admits deformations that are physically inadmissible.

This example highlights an important consideration when formulating peridynamic models: whereas one of the basic premises of peridynamics is that it contemplates the presence of discontinuities in a natural way, it actually goes too far and allows for discontinuities that are unphysical. Based on this consideration we argue that in any valid peridynamic formulation suitable for finite deformations, discontinuities leading to matter interpenetration should be kinematically inadmissible. We have therefore shown that constitutive correspondence, as currently formulated, does not satisfy this requirement.

3. Zero-energy modes in 1D: In this example we demonstrate the presence of zero-energy modes<sup>2</sup> in the constitutive correspondence formulation. Consider the 1D case and an influence function of the form  $\omega(|x'-x|) =$  $|x'-x|^{-1}$  for  $|x'-x| < \delta$ . By equation (5) this influence function results in a nonlocal scalar deformation gradient given by:

$$
\bar{F}(x) = \frac{1}{\delta^2} \int_{x-\delta}^{x+\delta} \text{sign}(x'-x)(y(x') - y(x)) dx'\n= \frac{1}{\delta^2} \int_{x}^{x+\delta} y(x') - y(x) dx' - \frac{1}{\delta^2} \int_{x-\delta}^{x} y(x') - y(x) dx'\n= \frac{1}{\delta^2} \int_{x}^{x+\delta} y(x') dx' - \frac{1}{\delta^2} \int_{x-\delta}^{x} y(x') dx'.
$$

For deformations of the form  $y(x) = x + a \sin(2\pi kx/\delta + \phi)$ , the corresponding deformation gradient is

$$
\bar{F}(x) = \frac{1}{\delta^2} \int_x^{x+\delta} x' + a \sin(2\pi kx'/\delta + \phi) dx'
$$

$$
- \frac{1}{\delta^2} \int_{x-\delta}^x x' + a \sin(2\pi kx'/\delta + \phi) dx'
$$

$$
= \frac{2}{\delta^2} \int_x^{x+\delta} x' dx' = 1,
$$

for any integer  $k > 0$  and all  $a, \phi \in \mathbb{R}$ . In other words, there exist periodic deformation mappings for which the nonlocal deformation measure  $\bar{F}$  is unable to describe the state of deformation of the material and, thus, they do not contribute to the elastic energy of the material irrespective of the

<sup>&</sup>lt;sup>2</sup>It should be emphasized that here we refer to zero-energy modes that exist in the mathematical formulation of the peridynamics correspondence theory, which should not be confused with those appearing in numerical discretizations. We point out that the issue of zero-energy modes has been observed in numerical discretizations of peridynamics and can be alleviated using numerical stabilization techniques [19].

constitutive model.

4. Vanishing-energy modes in 1D: A related example demonstrates how more general influence functions allow for the existence of deformation modes with vanishing energy in the short wavelength limit. Consider influence functions  $\omega$  which satisfy

$$
\int_{\mathcal{H}} \left| \frac{d}{d\xi} \left( \xi \, \omega(|\xi|) \right) \right| \, d\xi < \infty. \tag{7}
$$

A deformation of  $y(x) = x + a \sin \left( \frac{2\pi kx}{s} \right)$ δ results in

$$
\bar{F}(x) = \frac{1}{\bar{K}(x)} \int_{\mathcal{H}} \omega(|\xi|) \left[ y(x + \xi) - y(x) \right] \xi \, d\xi
$$
\n
$$
= 1 + \frac{a}{\bar{K}} \int_{\mathcal{H}} \xi \, \omega(|\xi|) \sin\left(\frac{2\pi k(x + \xi)}{\delta}\right) \, d\xi - \frac{a}{\bar{K}} \int_{\mathcal{H}} \xi \, \omega(|\xi|) \sin\left(\frac{2\pi kx}{\delta}\right) \, d\xi
$$
\n
$$
= 1 + \frac{a}{\bar{K}} \int_{\mathcal{H}} \xi \, \omega(|\xi|) \cos\left(\frac{2\pi kx}{\delta}\right) \sin\left(\frac{2\pi k\xi}{\delta}\right) \, d\xi
$$
\n
$$
+ \frac{a}{\bar{K}} \int_{\mathcal{H}} \xi \, \omega(|\xi|) \cos\left(\frac{2\pi k\xi}{\delta}\right) \sin\left(\frac{2\pi kx}{\delta}\right) \, d\xi
$$
\n
$$
= 1 + \frac{\delta \, a \cos\left(\frac{2\pi kx}{\delta}\right)}{2\pi k \bar{K}} \int_{\mathcal{H}} \frac{d}{d\xi} \left(\xi \, \omega(|\xi|)\right) \cos\left(\frac{2\pi k\xi}{\delta}\right) \, d\xi,
$$

