# Bond-level Deformation Gradients and Energy Averaging in Peridynamics

Timothy Breitzman*, Kaushik Dayal†
*Composites Branch, Air Force Research Laboratory
†Center for Nonlinear Analysis, Carnegie Mellon University
†Department of Civil and Environmental Engineering, Carnegie Mellon University
†Department of Materials Science and Engineering, Carnegie Mellon University

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**Abstract**

Peridynamic models that aim to incorporate a given classical local continuum stress-deformation response function typically start with a nonlocal averaged analog to the deformation gradient as input to the given local stress-deformation response function. This approach has been observed to allow unphysical deformations such as interpenetration and cause loss of linear stability. This paper describes an approach to deal with this shortcoming. The strategy is based on (1) defining a bond-level analog to the deformation gradient tensor – in contrast to the usual vector deformation measure in peridynamics – that captures both the average deformation in the neighborhood of the bond as well as the deviation of the bond stretch from this average deformation, and (2) using this bond-level deformation gradient in the classical local strain energy response to obtain the energy of each bond. Compared to the standard approach that applies the energy to the averaged deformation gradient, this approach instead averages the energy applied to the bond-level deformation gradient.

**Keywords: peridynamics, nonlocal, interpenetration, stability**

## 1 Introduction

Peridynamics is a nonlocal continuum model that appears well-suited to model discontinuous deformations such as occur in fracture, introduced in the foundational article by Silling [Sil00]. It was first formulated in terms of long-range bonds that connect material particles in a continuum body, with the force in each bond depending only on the reference and current positions of the material particles that it connects. However, the assumption that each bond is independent of the other bonds was recognized right in [Sil00] as being very restrictive in the types of material behavior that can be modeled; e.g., the Poissons ratio is $1/4$. A very similar restriction occurs also in pair-interaction models of atoms. In rough analogy with atomic models, one requires multibody interactions to be able to describe more complex and realistic material behavior; in essence, the force in a bond depends not only on the relative displacement of the atoms that it connects, but also on the positions of other atoms in the local environment [TM11, SPG14]. While extensions of peridynamics provide a framework [SEW$^+$07] that can in principle account for these multi-body interactions, an important challenge is to develop a nonlocal peridynamic model that will display a desired stress-deformation response under uniform deformation. Loosely speaking, this

*Email: timothy.breitzman.1@us.af.mil
†Email: Kaushik.Dayal@cmu.edu

is an inverse problem: given a classical local continuum stress-deformation response, how does one construct a peridynamic model that has the same behavior (i.e., stress and energy) under uniform deformation states?

Recent extensions of peridynamics – co-called *correspondence models* – have aimed to develop a systematic approach to incorporate classical local continuum stress-deformation response into the nonlocal setting [WSA$^+$09]. Correspondence models loosely work with the following procedure: (1) define a nonlocal averaged quantity that is analogous to the deformation gradient; (2) use this nonlocal averaged deformation gradient in the local continuum stress-deformation relations to obtain a stress tensor; and (3) average the stress tensor to obtain the force density. This approach has been observed to allow unphysical deformations such as interpenetration [TR14], and loss of linear stability [BLCB16, Sil17]. Key prior efforts towards dealing with interpenetration and linear instability are, first, [TR14] who prevent interpenetration through using nonlocal analogs of strain measures that become singular when the stretch goes to 0; and, second, [Sil17] who applies a quadratic penalty to penalize zero-energy deformations related to local deviation from the nonlocal average deformation state.

In this article, we present an approach[1] to account for these issues, based on (1) defining a bond-level analog to the deformation gradient that captures both the average deformation in the neighborhood of the bond as well as the deviation of the bond stretch from this average deformation; and (2) using this bond-level deformation gradient in the classical local strain energy response to obtain the energy of each bond, and then summing over all bonds in the body. Together, these elements impose naturally an energetic cost for any deformation that deviates locally from the average deformation, thus eliminating the linear instability observed in conventional correspondence models. In addition, when interpenetration occurs, the bond-level deformation gradient will be seen to have zero determinant, and standard local strain energy functions are typically singular when the argument has zero determinant. The key distinction from the prior efforts mentioned above is that our formulation is able to prevent both interpenetration as well as linear instability using a single framework based solely on the classical local strain energy density: we do not introduce any extra quadratic penalty terms, and interpenetration is forbidden by the use of appropriate standard local strain energy response functions. That is, we are given a local strain energy density function that we wish to mimic in peridynamics, and we do not introduce any further parameters besides those related to nonlocality.

## 1.1 Notation

- Hats denote vectors normalized to have unit magnitude: e.g., $\widehat{\breve{\boldsymbol{x}}-\boldsymbol{x}} := \dfrac{\breve{\boldsymbol{x}}-\boldsymbol{x}}{|\breve{\boldsymbol{x}}-\boldsymbol{x}|}$.
- Tildes denote constitutive response functions: e.g., $\boldsymbol{T}(\boldsymbol{x}) = \tilde{\boldsymbol{T}}(\boldsymbol{F}(\boldsymbol{x}))$.
- Dots denote time derivatives: e.g., $\dot{\boldsymbol{y}}$ and $\ddot{\boldsymbol{y}}$.
- The specimen is denoted $\Omega$.
- $\boldsymbol{x}$ and $\boldsymbol{y}(\boldsymbol{x})$ denote the reference coordinates and deformation. We use $\breve{\boldsymbol{x}}, \mathring{\boldsymbol{x}}$ as dummy variables of integration in the reference configuration, and for conciseness we write $\breve{\boldsymbol{y}} \equiv \boldsymbol{y}(\breve{\boldsymbol{x}}), \mathring{\boldsymbol{y}} \equiv \boldsymbol{y}(\mathring{\boldsymbol{x}})$ and similarly for $\boldsymbol{w}$ which is a test function for the deformation.
- $\alpha(\breve{\boldsymbol{x}}-\boldsymbol{x}) = \alpha(|\breve{\boldsymbol{x}}-\boldsymbol{x}|) \geq 0$ is a weight function satisfying the normalization $\displaystyle\int_{\breve{\boldsymbol{x}}\in\Omega} \alpha(\breve{\boldsymbol{x}}-\boldsymbol{x})\, dV_{\breve{\boldsymbol{x}}} = 1$. We further assume that it has compact support over a region with characteristic lengthscale $\ell$. We do not consider boundaries in this paper to avoid tedious algebraic manipulations that can obscure the key points.

[1] For clarity, we will refer to the approach proposed in this paper as the bond-level deformation gradient model.

- From the isotropy of $\alpha$, it follows that

$$\int_{\breve{\boldsymbol{x}}\in\Omega} \alpha(\breve{\boldsymbol{x}}-\boldsymbol{x})(\breve{\boldsymbol{x}}-\boldsymbol{x})\, dV_{\breve{\boldsymbol{x}}} = \boldsymbol{0}$$

$$\int_{\breve{\boldsymbol{x}}\in\Omega} \alpha(\breve{\boldsymbol{x}}-\boldsymbol{x})\widehat{\breve{\boldsymbol{x}}-\boldsymbol{x}}\otimes\widehat{\breve{\boldsymbol{x}}-\boldsymbol{x}}\, dV_{\breve{\boldsymbol{x}}} = \begin{cases} \frac{1}{2}\boldsymbol{I} \text{ (in 2D)} \\ \frac{1}{3}\boldsymbol{I} \text{ (in 3D)} \end{cases} \tag{1.1}$$

  away from the boundaries.

## 2 Summary of State-Based Correspondence Models

The original formulation of peridynamics was *bond-based*, i.e., the interactions between material particles was assumed to be independent of the deformation of all other material particles [Sil00]. This is closely analogous to pair-potentials in atomic models, and both bond-based peridynamics and pair-potential atomistics have similar failings in describing elastic response: for instance, as noted in [Sil00] itself, the Poisson ratio is constrained to be $1/4$ in both these models. In the context of inelastic response, for instance bonds that yield at a certain critical stretch, the application of hydrostatic loads could lead to yield. To remedy these failings, *state-based* peridynamic models were introduced in [SEW$^+$07]; in brief, these models incorporate the effect of the local deformation environment into the interactions between pairs of material particles. In the context of atomistics, these loosely correspond to multibody atomic potentials.

While the state-based models provide a very general framework, it is challenging to systematically construct models that display a desired macroscopic behavior, even when focusing exclusively on uniform deformations. This again parallels the situation in atomic models where there are few systematic methods – beside brute-force fitting – to develop atomic interaction potentials. But the continuum setting is more challenging in some ways, because inelastic behavior must also be captured in continuum models, whereas they are expected to appear naturally in the atomic setting. That is, given an inelastic response model, say from plasticity, how does one construct a peridynamic model that displays the same behavior at least in the limit of uniform deformations? Correspondence peridynamic models, first developed in [WSA$^+$09], provided a first attempt to address this issue. As we describe below, essentially they define a nonlocal analog to the deformation gradient, and then use the nonlocal analog as the argument for classical local energy or stress response functions. This allows correspondence models to directly and easily build on the vast literature of available classical local continuum strain energy density functions and stress response functions. We describe the essence of the correspondence approach below.

The equation of motion from linear momentum balance is:

$$\rho\ddot{\boldsymbol{y}}(\boldsymbol{x}) = \int_{\breve{\boldsymbol{x}}\in\Omega} \alpha(\breve{\boldsymbol{x}}-\boldsymbol{x})\left[\boldsymbol{T}(\breve{\boldsymbol{x}})\cdot\boldsymbol{K}^{-1}(\breve{\boldsymbol{x}}) + \boldsymbol{T}(\boldsymbol{x})\cdot\boldsymbol{K}^{-1}(\boldsymbol{x})\right]\cdot(\breve{\boldsymbol{x}}-\boldsymbol{x})\, dV_{\breve{\boldsymbol{x}}} + \boldsymbol{b}(\boldsymbol{x}) \tag{2.1}$$

where

$$\boldsymbol{K}(\boldsymbol{x}) = \int_{\mathring{\boldsymbol{x}}\in\Omega} \alpha(\mathring{\boldsymbol{x}}-\boldsymbol{x})\left(\mathring{\boldsymbol{x}}-\boldsymbol{x}\right)\otimes\left(\mathring{\boldsymbol{x}}-\boldsymbol{x}\right)\, dV_{\mathring{\boldsymbol{x}}} \tag{2.2}$$

The correspondence stress is given by $\boldsymbol{T}(\boldsymbol{x}) = \tilde{\boldsymbol{T}}(\boldsymbol{F}_{ave}(\boldsymbol{x}))$ where $\tilde{\boldsymbol{T}}$ is the classical local continuum Piola stress response function. The nonlocal averaged deformation gradient $\boldsymbol{F}_{ave}(\boldsymbol{x})$ given by:

$$\boldsymbol{F}_{ave}(\boldsymbol{x}) = \left(\int_{\mathring{\boldsymbol{x}}\in\Omega} \alpha(\mathring{\boldsymbol{x}}-\boldsymbol{x})\left(\mathring{\boldsymbol{y}}-\boldsymbol{y}\right)\otimes\left(\mathring{\boldsymbol{x}}-\boldsymbol{x}\right)\, dV_{\mathring{\boldsymbol{x}}}\right)\cdot\boldsymbol{K}^{-1}(\boldsymbol{x}) \tag{2.3}$$

Interestingly, similar expressions were proposed in [DO15] and [FJ06] in the context of Structured Deformations and Objective Structures respectively.

Notice that we can rewrite the nonlocal term in (2.1) as:

$$\begin{aligned}\int_{\breve{\boldsymbol{x}}\in\Omega} \alpha(\breve{\boldsymbol{x}}-\boldsymbol{x})\boldsymbol{T}(\breve{\boldsymbol{x}})\cdot\boldsymbol{K}^{-1}(\breve{\boldsymbol{x}})\cdot(\breve{\boldsymbol{x}}-\boldsymbol{x})\,dV_{\breve{\boldsymbol{x}}} + \boldsymbol{T}(\boldsymbol{x})\cdot\boldsymbol{K}^{-1}(\boldsymbol{x})\cdot\int_{\breve{\boldsymbol{x}}\in\Omega}\alpha(\breve{\boldsymbol{x}}-\boldsymbol{x})(\breve{\boldsymbol{x}}-\boldsymbol{x})\,dV_{\breve{\boldsymbol{x}}} \\ = \int_{\breve{\boldsymbol{x}}\in\Omega}\alpha(\breve{\boldsymbol{x}}-\boldsymbol{x})\boldsymbol{T}(\breve{\boldsymbol{x}})\cdot\boldsymbol{K}^{-1}(\breve{\boldsymbol{x}})\cdot(\breve{\boldsymbol{x}}-\boldsymbol{x})\,dV_{\breve{\boldsymbol{x}}}\end{aligned} \tag{2.4}$$

We have used here that $\displaystyle\int_{\breve{\boldsymbol{x}}\in\Omega}\alpha(\breve{\boldsymbol{x}}-\boldsymbol{x})(\breve{\boldsymbol{x}}-\boldsymbol{x})\,dV_{\breve{\boldsymbol{x}}} = \boldsymbol{0}$ in the interior, and ignored boundaries.

## 2.1 Observation of Zero-Energy Modes

We discuss the reason for the appearance of zero-energy modes in correspondence models of peridynamics, following closely [MPD].

Consider the setting of 1D linear elasticity for simplicity. Define the integral operator $D_{int}$ that acts on the displacement $u(x)$ as follows:

$$D_{int}u(x) = \frac{3}{2\ell^3}\int_{x-\ell}^{x+\ell}(u(x)-u(\breve{x}))\,(x-\breve{x})\;d\breve{x} \tag{2.5}$$

Consider the Taylor expansion $u(x)-u(\breve{x}) = (x-\breve{x})\dfrac{du}{dx}+\dfrac{1}{2}(x-\breve{x})^2\dfrac{d^2u}{dx^2}+\ldots$. Then, $D_{int}u(x) = \dfrac{du}{dx} + C_3\ell^2\dfrac{d^3u}{dx^3}+\ldots$, where the even derivatives vanish by symmetry. Therefore, $D_{int}u$ provides a nonlocal approximation to the strain $du/dx$ when $\ell$ – the lengthscale of the nonlocality – and the higher derivatives are sufficiently small. However, $D_{int}u$ continues to be well-defined at discontinuities where the derivative is not well-defined.

Geometrically, $D_{int}u$ can be understood as averaging the slope of $u(x)$ over a neighborhood of $x$ of size $\ell$, i.e., averaging $\dfrac{u(x)-u(\breve{x})}{x-\breve{x}}$. However, to avoid singularities from the denominator, we use the weight $(x-\breve{x})^2$ in the process of averaging. When the slope is constant, i.e. a linear function, we recover exactly the derivative; when the function is slowly varying, we get higher-order contributions; and when the function does not have well-defined derivatives due to insufficient smoothness, we obtain a finite value that captures some information about the average slope in the neighborhood.

While $D_{int}u$ appears to provide an attractive alternative to $du/dx$, there is one key failing. The classical derivative $du/dx$ is 0 only when $u = \text{const.}$ and not otherwise. However, while $D_{int}u = 0$ when $u = \text{const.}$, it can also be 0 for numerous other functions: in fact, any function for which the slopes cancel out on averaging. Therefore, one can have nontrivial displacement fields $u(x)$ with vanishing nonlocal strain, and consequently vanishing energy in a linear model. The analog of this argument in higher dimensions is precisely the reason for spurious unphysical zero-energy soft modes in correspondence models of peridynamics.

The possibility of these zero-energy modes had been noted in [TR14] and [Sil17]. In [TR14], they focus particularly on the possibility of interpenetration, and use a strain measure that becomes singular at interpenetration to prevent such deformations. In [Sil17], he introduces a quadratic penalty for the zero-energy modes, but this still appears to allow interpenetration at a finite energy cost.

This paper proposes a different approach. In the simplified 1D setting, we begin by noting that the cancellation described above can be avoided by averaging a quantity that is constrained to be positive; e.g., a natural quantity

with this property is the nonlocal analog of the elastic energy density[2] $\left(\frac{du}{dx}\right)^2$. That is, the operator

$$D_{2int}u = \int_{x-\ell}^{x+\ell} \left(\frac{u(x) - u(\breve{x})}{x - \breve{x}}\right)^2 d\breve{x} \tag{2.6}$$

provides a nonlocal regularized approximation of the elastic energy density $\left(\frac{du}{dx}\right)^2$ up to normalization. The integrand is always non-negative, thereby not allowing any cancellations. For the nonlocal elastic energy density $D_{2int}u$ to evaluate to 0, the integrand must be 0 everywhere, ensuring that $u = \text{const.}$ is the only possibility. A key element of our approach described below is a generalization of this idea.

# 3 Proposed Bond-Level Deformation Gradient and Energy Averaging Model

Our proposed model has two key ingredients: first, a definition of an analog to the deformation gradient for every pair of material particles, i.e. *bond-level*, that has information both about the average deformation in a nonlocal region as well as the deviation of the bond from this average deformation; and, second, the use of this deformation gradient in the local energy density function without any further extra penalties to account for interpenetration, linear zero-energy modes, and so on.

We then further include the bond stretch explicitly as an argument in the bond energy density, in addition to its contribution through the bond-wise deformation gradient. This is to fit our bond-level deformation gradient model into the framework of fracture in peridynamics that typically is modeled through dependence on bond stretch. We then find the peridynamic equation of motion for our model consisting of these ingredients.

## 3.1 Deformation Gradient Defined for Each Bond: Kinematic Augmentation to Detect Deviations from the Average

The nonlocal averaged deformation gradient $\boldsymbol{F}_{ave}(\boldsymbol{x})$ gives the average deformation of the neighborhood around $\boldsymbol{x}$. As discussed above, this implies that deviations from the mean are not captured in the kinematics. Consequently, there is no energetic penalty for these deviations thereby permitting zero-energy nontrivial deformations. We aim to account for the energetics of these deviations as described below. In [Sil17], these deviations are similarly captured and a quadratic energetic penalty is ascribed to them. Our model and [Sil17] use a similar approach to identify the deviations, but then we construct a bond-level deformation gradient and use it in the strain energy density which inherently accounts for deviations. As we discuss further below, our approach also enables us to account for the energetics of inter-penetration and related deformation modes that were identified to be problematic in the correspondence models [TR14]. Therefore, our approach builds on the advances of [Sil17] and [TR14] while eliminating the extraneous quadratic penalty in favor of the strain energy density that is already a part of the model.