where we've used standard trigonometric identities, the fact that  $\omega$  is an even function and the last step results from an integration by parts using  $\omega=0$  on  $\partial\mathcal{H}.$  Taking the limit of vanishingly-small wavelengths by increasing  $k$  for fixed oscillation amplitude,  $a$ , gives

$$
\lim_{k \to \infty} \left| \frac{a}{k} \int_{\mathcal{H}} \frac{d}{d\xi} \left( \xi \, \omega(|\xi|) \right) \cos \left( \frac{2\pi k \, \xi}{\delta} \right) \, d\xi \right| \leq \lim_{k \to \infty} \frac{|a|}{k} \int_{\mathcal{H}} \left| \frac{d}{d\xi} \left( \xi \, \omega(|\xi|) \right) \right| \, d\xi = 0,
$$

and we find:  $\lim_{k \to \infty} \bar{F}(x) = 1$ .

This shows that for sufficiently well behaved influence functions, equation (7), rapidly oscillating displacement fields contribute negligibly to the nonlocal deformation gradient  $\overline{F}$ . It should be noted that this example also embodies the case of local matter interpenetration for large values of the amplitude a.

This example has important implications for numerical discretizations of the constitutive correspondence formulation: for a fixed peridynamic horizon size, as the discretization is refined such that high-frequency oscillations become increasingly resolved within the horizon, additional zeroenergy modes emerge, which inevitably leads to instability.

As is known, [19], numerical implementations of peridynamic correspondence formulations are mired with instabilities commonly attributed to artifacts in particle-based discretizations of continuum mechanics [22, 23]. This example demonstrates that even when the numerical issues are properly addressed, more fundamental instabilities of a theoretical nature remain in the peridynamic correspondence formulation as currently stated. We also mention that an alternative interpretation of this result is that the length scale in the dynamics of interest sets an upper bound on the choice of peridynamic horizon size. This is because physical responses with characteristic length scales significantly smaller than the horizon size may be undetectable by the constitutive correspondence deformation measure  $\overline{F}$ . We also want to point out that this issue may be related to previous observations in the bond-based theory of peridynamics, where it was found that the choice of influence function critically affects the dispersion behavior of linear waves [20, 21].

#### 4. Peridynamic bond-strain measures

In the previous section, we concluded that in the existing constitutive correspondence framework unphysical deformations may result in a kinematically admissible  $\bf{F}$ . In other words, violating the kinematic constraint (2) on the bond-level does not imply that the resulting nonlocal deformation gradient violates the tensor-level kinematic constraint (1), i.e.

$$
\underline{\mathbf{Y}}[\mathbf{x}]\langle \xi \rangle = \mathbf{0} \text{ for some } \xi \in \mathcal{H}(\mathbf{x}) \implies \det(\overline{\mathbf{F}}(\mathbf{x})) \leq 0.
$$

The source of this limitation is that  $\bar{F}$  averages the material deformation over the horizon in such a way that localized misbehavior may contribute negligibly or be compensated for elsewhere in the integral. In order to fix this issue, we propose a nonlocal measure of strain which is sensitive to any violation of the bond-level kinematic constraint (2). To achieve this, we introduce strain measures on a bond-by-bond basis which have the appropriate kinematic behavior in the fully compressed limit.