Our starting point is to associate a deformation gradient to *every* bond connected to $\boldsymbol{x}$ that we denote by $\boldsymbol{F}_{bond}(\boldsymbol{x}, \breve{\boldsymbol{x}})$. However, a single bond is described only by $\breve{\boldsymbol{y}} - \boldsymbol{y}$ and $\breve{\boldsymbol{x}} - \boldsymbol{x}$, and the simplistic attempt to define a deformation gradient as $(\breve{\boldsymbol{y}} - \boldsymbol{y}) \otimes (\breve{\boldsymbol{x}} - \boldsymbol{x})$ leads to a rank-deficient tensor. An alternative that would capture the correct physics but be very expensive computationally is to start with the expression:

$$(\breve{\boldsymbol{y}} - \boldsymbol{y}) \otimes (\breve{\boldsymbol{x}} - \boldsymbol{x}) + (\breve{\breve{\boldsymbol{y}}} - \boldsymbol{y}) \otimes (\breve{\breve{\boldsymbol{x}}} - \boldsymbol{x}) + (\breve{\breve{\breve{\boldsymbol{y}}}} - \boldsymbol{y}) \otimes (\breve{\breve{\breve{\boldsymbol{x}}}} - \boldsymbol{x}) \tag{3.1}$$

where $\breve{\breve{\boldsymbol{x}}} - \boldsymbol{x}$ and $\breve{\boldsymbol{x}} - \boldsymbol{x}$ are in the plane normal to $\breve{\boldsymbol{x}} - \boldsymbol{x}$, and then average over all $\breve{\breve{\boldsymbol{x}}}$ and $\breve{\boldsymbol{x}}$. This would require integrations over a different plane for *every* bond at $\boldsymbol{x}$, unlike $\boldsymbol{F}_{ave}$ which is computed once and then defined for all bonds at $\boldsymbol{x}$.

[2] [MPD] discusses a similar situation for liquid crystals.

Motivated by the expression in the previous paragraph but to also balance computational efficiency, we capture the deviations from uniform deformation through the difference between: (1) the actual stretch of a bond, $\breve{\boldsymbol{y}} - \boldsymbol{y}$, and (2) the stretch that the bond would undergo as a material line element mapped under $\boldsymbol{F}_{ave}$ if the deformation was uniform. We then use this difference to "correct" $\boldsymbol{F}_{ave}$ for each bond to obtain $\boldsymbol{F}_{bond}$ that is a useful full-rank deformation gradient. To perform this correction in a way that captures the physics yet is reasonably efficient, rather than integrating over an entire plane for each bond, we approximate this operation by starting with $\boldsymbol{F}_{ave}$ and "correcting" it for each bond by first removing the contribution due to the uniform deformation assumption and replacing it by the actual deformation. That is, we define $\boldsymbol{F}_{bond}(\boldsymbol{x}, \breve{\boldsymbol{x}})$ centered at $\boldsymbol{x}$ as:

$$\begin{aligned}\boldsymbol{F}_{bond}(\boldsymbol{x}, \breve{\boldsymbol{x}}) &= \boldsymbol{F}_{ave}(\boldsymbol{x}) - \left(\boldsymbol{F}_{ave}(\boldsymbol{x}) \cdot \widehat{\breve{\boldsymbol{x}} - \boldsymbol{x}}\right) \otimes \widehat{\breve{\boldsymbol{x}} - \boldsymbol{x}} + \frac{\breve{\boldsymbol{y}} - \boldsymbol{y}}{|\breve{\boldsymbol{x}} - \boldsymbol{x}|} \otimes \widehat{\breve{\boldsymbol{x}} - \boldsymbol{x}} \\ &= \boldsymbol{F}_{ave}(\boldsymbol{x}) \left(\boldsymbol{I} - \widehat{\breve{\boldsymbol{x}} - \boldsymbol{x}} \otimes \widehat{\breve{\boldsymbol{x}} - \boldsymbol{x}}\right) + \frac{\breve{\boldsymbol{y}} - \boldsymbol{y}}{|\breve{\boldsymbol{x}} - \boldsymbol{x}|} \otimes \widehat{\breve{\boldsymbol{x}} - \boldsymbol{x}}\end{aligned} \tag{3.2}$$

This definition satisfies $\boldsymbol{F}_{bond} \cdot (\breve{\boldsymbol{x}} - \boldsymbol{x}) = \breve{\boldsymbol{y}} - \boldsymbol{y}$. Also $\boldsymbol{F}_{bond}$ has information about the average deformation in the plane normal to the bond as well as information about the deviation of the bond from the average in the bond direction.

Notice that $\left(\boldsymbol{I} - \widehat{\breve{\boldsymbol{x}} - \boldsymbol{x}} \otimes \widehat{\breve{\boldsymbol{x}} - \boldsymbol{x}}\right)$ is a rank-deficient tensor. Therefore, if $\breve{\boldsymbol{y}} - \boldsymbol{y} = \boldsymbol{0}$, implying interpenetration, then $\det \boldsymbol{F}_{bond} = 0$ and a suitable standard hyperelastic energy density using $\boldsymbol{F}_{bond}$ as argument will become singular. Therefore, this kinematics can capture the essential aspects of [TR14], as we discuss further in Section 4.4.

Notice that in general $\boldsymbol{F}_{ave}(\boldsymbol{x}) \neq \boldsymbol{F}_{ave}(\breve{\boldsymbol{x}})$, implying $\boldsymbol{F}_{bond}(\boldsymbol{x}, \breve{\boldsymbol{x}}) \neq \boldsymbol{F}_{bond}(\breve{\boldsymbol{x}}, \boldsymbol{x})$.

In [Sil17], $\boldsymbol{F}_{bond} \cdot (\breve{\boldsymbol{x}} - \boldsymbol{x}) - (\breve{\boldsymbol{y}} - \boldsymbol{y})$ is used as a measure of the deviations from the average deformation. However, he then directly penalizes this deviation with a quadratic penalty by introducing a stiffness corresponding to the penalty that is unrelated to the elastic energy density.

## 3.2 Energetic Nonlocal Averaging Using Classical Local Energy Densities

We consider next the energy associated to each bond. Our development is based on the assumption that a classical local hyperelastic strain energy density response $\tilde{W}_{loc}(\boldsymbol{F}) \geq 0$ is available, well-characterized, and well-behaved in the classical local continuum setting. Our association of a deformation gradient $\boldsymbol{F}_{bond}$ to each bond enables us to simply use $\tilde{W}_{loc}$ to find the bond energy[3]. As discussed in Section 2.1, $\tilde{W}_{loc} \geq 0$ enables us to avoid the cancellations that permit zero-energy modes.

Therefore, we define the energy of the bond between $\boldsymbol{x}$ and $\breve{\boldsymbol{x}}$, centered at $\boldsymbol{x}$, simply as $\tilde{W}_{loc}(\boldsymbol{F}_{bond}(\boldsymbol{x}, \breve{\boldsymbol{x}}))$. We then further define the averaged energy density as:

$$W_{ave}(\boldsymbol{x}) = \frac{1}{2} \int_{\breve{\boldsymbol{x}} \in \Omega} \alpha(\breve{\boldsymbol{x}} - \boldsymbol{x}) \tilde{W}_{loc}(\boldsymbol{F}_{bond}(\boldsymbol{x}, \breve{\boldsymbol{x}}))\, dV_{\breve{\boldsymbol{x}}} \tag{3.3}$$

where the factor of $\frac{1}{2}$ accounts for splitting the energy equally between $\boldsymbol{x}$ and $\breve{\boldsymbol{x}}$. The free energy of the body is then:

$$E[\boldsymbol{y}] = \int_{\boldsymbol{x} \in \Omega} \left( \frac{1}{2} \int_{\breve{\boldsymbol{x}} \in \Omega} \alpha(\breve{\boldsymbol{x}} - \boldsymbol{x}) \tilde{W}_{loc}(\boldsymbol{F}_{bond}(\boldsymbol{x}, \breve{\boldsymbol{x}}))\, dV_{\breve{\boldsymbol{x}}} \right) - \boldsymbol{b} \cdot \boldsymbol{y}\, dV_{\boldsymbol{x}} \tag{3.4}$$

[3] For dimensional consistency, the hyperelastic volume energy density must be divided by a characteristic volume $\ell^3$ to obtain a bond energy density, but we do not write this explicitly for clarity of notation.

### 3.3 Bond Stretch Dependence for Fracture

While Section 3.2 provides an approach to incorporate classical local strain energy density response functions into peridynamics, that model alone is insufficient to permit fracture. In particular, standard local elastic energies $W_{loc}(\boldsymbol{F})$ typically have superlinear growth as $|\boldsymbol{F}| \to \infty$ to obtain good mathematical properties of solutions, e.g. [Ant13, Cia88]. One approach to introduce the ability to fracture may be to relax this growth condition. However, a far more popular approach in peridynamics is to use the bond stretch as an indicator of failure: as the stretch increases, the ability of the bond to bear load degrades, e.g. [WOG17, FSC11, Lip14, Lip16] and numerous others. This degradation may be sharp or gradual, and is generally irreversible. The irreversibility makes it debatable if we can implement fracture in an energetic setting in peridynamics; in fact, even inelasticity in a classical local setting is often not well-described in an energy framework. However, we nonetheless do this here because the energy provides a simple approach to obtaining the equations of motion and restrictions on various quantities (e.g., Sections 4.2, 4.1); once we have these equations, we can use stress-response functions with the appropriate restrictions for inelastic settings.

Therefore, we begin with an elastic energy density $\tilde{W}_{loc}(\boldsymbol{F}_{bond}(\boldsymbol{x},\breve{\boldsymbol{x}}),\boldsymbol{x},\breve{\boldsymbol{x}},\breve{\boldsymbol{y}}-\boldsymbol{y})$, where the first argument is as discussed above, the second and third arguments represent inhomogeneity if present, and the fourth argument represents the bond stretch explicitly. Alternatively, one could use a stress response function $\tilde{\boldsymbol{T}}(\boldsymbol{F}_{bond}(\boldsymbol{x},\breve{\boldsymbol{x}}),\boldsymbol{x},\breve{\boldsymbol{x}},\breve{\boldsymbol{y}}-\boldsymbol{y})$, and incorporate failure through the form:

$$\tilde{\boldsymbol{T}}(\boldsymbol{F}_{bond}(\boldsymbol{x},\breve{\boldsymbol{x}}),\boldsymbol{x},\breve{\boldsymbol{x}},\breve{\boldsymbol{y}}-\boldsymbol{y}) = \tilde{\boldsymbol{T}}_{loc}(\boldsymbol{F}_{bond}(\boldsymbol{x},\breve{\boldsymbol{x}}),\boldsymbol{x},\breve{\boldsymbol{x}})\cdot f(\breve{\boldsymbol{y}}-\boldsymbol{y},\boldsymbol{F}_{bond}(\boldsymbol{x},\breve{\boldsymbol{x}}),\boldsymbol{x},\breve{\boldsymbol{x}}) \tag{3.5}$$

where $\tilde{\boldsymbol{T}}_{loc}$ is the classical local Piola stress response function, and $f$ is a function that is 1 when the bond stretch is small and 0 when the bond stretch is large. The functional form of $f$ defines the failure, and it can in general be inhomogeneous as well as depend on the state of strain in the neighborhood through $\boldsymbol{F}_{bond}$.

### 3.4 Equation of Motion

We obtain the balance of linear momentum from the first variation of $E$ with respect to $\boldsymbol{y}$ from (3.4), but with the additional arguments in $\tilde{W}_{loc}(\boldsymbol{F}_{bond}(\boldsymbol{x},\breve{\boldsymbol{x}}),\boldsymbol{x},\breve{\boldsymbol{x}},\breve{\boldsymbol{y}}-\boldsymbol{y})$.

We begin with $\boldsymbol{y}\mapsto\boldsymbol{y}+\epsilon\boldsymbol{w}$, implying

$$\boldsymbol{F}_{ave}(\boldsymbol{x})\mapsto\boldsymbol{F}_{ave}(\boldsymbol{x})+\epsilon\int_{\mathring{\boldsymbol{x}}\in\Omega}\alpha(\boldsymbol{x}-\mathring{\boldsymbol{x}})\left(\mathring{\boldsymbol{w}}-\boldsymbol{w}\right)\otimes\left(\mathring{\boldsymbol{x}}-\boldsymbol{x}\right)\,dV_{\mathring{\boldsymbol{x}}}\cdot\boldsymbol{K}^{-1}(\boldsymbol{x}) \tag{3.6}$$

and

$$\begin{aligned}(F_{bond}(\boldsymbol{x},\breve{\boldsymbol{x}}))_{ij}\mapsto&(F_{bond}(\boldsymbol{x},\breve{\boldsymbol{x}}))_{ij}+\epsilon\frac{(\breve{w}-w)_i}{|\breve{\boldsymbol{x}}-\boldsymbol{x}|}\widehat{(\breve{x}-x)}_j\\&+\epsilon(K^{-1}(\boldsymbol{x}))_{lk}\left(\delta_{kj}-\widehat{(\breve{x}-x)}_k\widehat{(\breve{x}-x)}_j\right)\int_{\mathring{\boldsymbol{x}}\in\Omega}\alpha(\boldsymbol{x}-\mathring{\boldsymbol{x}})\left(\mathring{w}-w\right)_i\left(\mathring{x}-x\right)_l\,dV_{\mathring{\boldsymbol{x}}}\end{aligned} \tag{3.7}$$

The variation of $E$ up to linear order in $\epsilon$ is therefore:

$$\begin{aligned}&E\mapsto E+\epsilon\int_{\boldsymbol{x}\in\Omega}w_ib_i+\frac{\epsilon}{2}\int_{\boldsymbol{x}\in\Omega}\int_{\breve{\boldsymbol{x}}\in\Omega}\alpha(\breve{\boldsymbol{x}}-\boldsymbol{x})\frac{\partial\tilde{W}_{loc}}{\partial(\breve{y}-y)_i}(\breve{w}-w)_i\,dV_{\boldsymbol{x}}\,dV_{\breve{\boldsymbol{x}}}\\&+\frac{\epsilon}{2}\int_{\boldsymbol{x}\in\Omega}\int_{\breve{\boldsymbol{x}}\in\Omega}\alpha(\breve{\boldsymbol{x}}-\boldsymbol{x})(T_{bond}(\boldsymbol{x},\breve{\boldsymbol{x}}))_{ij}\frac{(\breve{w}-w)_i}{|\breve{\boldsymbol{x}}-\boldsymbol{x}|}\widehat{(\breve{x}-x)}_j\,dV_{\boldsymbol{x}}\,dV_{\breve{\boldsymbol{x}}}\\&+\frac{\epsilon}{2}\int_{\boldsymbol{x}\in\Omega}\int_{\breve{\boldsymbol{x}}\in\Omega}\alpha(\breve{\boldsymbol{x}}-\boldsymbol{x})(T_{bond}(\boldsymbol{x},\breve{\boldsymbol{x}}))_{ij}(K^{-1}(\boldsymbol{x}))_{lk}\delta_{kj}\int_{\mathring{\boldsymbol{x}}\in\Omega}\alpha(\boldsymbol{x}-\mathring{\boldsymbol{x}})\left(\mathring{w}-w\right)_i\left(\mathring{x}-x\right)_l\,dV_{\mathring{\boldsymbol{x}}}\,dV_{\breve{\boldsymbol{x}}}\,dV_{\boldsymbol{x}}\\&-\frac{\epsilon}{2}\int_{\boldsymbol{x}\in\Omega}\int_{\breve{\boldsymbol{x}}\in\Omega}\alpha(\breve{\boldsymbol{x}}-\boldsymbol{x})(T_{bond}(\boldsymbol{x},\breve{\boldsymbol{x}}))_{ij}(K^{-1}(\boldsymbol{x}))_{lk}\widehat{(\breve{x}-x)}_k\widehat{(\breve{x}-x)}_j\int_{\mathring{\boldsymbol{x}}\in\Omega}\alpha(\boldsymbol{x}-\mathring{\boldsymbol{x}})\left(\mathring{w}-w\right)_i\left(\mathring{x}-x\right)_l\,dV_{\mathring{\boldsymbol{x}}}\,dV_{\breve{\boldsymbol{x}}}\,dV_{\boldsymbol{x}}\end{aligned} \tag{3.8}$$

We have defined the bond Piola stress $\boldsymbol{T}_{bond}(\boldsymbol{x},\hat{\boldsymbol{x}}) = \dfrac{\partial \tilde{W}_{loc}}{\partial \boldsymbol{F}}(\boldsymbol{F})\Big|_{\boldsymbol{F}=\boldsymbol{F}_{bond}(\boldsymbol{x},\hat{\boldsymbol{x}})}$. Note the difference in physical dimension from the classical Piola stress.