We propose a family of bond-strain measures inspired by the Seth-Hill<sup>3</sup> strain measures  $[16, 17]$ :

$$
\underline{\varepsilon}_{(m)}\langle \xi \rangle := \frac{1}{2m} \left[ \underline{c} \langle \xi \rangle^m - 1 \right],\tag{8}
$$

where we have defined  $\underline{\varepsilon}$  as the strain scalar-state and

$$
\underline{c}\langle \boldsymbol{\xi}\rangle := \frac{\boldsymbol{\underline{Y}}\langle \boldsymbol{\xi}\rangle\cdot \boldsymbol{\underline{Y}}\langle \boldsymbol{\xi}\rangle}{\boldsymbol{\xi}\cdot \boldsymbol{\xi}},
$$

as the Cauchy-Green deformation scalar-state which measures the bond elonga-

<sup>&</sup>lt;sup>3</sup>Recall the classical Seth-Hill strain tensors,  $\mathbf{E}_{(m)} = \frac{1}{2m} (\mathbf{C}^m - \mathbf{1})$ , and right Cauchy-Green deformation tensor  $\mathbf{C} = \mathbf{F}^T \mathbf{F}$ .

tion.

For the degenerate case  $m = 0$ , we obtain:

$$
\underline{\varepsilon}_{(0)}\langle \xi \rangle := \frac{1}{2}\log(\underline{c}\langle \xi \rangle),
$$

which we define as the logarithmic (also Hencky or true) strain scalar-state. For infinitesimal bond strains all of these measures reduce to the same scalar-state. For  $m \leq 0$ , these strain measures have the proper kinematic behavior in the fully compressed limit, i.e.

$$
\underline{\mathbf{Y}}\langle \xi \rangle \to 0 \implies \underline{\varepsilon}_{(m)}\langle \xi \rangle \to -\infty.
$$

As a result, these bond-strain measures for  $m \leq 0$  naturally allow for the enforcement of non-interpenetration (2) on a bond-by-bond basis. This is in contrast to constitutive correspondence, which only allows for an averaged enforcement of the tensorial kinematic constraint (1).

#### 4.1. Nonlocal peridynamic strain tensor

In order to use established constitutive models formulated in terms of a strain tensor, it is convenient to formulate a tensorial measure of the nonlocal strain. This is accomplished by defining a nonlocal peridynamic strain tensor  $\bar{\mathbf{E}}_{(m)} \in \mathbb{R}^3 \times \mathbb{R}^3$  parametrized by m as

$$
\bar{\mathbf{E}}_{(m)} := \int_{\mathcal{H}} \underline{\omega} \langle \xi \rangle \underline{\varepsilon}_{(m)} \langle \xi \rangle \underline{\mathbf{H}} \langle \xi \rangle d\xi, \tag{9}
$$

where we define the shape tensor-state  $\mathbf{H} \in \mathcal{H} \times \mathbb{R}^3 \times \mathbb{R}^3$  by

$$
\underline{\mathbf{H}}\langle \xi \rangle := \frac{5}{2} \frac{\xi \otimes \xi}{\xi \cdot \xi} - \frac{1}{2} \mathbf{1},\tag{10}
$$

and without loss of generality we normalize the influence function in 3D as follows:

$$
\int_{\mathcal{H}} \underline{\omega} \langle \xi \rangle d\xi = 3. \tag{11}
$$

### 4.2. Properties of the family of nonlocal strain tensors  $\bar{\mathbf{E}}_{(m)}$

1. Correspondence for infinitesimal strains: The specific forms of (10) and (11) ensure that the nonlocal strain tensor  $\bar{\mathbf{E}}_{(m)}$  reduces to the classical value for infinitesimal uniform strains. This can be shown as follows. Start by noting that in this case  $\epsilon_{(m)}\langle \xi \rangle = \epsilon_{ij} \xi_i \xi_j / |\xi|^2$  for any m. Here we drop the *m* subscript, as in this limit the strain measures are all identical. Using index notation and the summation convention, the nonlocal strain tensor for uniform infinitesimal strains is

$$
\bar{E}_{ij} = \mathcal{I}_{ijkl} \,\epsilon_{kl} - \mathcal{J}_{kl} \,\epsilon_{kl} \,\delta_{ij},
$$

where

$$
\mathcal{I}_{ijkl} := \frac{5}{2} \int_{\mathcal{H}} \underline{\omega} \langle \xi \rangle \, \frac{\xi_i \xi_j \xi_k \xi_l}{|\xi|^4} \, d\xi \text{ and } \mathcal{J}_{kl} := \frac{1}{2} \int_{\mathcal{H}} \underline{\omega} \langle \xi \rangle \, \frac{\xi_k \xi_l}{|\xi|^2} \, d\xi.
$$

These integrals can be computed analytically using symmetry arguments and by transforming to spherical coordinates, as in [10]. It follows from the symmetry of the influence function (6) that terms like  $\mathcal{I}_{1112}$ ,  $\mathcal{I}_{1233}$  and  $\mathcal{J}_{12}$ , where any index appears an odd number of times, are zero. Also by symmetry,  $\mathcal{I}_{1122} = \mathcal{I}_{1221} = \mathcal{I}_{2233}$ ,  $\mathcal{I}_{1111} = \mathcal{I}_{2222}$ ,  $\mathcal{J}_{11} = \mathcal{J}_{22}$ , etc. To compute the nonzero terms of  $J$ , note that

$$
\mathcal{J}_{ii} = \frac{1}{2} \int_{\mathcal{H}} \underline{\omega} \langle \xi \rangle \, \frac{\xi_i \xi_i}{|\xi|^2} \, d\xi = \frac{1}{2} \int_{\mathcal{H}} \underline{\omega} \langle \xi \rangle \, d\xi = \frac{3}{2},
$$

where we have used the normalization constraint (11), and therefore

$$
\mathcal{J}_{11} = \mathcal{J}_{22} = \mathcal{J}_{33} = \frac{1}{3}\mathcal{J}_{ii} = \frac{1}{2}.
$$
 (12)

The nonzero terms of  $\mathcal I$  can be found by noting that

$$
5\,\mathcal{J}_{11} = \frac{5}{2}\int_{\mathcal{H}} \underline{\omega}\langle \xi \rangle \, \frac{\xi_1 \xi_1 |\xi|^2}{|\xi|^4} \, d\xi = \mathcal{I}_{1111} + \mathcal{I}_{1122} + \mathcal{I}_{3311},
$$

and

$$
\mathcal{I}_{3333} = \frac{5}{2} \int_0^{2\pi} \int_0^{\pi} \int_0^{\delta} \omega(r) \cos^4 \phi \sin \phi r^2 dr d\phi d\theta
$$

$$
= \left(\frac{5}{4} \int_{\mathcal{H}} \underline{\omega} \langle \xi \rangle d\xi\right) \int_0^{\pi} \cos^4 \phi \sin \phi d\phi = \frac{15}{4} \frac{2}{5},
$$

to find

$$
\mathcal{I}_{1111} = \mathcal{I}_{2222} = \mathcal{I}_{3333} = \frac{3}{2}
$$
 and  $\mathcal{I}_{1122} = \mathcal{I}_{2233} = \mathcal{I}_{3311} = \frac{1}{2}$ .

The off-diagonal terms of the nonlocal strain tensor evaluate as

$$
\bar{E}_{12} = \bar{E}_{21} = \mathcal{I}_{1212} \epsilon_{12} + \mathcal{I}_{1221} \epsilon_{21} = \frac{\epsilon_{12}}{2} + \frac{\epsilon_{21}}{2} = \epsilon_{12},
$$

and similarly for  $\bar{E}_{23}$  and  $\bar{E}_{31}$ . We find for the diagonal terms that

$$
\bar{E}_{11} = \mathcal{I}_{1111} \epsilon_{11} + \mathcal{I}_{1122} \epsilon_{22} + \mathcal{I}_{1133} \epsilon_{33} - \mathcal{J}_{11} \epsilon_{11} - \mathcal{J}_{22} \epsilon_{22} - \mathcal{J}_{33} \epsilon_{33} = \epsilon_{11},
$$

and similarly for  $\bar{E}_{22}$  and  $\bar{E}_{33}$ . We conclude that in the limit of uniform infinitesimal strains, the nonlocal strain tensor is identical to the actual (classical) strain tensor,  $\bar{\mathbf{E}} = \boldsymbol{\epsilon}$ .