We now relabel in the standard way and rearrange to reach the form for $\dfrac{dE}{d\epsilon}\Big|_{\epsilon=0}$:

$$\int_{\boldsymbol{x}\in\Omega} w_i \left( \begin{array}{l} \displaystyle\int_{\breve{\boldsymbol{x}}\in\Omega} \alpha(\breve{\boldsymbol{x}}-\boldsymbol{x}) \frac{\partial \tilde{W}_{loc}}{\partial (y-\breve{y})_i}\, dV_{\breve{\boldsymbol{x}}} \\ \displaystyle + \int_{\breve{\boldsymbol{x}}\in\Omega} \alpha(\breve{\boldsymbol{x}}-\boldsymbol{x}) \frac{1}{2} \left(T_{bond}(\boldsymbol{x},\breve{\boldsymbol{x}}) + T_{bond}(\breve{\boldsymbol{x}},\boldsymbol{x})\right)_{ij} \frac{\widehat{(\breve{x}-x)}_j}{|\breve{\boldsymbol{x}}-\boldsymbol{x}|}\, dV_{\breve{\boldsymbol{x}}} \\ \displaystyle - \frac{1}{2}\int_{\breve{\boldsymbol{x}}\in\Omega}\int_{\mathring{\boldsymbol{x}}\in\Omega} \alpha(\breve{\boldsymbol{x}}-\mathring{\boldsymbol{x}})\alpha(\boldsymbol{x}-\mathring{\boldsymbol{x}})(T_{bond}(\mathring{\boldsymbol{x}},\breve{\boldsymbol{x}}))_{ij}(K^{-1}(\mathring{\boldsymbol{x}}))_{lk}\widehat{(\breve{x}-\mathring{x})}_k\widehat{(\breve{x}-\mathring{x})}_j \left(x-\mathring{x}\right)_l\, dV_{\mathring{\boldsymbol{x}}}\, dV_{\breve{\boldsymbol{x}}} \\ \displaystyle + \frac{1}{2}\int_{\breve{\boldsymbol{x}}\in\Omega}\int_{\mathring{\boldsymbol{x}}\in\Omega} \alpha(\breve{\boldsymbol{x}}-\mathring{\boldsymbol{x}})\alpha(\boldsymbol{x}-\mathring{\boldsymbol{x}})(T_{bond}(\mathring{\boldsymbol{x}},\breve{\boldsymbol{x}}))_{ij}(K^{-1}(\mathring{\boldsymbol{x}}))_{lk}\delta_{kj} \left(x-\mathring{x}\right)_l\, dV_{\mathring{\boldsymbol{x}}}\, dV_{\breve{\boldsymbol{x}}} \\ + b_i \end{array} \right) dV_{\boldsymbol{x}} \tag{3.9}$$

We have used that $\displaystyle\int_{\breve{\boldsymbol{x}}\in\Omega} \alpha(\breve{\boldsymbol{x}}-\boldsymbol{x})(\breve{\boldsymbol{x}}-\boldsymbol{x})\, dV_{\breve{\boldsymbol{x}}} = \boldsymbol{0}$ to simplify the third term. For arbitrary $\boldsymbol{w}$, the expression in the brackets is the right side of the equation of motion. In static equilibrium this is set to $\boldsymbol{0}$, and in dynamics to $\rho\ddot{\boldsymbol{y}}$.

We examine the terms in (3.9). The first term is due to the explicit stretch dependence, and closely resembles bond-based peridynamics. The second and third terms are absent in standard correspondence models of peridynamics, and arise due to the approach proposed in this paper. The fourth term can be related to the standard correspondence model in (2.1) by rewriting it as follows:

$$\frac{1}{2}\int_{\mathring{\boldsymbol{x}}\in\Omega} \alpha(\boldsymbol{x}-\mathring{\boldsymbol{x}}) \underbrace{\left(\int_{\breve{\boldsymbol{x}}\in\Omega} \alpha(\breve{\boldsymbol{x}}-\mathring{\boldsymbol{x}})(T_{bond}(\mathring{\boldsymbol{x}},\breve{\boldsymbol{x}}))_{ij}\, dV_{\breve{\boldsymbol{x}}}\right)}_{=:\,(T_{corr}(\mathring{\boldsymbol{x}}))_{ij}} (K^{-1}(\mathring{\boldsymbol{x}}))_{lj} \left(x-\mathring{x}\right)_l\, dV_{\mathring{\boldsymbol{x}}} \tag{3.10}$$

The fifth term is the external body force.

# 4 Characterization of the Bond-Level Deformation Gradient Model

We begin first by noting that the bond-level deformation gradient model satisfies the simple but necessary constraint that it mimics classical local elasticity in the limit of uniform deformation. Consider the uniform deformation $\boldsymbol{y} = \boldsymbol{F}_0 \cdot \boldsymbol{x}$ where $\boldsymbol{F}_0$ is a constant tensor. This implies $\boldsymbol{F}_{ave} = \boldsymbol{F}_{bond} = \boldsymbol{F}_0$. Assume that the deformation is not in the regime where the pairwise stretch-dependence is active. Then, the energy density $W_{ave}(\boldsymbol{x}) = \dfrac{1}{2}\displaystyle\int_{\breve{\boldsymbol{x}}\in\Omega} \alpha(\boldsymbol{x}-\breve{\boldsymbol{x}})\tilde{W}_{loc}(\boldsymbol{F}_0)\, dV_{\breve{\boldsymbol{x}}} = \tilde{W}_{loc}(\boldsymbol{F}_0)$ recovers the classical continuum expression.

We briefly consider the setting of one dimension. First, as discussed in, for example, Section 2 of [DB06], arbitrary stress-strain responses can be easily incorporated in pairwise bond interaction peridynamics; there is no need to use multi-body interactions. Second, the proposed bond-level deformation gradient model is trivial because $\left(\boldsymbol{I} - \widehat{\breve{\boldsymbol{x}}-\boldsymbol{x}} \otimes \widehat{\breve{\boldsymbol{x}}-\boldsymbol{x}}\right) = 0$, and consequently $\boldsymbol{F}_{bond}$ is simply the stretch of individual bonds; geometrically, $\boldsymbol{F}_{bond}$ uses information in $\boldsymbol{F}_{ave}$ in directions orthogonal to the bond direction and corrects along the bond but this geometric interpretation is of course degenerate in 1D. Third, another interpretation is that all bonds undergo the same deformation in a homogeneous deformation in 1D, whereas bonds in different directions undergo different deformations in 2D / 3D.

The stability and other properties of the bond-level deformation gradient model depend strongly on the properties of the local strain energy density $\tilde{W}_{loc}$ on which it is based. One immediate consequence is that we should *not* generally expect stability for all deformations in the finite deformation setting. A simple example is that frame-indifference requires invariance of the energy under rigid rotations, implying nonconvexity; imposing convexity could rule out physically-relevant instabilities such as buckling and snap-through altogether [Ant13][4]. This is a key motivation for us to propose the current alternative – based solely on the classical local energy density – to the approach in [Sil17] using a quadratic penalty. However, we also emphasize that we are to date unaware of any specific physically-reasonable instabilities that are suppressed by the quadratic penalty approach, and also it does not violate frame-indifference.

A further example is the use of nonconvex local elastic energy functions to model materials with multiple phases that can lead to the formation of complex fine microstructures [BJ87]. When the deformation varies over length-scales much larger than the intrinsic nonlocal lengthscale, the bond-level deformation gradient model mimics the local model. Consequently, the formation of microstructure with refinement much larger than the intrinsic nonlocal lengthscale may be expected. It is certainly also a possibility that the bond-level deformation gradient model will permit the formation of complex microstructure at even smaller scales.

Beyond these well-known examples, nonlinear elasticity leads to an extremely rich and complex structure in terms of microstructure and stability that is very far from complete characterization [Ant13]. It is reasonable to expect that the peridynamic bond-level deformation gradient model based on such local energies will be at least as complex, and we therefore focus below on examining only specific key deformation modes. We characterize the bond-level deformation gradient model by confirming the consistency with balances of linear and angular momentum, the energetics of linear perturbations, and the energetics of idealized discontinuous deformations.

## 4.1 Balance of Linear Momentum

We ensure that the equation of motion implied by (3.9) is consistent with conservation of linear momentum. This is of course to be anticipated given its energetic basis.

We simply integrate the equation of motion over the body:

$$\begin{aligned}
&\int_{\boldsymbol{x}\in\Omega} \rho\ddot{\boldsymbol{y}}\, dV_{\boldsymbol{x}} = \int_{\boldsymbol{x}\in\Omega} b_i\, dV_{\boldsymbol{x}} \\
&\int_{\boldsymbol{x}\in\Omega}\int_{\breve{\boldsymbol{x}}\in\Omega} \alpha(\breve{\boldsymbol{x}}-\boldsymbol{x})\frac{\partial \tilde{W}_{loc}}{\partial(y-\breve{y})_i}\, dV_{\breve{\boldsymbol{x}}}\, dV_{\boldsymbol{x}} \\
&+\int_{\boldsymbol{x}\in\Omega}\int_{\breve{\boldsymbol{x}}\in\Omega} \alpha(\breve{\boldsymbol{x}}-\boldsymbol{x})\frac{1}{2}\left(T_{bond}(\boldsymbol{x},\breve{\boldsymbol{x}})+T_{bond}(\breve{\boldsymbol{x}},\boldsymbol{x})\right)_{ij}\frac{\widehat{(\breve{x}-x)}_j}{|\breve{\boldsymbol{x}}-\boldsymbol{x}|}\, dV_{\breve{\boldsymbol{x}}}\, dV_{\boldsymbol{x}} \\
&-\frac{1}{2}\int_{\boldsymbol{x}\in\Omega}\int_{\breve{\boldsymbol{x}}\in\Omega}\int_{\mathring{\boldsymbol{x}}\in\Omega} \alpha(\breve{\boldsymbol{x}}-\mathring{\boldsymbol{x}})\alpha(\boldsymbol{x}-\mathring{\boldsymbol{x}})(T_{bond}(\mathring{\boldsymbol{x}},\breve{\boldsymbol{x}}))_{ij}(K^{-1}(\mathring{\boldsymbol{x}}))_{lk}\widehat{(\breve{x}-\mathring{x})}_k\widehat{(\breve{x}-\mathring{x})}_j\left(x-\mathring{x}\right)_l\, dV_{\mathring{\boldsymbol{x}}}\, dV_{\breve{\boldsymbol{x}}}\, dV_{\boldsymbol{x}} \\
&+\frac{1}{2}\int_{\boldsymbol{x}\in\Omega}\int_{\breve{\boldsymbol{x}}\in\Omega}\int_{\mathring{\boldsymbol{x}}\in\Omega} \alpha(\breve{\boldsymbol{x}}-\mathring{\boldsymbol{x}})\alpha(\boldsymbol{x}-\mathring{\boldsymbol{x}})(T_{bond}(\mathring{\boldsymbol{x}},\breve{\boldsymbol{x}}))_{ij}(K^{-1}(\mathring{\boldsymbol{x}}))_{lk}\delta_{kj}\left(x-\mathring{x}\right)_l\, dV_{\mathring{\boldsymbol{x}}}\, dV_{\breve{\boldsymbol{x}}}\, dV_{\boldsymbol{x}}
\end{aligned} \tag{4.1}$$

We consider this equation term by term. The second and third terms on the right vanish because the integrand changes sign under the relabeling $\boldsymbol{x}\leftrightarrow\breve{\boldsymbol{x}}$. The fourth and fifth terms on the right vanish because one can isolate terms of the form $\int_{\mathring{\boldsymbol{x}}\in\Omega}\alpha(\mathring{\boldsymbol{x}}-\boldsymbol{x})(\mathring{\boldsymbol{x}}-\boldsymbol{x})\, dV_{\mathring{\boldsymbol{x}}} = \boldsymbol{0}$. This leaves only the term on the left – the rate of change of the total angular momentum – equal to the first term on the right – the total external force.

[4]The requirements for general peridynamic energies can be different from classical elasticity [EP14].

We notice that the Piola stress makes an appearance above. Therefore, to adapt local inelastic models – where the energy is not meaningful – to peridynamics, we can instead simply treat the equation of motion as the starting point and use the local stress response function.

We recall that peridynamics has no role for boundary tractions. All external forces are modeled as applied through $\boldsymbol{b}$.

## 4.2 Balance of Angular Momentum

We next ensure that the equation of motion implied by (3.9) is consistent with conservation of angular momentum. In principle, we could take the cross product of the equation of motion with $\boldsymbol{y}$ and then integrate over the body. However, this is extremely formidable algebraically, in particular because the bond force need not be directed along the bond in general peridynamic models. In bond-based peridynamics, bond forces are always directed along bonds, and this property immediately implies consistency – at the level of each bond – with angular momentum balance. Therefore, here we instead use Noether's theorem, following the presentation in [KS72, LM00], to show this consistency as well as the restrictions required of the constitutive response functions.

One perspective of Noether's theorem is that continuous invariances imply balance laws. We therefore begin by showing that the strain energy

$$U = \int_{\boldsymbol{x}\in\Omega} \left( \frac{1}{2} \int_{\breve{\boldsymbol{x}}\in\Omega} \alpha(\breve{\boldsymbol{x}}-\boldsymbol{x}) \tilde{W}_{loc}(\boldsymbol{F}_{bond}(\boldsymbol{x},\breve{\boldsymbol{x}}),\boldsymbol{x},\breve{\boldsymbol{x}},\breve{\boldsymbol{y}}-\boldsymbol{y})\, dV_{\breve{\boldsymbol{x}}} \right) dV_{\boldsymbol{x}} \tag{4.2}$$

is invariant under rigid rotations $\boldsymbol{Q}$ acting on the current configuration: $\boldsymbol{y} \mapsto \boldsymbol{Q}\cdot\boldsymbol{y}$. This implies that the bond stretch transforms as $\breve{\boldsymbol{y}}-\boldsymbol{y} \mapsto \boldsymbol{Q}\cdot(\breve{\boldsymbol{y}}-\boldsymbol{y})$, and the average deformation gradient and the bond deformation gradient both transform as $\boldsymbol{F}_{ave} \mapsto \boldsymbol{Q}\cdot\boldsymbol{F}_{ave}, \boldsymbol{F}_{bond} \mapsto \boldsymbol{Q}\cdot\boldsymbol{F}_{ave}$. If the strain energy density is invariant under such a transformation – i.e., $\tilde{W}_{loc}(\boldsymbol{Q}\cdot\boldsymbol{F}_{bond}(\boldsymbol{x},\breve{\boldsymbol{x}}),\boldsymbol{x},\breve{\boldsymbol{x}},\boldsymbol{Q}\cdot(\breve{\boldsymbol{y}}-\boldsymbol{y})) = \tilde{W}_{loc}(\boldsymbol{F}_{bond}(\boldsymbol{x},\breve{\boldsymbol{x}}),\boldsymbol{x},\breve{\boldsymbol{x}},\breve{\boldsymbol{y}}-\boldsymbol{y})$ – then the strain energy $U$ is also invariant. The constraints on $\tilde{W}_{loc}$ implied by the restriction $\tilde{W}_{loc}(\boldsymbol{Q}\cdot\boldsymbol{F}_{bond}(\boldsymbol{x},\breve{\boldsymbol{x}}),\boldsymbol{x},\breve{\boldsymbol{x}},\boldsymbol{Q}\cdot(\breve{\boldsymbol{y}}-\boldsymbol{y})) = \tilde{W}_{loc}(\boldsymbol{F}_{bond}(\boldsymbol{x},\breve{\boldsymbol{x}}),\boldsymbol{x},\breve{\boldsymbol{x}},\breve{\boldsymbol{y}}-\boldsymbol{y})$ in terms of the first argument are standard frame indifference in the local continuum models, and standard in peridynamics in terms of the fourth argument.

Now consider the family of deformations $\boldsymbol{w}(s,\boldsymbol{x}) = \boldsymbol{Q}(s)\cdot\boldsymbol{y}(\boldsymbol{x})$ indexed by the parameter $s$ and $\boldsymbol{Q}(0)=\boldsymbol{I}$. This implies $\left.\dfrac{d\boldsymbol{F}_{bond}}{ds}\right|_{s=0} = \left.\dfrac{d\boldsymbol{Q}}{ds}\right|_{s=0}\cdot\boldsymbol{F}_{bond}$. The derivative of the strain energy can be written:

$$\begin{aligned}
\left.\frac{dU}{ds}[w(s)]\right|_{s=0} &= \left.\frac{dQ_{ik}}{ds}\right|_{s=0} \int_{\boldsymbol{x}\in\Omega}\int_{\breve{\boldsymbol{x}}\in\Omega} \left( \frac{\partial\tilde{W}_{loc}}{\partial(F_{bond})_{ij}}(F_{bond})_{kj} + \frac{\partial\tilde{W}_{loc}}{\partial(\breve{y}-y)_i}\cdot(\breve{y}-y)_k \right) dV_{\breve{\boldsymbol{x}}}\, dV_{\boldsymbol{x}} \\
&= \left.\frac{dQ_{ik}}{ds}\right|_{s=0} \int_{\boldsymbol{x}\in\Omega} y_k \int_{\breve{\boldsymbol{x}}\in\Omega} \left(\ldots \text{ nonlocal terms from the equation of motion (3.9)} \ldots\right)_i \, dV_{\breve{\boldsymbol{x}}}\, dV_{\boldsymbol{x}}
\end{aligned} \tag{4.3}$$

where the final form is obtained through the usual relabeling. Noting that $U$ is invariant over the family of transformations $s$, it follows that the expression above is 0. Further, since $\boldsymbol{Q}(s)$ is a rotation, it follows that $\left.\dfrac{dQ_{ik}}{ds}\right|_{s=0}$ is a skew tensor, which we can write in terms of an axial vector: $\dfrac{dQ_{ik}}{ds} = \epsilon_{ijk}\omega_j$. Finally, we replace the nonlocal terms in the final expression above by the inertia and body force terms using (3.9). All of these give us:

$$\boldsymbol{\omega}\cdot\int_{\boldsymbol{x}\in\Omega} \boldsymbol{y}\times(\rho\ddot{\boldsymbol{y}}-\boldsymbol{b})\, dV_{\boldsymbol{x}} = \boldsymbol{0} \Rightarrow \frac{d}{dt}\int_{\boldsymbol{x}\in\Omega} \boldsymbol{y}\times\rho\dot{\boldsymbol{y}}\, dV_{\boldsymbol{x}} = \int_{\boldsymbol{x}\in\Omega} \boldsymbol{y}\times\boldsymbol{b}\, dV_{\boldsymbol{x}} \tag{4.4}$$

where we have used that $\boldsymbol{\omega}$ is arbitrary. That is, the rate of change of angular momentum is equal to the external applied moment.

We briefly consider the setting where we do not have a strain energy density but only a stress response function, e.g. due to inelasticity. The constraint above on $\tilde{W}_{loc}(\boldsymbol{F}_{bond}, \ldots)$ that it must be frame indifferent with respect to $\boldsymbol{F}_{bond}$ implies that the Piola stress $\boldsymbol{T}_{bond} = \tilde{\boldsymbol{T}}_{bond}(\boldsymbol{F}_{bond}) = \boldsymbol{F}_{bond} \cdot \tilde{\boldsymbol{S}}_{bond}(\boldsymbol{F}_{bond})$, where $\tilde{\boldsymbol{S}}_{bond}(\boldsymbol{F}_{bond})$ is the analog to the second Piola Kirchoff stress tensor response function and must return a symmetric tensor. Alternately, we can use $\tilde{\boldsymbol{S}}_{bond}(\boldsymbol{F}_{bond}) = \det \boldsymbol{F}_{bond} \left( \boldsymbol{F}_{bond}^{-1} \cdot \tilde{\boldsymbol{\sigma}}_{bond}(\boldsymbol{F}_{bond}) \cdot \boldsymbol{F}_{bond}^{-T} \right)$ where $\tilde{\boldsymbol{\sigma}}_{bond}(\boldsymbol{F}_{bond})$ is the Cauchy stress response. These relations have a direct and obvious parallel with large-deformation local constitutive models, e.g. [Hol00, Ogd97].