#### 2. Correspondence of the nonlocal log strain tensor for pure dilata-

tion: In addition to being exact in the limit of infinitesimal strains, we show that for the case  $m = 0$ ,  $\bar{\mathbf{E}}_{(0)}$  is exactly the log strain tensor for large uniform volumetric deformations. Consider a uniform volumetric strain with deformation gradient  $\mathbf{F} = J^{\frac{1}{3}}\mathbf{R}$ , where **R** is a rotation vector,  $\mathbf{R} \mathbf{R}^T = \mathbf{R}^T \mathbf{R} = \mathbf{1}$ , and J represents the volume change between reference and deformed configurations. The actual log strain tensor  $\mathbf{E}_{(0)}$  for this deformation gradient is

$$
\mathbf{E}_{(0)} = \frac{1}{2}\log(\mathbf{F}^T\mathbf{F}) = \frac{1}{2}\log(J^{\frac{2}{3}}\mathbf{R}^T\mathbf{R}) = \frac{1}{3}\log(J)\mathbf{1}.
$$

For this case, the peridynamic deformation vector-state is:

$$
\underline{\mathbf{Y}}\langle \boldsymbol{\xi} \rangle = \mathbf{F} \boldsymbol{\xi} = J^{\frac{1}{3}} \mathbf{R} \boldsymbol{\xi},
$$

which results in the log bond-strain:

$$
\underline{\varepsilon}_{(0)}\langle \xi \rangle = \log(J^{\frac{1}{3}}) = \frac{1}{3}\log(J), \quad \forall \xi \in \mathcal{H},
$$

and the nonlocal strain tensor:

$$
\begin{aligned} \mathbf{\bar{E}}_{(0)} &= \frac{1}{3} \log(J) \int_{\mathcal{H}} \underline{\omega} \langle \xi \rangle \left( \frac{5}{2} \frac{\xi \otimes \xi}{\xi \cdot \xi} - \frac{1}{2} \mathbf{1} \right) \, d\xi \\ &= \frac{1}{3} \log(J) \left( 5 \, \mathcal{J}_{11} \mathbf{1} - \frac{3}{2} \mathbf{1} \right) \\ &= \frac{1}{3} \log(J) \mathbf{1} = \mathbf{E}_{(0)}, \end{aligned}
$$

where the integral  $\mathcal{J}_{11}$  is given by equation (12).

### 4.3. A fix to the issue of matter interpenetration

We revisit the issue of matter interpenetration and explore how the nonlocal strain tensor in equation (9) behaves for some of the examples described in Section 3.

1. Sub-horizon material collapse: Consider again Figure 2, which depicts a small finite volume of material  $\mathcal{G} \subset \mathcal{B}_0$  collapsing to a single point  $\mathbf{z} \in \mathcal{B}_t$ . For  $m \leq 0$ , it is easy to see from equation (8) that at a point  $\mathbf{x} \in \mathcal{G}$ ,  $\mathfrak{S}_{(m)}[\mathbf{x}]\langle \boldsymbol{\xi} \rangle \to -\infty$  for  $\mathbf{x} + \boldsymbol{\xi} \in \mathcal{G}$ , and therefore

$$
\mathrm{tr}\left(\bar{\mathbf{E}}_{(m)}(\mathbf{x})\right) = \int_{\mathcal{H}} \underline{\omega}\langle \boldsymbol{\xi} \rangle \underline{\varepsilon} \left[\mathbf{x}\right] \langle \boldsymbol{\xi} \rangle d\boldsymbol{\xi} \to -\infty,
$$

which follows from (9) provided that  $|\underline{\mathbf{Y}}\langle \xi \rangle| < \infty$ ,  $\forall \xi \in \mathcal{H}$ . This shows that if any finite volume  $G$  collapses to a single point, the nonlocal strain tensor  $\bar{\mathbf{E}}_{(m)}$  exhibits the expected behavior.

2. Interpenetrating jump discontinuities in 1D: In this example, we consider a displacement jump discontinuity with a deformation field of the form  $y(x) = x + a$  for  $x > 0$  and  $y(x) = x$  for  $x < 0$ . The nonlocal strain in 1D is

$$
\bar{\varepsilon}_{(m)}(x) := \int_{\mathcal{H}} \omega(|\xi|) \, \underline{\varepsilon}_{(m)}[x] \, \langle \xi \rangle \, d\xi
$$
\n
$$
= \frac{1}{2m} \int_{\mathcal{H}} \omega(|\xi|) \left[ \left( \frac{|y(x+\xi) - y(x)|}{|\xi|} \right)^{2m} - 1 \right] \, d\xi,
$$

where in 1D we constrain the influence function by  $\int_{\mathcal{H}} \omega(|\xi|) d\xi = 1$ . We consider the case  $a < 0$ ,  $|a| < \delta$ , corresponding to a small interpenetrating jump discontinuity. The nonlocal strain at a point  $x \leq 0$  for  $|x| < |a|$  is

$$
2m\,\bar{\varepsilon}_{(m)}(x) = \int_{-x}^{\delta} \omega(\xi) \left(\frac{|\xi + a|}{\xi}\right)^{2m} d\xi - \int_{-x}^{\delta} \omega(\xi) d\xi
$$

$$
= \int_{-x}^{-a} \frac{\omega(\xi)}{\xi^{2m}} \left(-\xi - a\right)^{2m} d\xi + \int_{-a}^{\delta} \frac{\omega(\xi)}{\xi^{2m}} \left(\xi + a\right)^{2m} d\xi
$$

$$
- \int_{-x}^{\delta} \omega(\xi) d\xi.
$$

This shows that for  $m < -1/2$ , matter interpenetration near surfaces of discontinuity results in an unbounded nonlocal strain scalar, at least in 1D, i.e.  $\bar{\varepsilon}_{(m)}(x) \to -\infty$  for  $-|a| < x \le 0$  and by symmetry for  $-|a| < x < |a|$ .

3. Opening jump discontinuities in 1D: In addition, we consider the case  $a > 0$ , corresponding to an opening displacement jump discontinuity as would occur in the presence of fracture. In this case, the nonlocal strain tensor at  $x\leq 0,\,|x|<\delta$  is

$$
2m\,\bar{\varepsilon}(x) = \int_{-x}^{\delta} \omega(|\xi|) \left(\frac{|\xi + a|}{\xi}\right)^{2m} - \omega(|\xi|) \, d\xi
$$
  
< 
$$
< \infty,
$$

provided that

$$
\omega(|\xi|) < C|\xi|^{2m-1}, \ \ \forall \xi \in \mathcal{H}, \text{ for some } C > 0.
$$

This example shows that for sufficiently well behaved influence functions, opening fracture-type discontinuities are allowed and result in a finite nonlocal strain scalar.

These previous examples show that use of appropriate bond-strain measures ensures that unphysical deformations are ruled out from the peridynamic theory, i.e. the nonlocal strains become undefined, as expected. This is accomplished without sacrificing the key advantage of peridynamics for problems involving physically admissible discontinuities such as those which occur during fracture.

#### 5. Constitutive models based on the nonlocal strain tensor

A straightforward approach for formulating constitutive models in terms of the proposed strain measures is based on the peridynamic correspondence

concept: the classical strain energy density function  $\hat{\psi}(\mathbf{E}_{(m)})$  as originally formulated in terms of a classical strain tensor  $\mathbf{E}_{(m)}$  must be evaluated using the corresponding nonlocal strain tensor  $\bar{\mathbf{E}}_{(m)}$ , i.e.  $\psi(\underline{\mathbf{Y}}) = \hat{\psi}(\bar{\mathbf{E}}_{(m)})$ . The workconjugate stress measure then follows as:

$$
\bar{\boldsymbol{\sigma}}_{(m)}:=\hat{\boldsymbol{\sigma}}\left(\bar{\mathbf{E}}_{(m)}\right)=\nabla\hat{\psi}\left(\bar{\mathbf{E}}_{(m)}\right).
$$

Finally, the peridynamic force vector-state follows from work conjugacy and using equations  $(8)$ ,  $(9)$  and  $(10)$  as:

$$
\underline{\mathbf{T}}_{(m)}\langle \xi \rangle = \psi, \underline{\mathbf{Y}} \langle \xi \rangle \left( \bar{\mathbf{E}}_{(m)} \right)
$$
  
\n
$$
= \nabla \hat{\psi} \left( \bar{\mathbf{E}}_{(m)} \right) : \bar{\mathbf{E}}_{(m), \underline{\mathbf{Y}}} \langle \xi \rangle
$$
  
\n
$$
= \left( \bar{\boldsymbol{\sigma}}_{(m)} : \underline{\mathbf{H}} \langle \xi \rangle \right) \underline{\omega} \langle \xi \rangle \underline{c} \langle \xi \rangle^{m-1} |\xi|^{-2} \underline{\mathbf{Y}} \langle \xi \rangle . \tag{13}
$$

It should be noted that this extended correspondence formulation generalizes to materials exhibiting anisotropy and inelasticity as long as they are formulated within an internal variable framework. Another important observation is that the resulting material models are ordinary (which can be clearly seen by noting that the force vector-state is parallel to the deformation vector-state, i.e.  $\underline{\mathbf{T}}\langle \boldsymbol{\xi} \rangle \times$  $\underline{\mathbf{Y}}\langle \xi \rangle = 0, \, \forall \xi \in \mathcal{H}),$  and therefore conserve angular momentum.