### 4.3 Linear Stability

We consider the linearized setting here. Assume that we have linearized a nonlinear material about an equilibrium state to examine stability (i.e., "small-on-large"). The linearized material will generally be inhomogeneous with the local stiffness tensor corresponding to the tangent modulus of the nonlinear energy at that point. If the local stiffness is everywhere positive definite, then it is immediately apparent from (3.4) that any deformation away from the equilibrium reference state increases the energy, and hence the material is linearly stable. Therefore, a linear peridynamic material in the bond-level deformation gradient approach is stable to all perturbations if the underlying local stiffness tensor is positive-definite for all bonds.

We examine numerically the stability of a homogeneous isotropic 2D linearized model against perturbations in the form of plane-waves of all wavelengths, i.e. $\boldsymbol{y}(\boldsymbol{x}) = \boldsymbol{A} e^{\imath(\boldsymbol{k}\cdot\boldsymbol{x})}$. Note that this does *not* probe the stability of uniform deformations such as biaxial or triaxial stretch, i.e. so-called non-rank-one modes [ADE13, ETS06], but that is in any case a property of the local energy density function and not the peridynamic model.

We nondimensionalize lengths by the peridynamic nonlocal lengthscale $\ell$, and use that $\alpha = \dfrac{1}{\pi}$ when the argument is less than 1 and $\alpha = 0$ otherwise. We use an isotropic local response function $\tilde{W}_{loc}(\boldsymbol{\epsilon}) = \dfrac{\lambda}{2} \operatorname{tr}(\boldsymbol{\epsilon})^2 + \mu \boldsymbol{\epsilon} : \boldsymbol{\epsilon}$, with $\lambda = \mu = 1$ and $\boldsymbol{\epsilon}$ is the linearized strain. Because it is isotropic, we need only test in one direction; we therefore align our coordinate direction such that the wave-vector $\boldsymbol{k} = k\boldsymbol{e}_1$. From symmetry, it is straightforward to see that the eigenvectors of the peridynamic operator correspond to classical P-waves ($\boldsymbol{A} \parallel \boldsymbol{k}$) and S-waves ($\boldsymbol{A} \cdot \boldsymbol{k} = 0$). We therefore focus on these specific choices of $\boldsymbol{A}$ as they provide bounds on the energy in other directions.

Fig. 1 shows the total stored energy of a specimen subjected to the deformation $\boldsymbol{y}$ as a function of $k$. The energy is computed over a large fixed domain (dimensions $\gg 1$) using a fine Cartesian mesh (of size $0.01$) for quadrature. We plot the energy for plane waves with P- and S-polarization for the standard correspondence peridynamic model and the bond-level deformation gradient model; the former has zero-energy modes – and in fact the energy tends to zero as $k \to \infty$ – whereas the latter does not have zero-energy modes. The bond-level deformation gradient model converges to a constant finite energy as $|k| \to \infty$, as expected in peridynamics [Sil00, WA05, Day17]. This is apparent at larger values of $k$ but we do not plot this as it would obscure the features shown in Fig. 1.

### 4.4 Interpenetration and Opening Discontinuities

We examine the behavior of the bond-level deformation gradient model for deformation modes with discontinuities, motivated by [TR14] who studied similar deformations in their approach.

First, we briefly examine what they denote sub-horizon material collapse, namely that a finite volume – with characteristic dimensions much smaller than $\ell$ – of material collapses to a point with zero volume. That is, $\breve{\boldsymbol{y}} = \boldsymbol{y}$ for all $\breve{\boldsymbol{x}}$ within the volume. We notice from (3.2) that $\boldsymbol{F}_{bond}$ will be rank-deficient and hence $\det \boldsymbol{F}_{bond} = 0$. Many standard large-deformation elastic energy densities will be singular when the argument has zero determinant.

Next, we consider discontinuous deformation fields of the form $\boldsymbol{y}(\boldsymbol{x}) = \boldsymbol{x} + c(\boldsymbol{x})\hat{\boldsymbol{e}}$, with $c(\boldsymbol{x}) = 0$ if $\boldsymbol{x} \cdot \hat{\boldsymbol{n}} < 0$ and

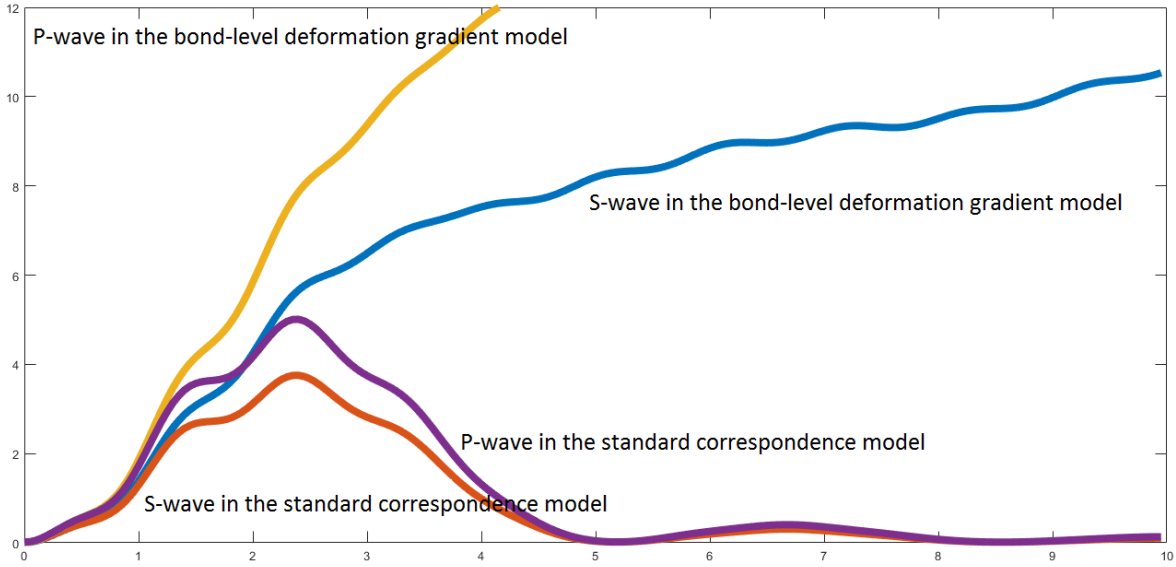


Figure 1: Total stored energy in a domain as a function of $|\boldsymbol{k}|$ for deformations of the type $\boldsymbol{y}(\boldsymbol{x}) = \boldsymbol{A}e^{\imath(\boldsymbol{k}\cdot\boldsymbol{x})}$. The curves correspond to a standard correspondence model and a bond-level deformation gradient model, with $\boldsymbol{A}$ corresponding to P- and S- plane-waves. The material is isotropic with $\lambda = \mu = 1$. Notice that both models have the same energy in the long wavelength limit for the P- and S- type waves respectively.

$c(\boldsymbol{x}) = C$ if $\boldsymbol{x}\cdot\hat{\boldsymbol{n}} \geq 0$. We consider a large body and ignore the issues at boundaries. This corresponds to rigid deformation on either side of the plane $\boldsymbol{x}\cdot\hat{\boldsymbol{n}} = 0$, with a rigid translation $C\hat{\boldsymbol{e}}$ on the positive side and no translation on the negative side, thereby causing a discontinuity along the plane. Notice that if $\hat{\boldsymbol{e}}\cdot\hat{\boldsymbol{n}} = 0$, this deformation corresponds to relative sliding in a direction tangential the separating plane; we expect this deformation to cost finite – nonzero and non-infinite – bond energy in peridynamics. If $\hat{\boldsymbol{e}} \parallel \hat{\boldsymbol{n}}$, this deformation corresponds to opening a gap if $C > 0$, and interpenetration if $C < 0$; the former should again cost finite bond energy while the latter should cause the bond energy to be singular.