The fact that this extended correspondence formulation is ordinary (in contrast to the original, non-ordinary correspondence theory) is a direct consequence of the fact that the proposed nonlocal strain tensors  $\bf{E}$  (for any m) are ultimately formulated solely in terms of the magnitude of the deformed bond lengths  $|\underline{\mathbf{Y}}\langle \xi\rangle|$ .<sup>4</sup> A direct consequence of this restriction is that the force vector-

<sup>&</sup>lt;sup>4</sup>In the original constitutive correspondence formulation, the nonlocal deformation gradient  $\overline{\mathbf{F}}$  also depends on the direction of  $\underline{\mathbf{Y}}$ , not just its magnitude.

state takes the form:

$$
\underline{\mathbf{T}}\langle \xi \rangle = \bar{\boldsymbol{\sigma}} : \bar{\mathbf{E}}, \underline{\mathbf{v}} \langle \xi \rangle = \left( \bar{\boldsymbol{\sigma}} : \bar{\mathbf{E}}, |\underline{\mathbf{v}}| \langle \xi \rangle \right) \frac{\underline{\mathbf{Y}} \langle \xi \rangle}{|\underline{\mathbf{Y}} \langle \xi \rangle|},
$$

where the term in parentheses is a scalar, so the resulting bond-force is clearly parallel to the direction of the deformation vector-state, thereby satisfying the definition of an ordinary peridynamic material. It is also interesting to note that in this correspondence formulation only the symmetric part of the stress tensor contributes to the force vector-state. This follows from (13) and the symmetry of  $\underline{\mathbf{H}}\langle \xi \rangle$ , see equation (10).

In summary, the proposed extended constitutive correspondence formulation shares the main features of the original version: it enables the direct use of classical constitutive models and is formulated entirely in terms of integrals of deformation, so that derivatives need not exist and no special treatment is required in the presence of discontinuities. In addition, the new formulation addresses the fundamental issues discussed in Section 3: 1) it avoids unphysical deformation modes present in the original formulation by introducing generalized bond-level strain measures, and 2) the formulation is extended in the sense that constitutive models are formulated directly in terms of generalized nonlocal peridynamic strain tensors  $\bar{\mathbf{E}}_{(m)}$  and their corresponding work-conjugate stress measures.

#### 6. Conclusion

The ability to naturally handle field discontinuities has previously been put forward as a key advantage of the peridynamic theory over classical continuum theories [10, 11]. However, without careful consideration this flexibility may go too far and result in peridynamic formulations in which highly unphysical deformation modes (i.e. matter interpenetration) are allowed. Although in previous numerical simulations these issues have been effectively handled by adding short-range forces, in this work we have tackled the problem at its theoretical root, i.e. we have addressed the fundamental limitations identified in the kinematic assumptions of constitutive correspondence.

We have shown in a number of analytical examples that the *constitutive* correspondence framework of peridynamics [10] fails to enforce the kinematic invertibility constraint and thus allows for a variety of unphysical deformation modes including material collapse, matter interpenetrating surfaces of discontinuity and zero-energy modes. To overcome this limitation, the constitutive correspondence framework of peridynamics [10] has been extended to a class of constitutive models which are formulated in terms of generalized nonlocal Seth-Hill strain tensors and their work-conjugate stresses. These nonlocal strain tensors are in turn based on nonlinear bond-strain measures which enforce the kinematic constraint at the individual bond level by design. The resulting extended constitutive correspondence framework supports general classic constitutive laws as originally intended and is also shown to be ordinary. Several examples are used to show that the modified theory avoids the associated issues of matter interpenetration in cases where the original theory fails.

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