We compute $\boldsymbol{F}_{ave}$ for this class of deformations:

$$\boldsymbol{F}_{ave} = \int_{\mathring{\boldsymbol{x}}\in\Omega} \alpha(\mathring{\boldsymbol{x}}-\boldsymbol{x})\left(\mathring{\boldsymbol{y}}-\boldsymbol{y}\right)\otimes\left(\mathring{\boldsymbol{x}}-\boldsymbol{x}\right)\, dV_{\mathring{\boldsymbol{x}}} = \boldsymbol{I} + \hat{\boldsymbol{e}}\otimes\int_{\mathring{\boldsymbol{x}}\in\Omega} \alpha(\mathring{\boldsymbol{x}}-\boldsymbol{x})\left(c(\mathring{\boldsymbol{x}})-c(\boldsymbol{x})\right)\left(\mathring{\boldsymbol{x}}-\boldsymbol{x}\right)\, dV_{\mathring{\boldsymbol{x}}} \quad (4.5)$$

We consider the quantity $\boldsymbol{r}(\boldsymbol{x}) := \int_{\mathring{\boldsymbol{x}}\in\Omega} \alpha(\mathring{\boldsymbol{x}}-\boldsymbol{x})\left(c(\mathring{\boldsymbol{x}})-c(\boldsymbol{x})\right)\left(\mathring{\boldsymbol{x}}-\boldsymbol{x}\right)\, dV_{\mathring{\boldsymbol{x}}}$. The only distinguished direction is $\hat{\boldsymbol{n}}$ and therefore $\boldsymbol{r} \parallel \hat{\boldsymbol{n}}$; if $\boldsymbol{r}$ were at some nonzero angle to $\hat{\boldsymbol{n}}$, by symmetry it could equally well be at the negative of that angle. Alternately, one can reach the same conclusion by noticing that the integrand in the definition of $\boldsymbol{r}$ is non-zero only when $\boldsymbol{x}$ and $\mathring{\boldsymbol{x}}$ are on opposite sides of $\boldsymbol{x}\cdot\hat{\boldsymbol{n}} = 0$; and $\left(c(\mathring{\boldsymbol{x}})-c(\boldsymbol{x})\right) = C$ in this case. Therefore, for a given $\boldsymbol{x}$, the integration over $\mathring{\boldsymbol{x}}$ on the other side of the plane can be decomposed into integrations over circular disks with normal $\hat{\boldsymbol{n}}$ and centered at $\boldsymbol{x} + \text{const.}\hat{\boldsymbol{n}}$. By symmetry, the part of $\left(\mathring{\boldsymbol{x}}-\boldsymbol{x}\right)$ normal to $\hat{\boldsymbol{n}}$ integrates to $\boldsymbol{0}$ over the disk, and only the contribution parallel to $\hat{\boldsymbol{n}}$ survives. Hence $\boldsymbol{r} \parallel \hat{\boldsymbol{n}}$, and $\boldsymbol{F}_{ave} = \boldsymbol{I} + \hat{\boldsymbol{e}}\otimes\boldsymbol{r}$.

We next use $\boldsymbol{F}_{ave}$ and the form of $\boldsymbol{y}$ to find $\boldsymbol{F}_{bond}$ using the definition from (3.2):

$$\begin{aligned}\boldsymbol{F}_{bond}(\boldsymbol{x},\breve{\boldsymbol{x}}) &= (\boldsymbol{I}+\hat{\boldsymbol{e}}\otimes\boldsymbol{r}(\boldsymbol{x}))\cdot\left(\boldsymbol{I}-\widehat{\boldsymbol{x}-\breve{\boldsymbol{x}}}\otimes\widehat{\boldsymbol{x}-\breve{\boldsymbol{x}}}\right)+\widehat{\boldsymbol{x}-\breve{\boldsymbol{x}}}\otimes\widehat{\boldsymbol{x}-\breve{\boldsymbol{x}}}+\frac{c(\boldsymbol{x})-c(\breve{\boldsymbol{x}})}{|\boldsymbol{x}-\breve{\boldsymbol{x}}|}\hat{\boldsymbol{e}}\otimes\widehat{\boldsymbol{x}-\breve{\boldsymbol{x}}} \\ &= \boldsymbol{I}+\hat{\boldsymbol{e}}\otimes\boldsymbol{r}(\boldsymbol{x})-\left(\boldsymbol{r}(\boldsymbol{x})\cdot\widehat{\boldsymbol{x}-\breve{\boldsymbol{x}}}\right)\hat{\boldsymbol{e}}\otimes\widehat{\boldsymbol{x}-\breve{\boldsymbol{x}}}+\frac{c(\boldsymbol{x})-c(\breve{\boldsymbol{x}})}{|\boldsymbol{x}-\breve{\boldsymbol{x}}|}\hat{\boldsymbol{e}}\otimes\widehat{\boldsymbol{x}-\breve{\boldsymbol{x}}}\end{aligned} \quad (4.6)$$

Consider now specifically bonds that connect points across the dividing plane; for specificity, consider $\boldsymbol{x}$ on the positive side and $\breve{\boldsymbol{x}}$ on the negative side. Further, consider those bonds whose reference directions are normal to the dividing plane: $\widehat{\boldsymbol{x}-\breve{\boldsymbol{x}}} = \hat{\boldsymbol{n}}$. For these bonds, using further that $\boldsymbol{r}(\boldsymbol{x}) \parallel \hat{\boldsymbol{n}}$, the bond deformation gradient reduces to:

$$\boldsymbol{F}_{bond}(\boldsymbol{x}, \breve{\boldsymbol{x}}) = \boldsymbol{I} + \frac{C}{|\boldsymbol{x}-\breve{\boldsymbol{x}}|}\hat{\boldsymbol{e}} \otimes \hat{\boldsymbol{n}} \tag{4.7}$$

Recall the spectral decomposition of $\boldsymbol{I} = \sum_i \hat{\boldsymbol{p}}_i \otimes \hat{\boldsymbol{p}}_i$, where $\{\hat{\boldsymbol{p}}_1, \hat{\boldsymbol{p}}_2, \hat{\boldsymbol{p}}_3\}$ are any set of orthonormal vectors; in particular, we choose $\hat{\boldsymbol{p}}_1 = \hat{\boldsymbol{e}}$. We use this to examine three distinguished cases below.

First, consider $\hat{\boldsymbol{n}} \parallel \hat{\boldsymbol{e}}$ with $C < 0$ which corresponds to interpenetration. We can then write $\boldsymbol{F}_{bond}(\boldsymbol{x}, \breve{\boldsymbol{x}}) = \left(1 + \frac{C}{|\boldsymbol{x}-\breve{\boldsymbol{x}}|}\right)\hat{\boldsymbol{p}}_1 \otimes \hat{\boldsymbol{p}}_1 + \hat{\boldsymbol{p}}_2 \otimes \hat{\boldsymbol{p}}_2 + \hat{\boldsymbol{p}}_3 \otimes \hat{\boldsymbol{p}}_3$. For any $C < 0$, we can find bonds that connect points that are sufficiently close to the dividing plane such that $C < -|\boldsymbol{x}-\breve{\boldsymbol{x}}|$. Therefore, there will be bonds with bond-level deformation gradients having negative determinant, and a standard local energy density will be singular. The "number" – or more strictly the measure – of singular bonds, and consequently the effect on the total energy, will depend on the level of interpenetration as measured by $C$.

Second, consider $\hat{\boldsymbol{n}} \parallel \hat{\boldsymbol{e}}$ with $C > 0$ which corresponds to opening of a gap. The bond deformation gradient (4.7) will have the same form as for interpenetration, but with the eigenvalue corresponding to $\hat{\boldsymbol{p}}_1$ being greater than 1. For a standard large-deformation local energy density that has minimum energy at $\boldsymbol{I}$, there will be a finite energetic cost for opening a gap.

Third, consider $\hat{\boldsymbol{n}} \cdot \hat{\boldsymbol{e}} = 0$ that corresponds to relative sliding between the two sides of the dividing plane. The bond deformation gradient (4.7) will have the form of a shear and a standard large-deformation local energy density will again impose a finite energetic cost for this deformation.

Finally, we briefly examine a specific example to show the interplay between the average deformation gradient and the deviation from the average of the particular bond. Consider in 2D the bond connecting the points $\boldsymbol{x} - \breve{\boldsymbol{x}} = \hat{\boldsymbol{e}}_1$ and with deformation $\boldsymbol{y} - \breve{\boldsymbol{y}} = \hat{\boldsymbol{e}}_2$, where $\hat{\boldsymbol{e}}_1$ and $\hat{\boldsymbol{e}}_2$ are orthonormal unit vectors. Consider first the case where the average deformation gradient $\boldsymbol{F}_{ave}(\boldsymbol{x}) = \boldsymbol{I}$: the bond deformation gradient $\boldsymbol{F}_{bond}(\boldsymbol{x}, \breve{\boldsymbol{x}}) = \hat{\boldsymbol{e}}_2 \otimes \hat{\boldsymbol{e}}_2 + \hat{\boldsymbol{e}}_2 \otimes \hat{\boldsymbol{e}}_1$ which has zero determinant and singular energy in a standard local large deformation elastic energy density. Physically, this corresponds to the bond collapsing to zero volume. Consider next the case where the average deformation gradient $\boldsymbol{F}_{ave}(\boldsymbol{x}) = \boldsymbol{Q}_{\hat{\boldsymbol{e}}_3, \pi/2}$ is a rotation that maps $\hat{\boldsymbol{e}}_1$ to $\hat{\boldsymbol{e}}_2$. Since this coincides precisely with the deformation experienced by the bond $\boldsymbol{x} - \breve{\boldsymbol{x}}$, it follows that $\boldsymbol{F}_{bond}(\boldsymbol{x}, \breve{\boldsymbol{x}}) = \boldsymbol{Q}_{\hat{\boldsymbol{e}}_3, \pi/2}$. Physically, the material element has, on average, undergone a rigid rotation and the bond has followed this rigid rotation. A standard local large-deformation frame-indifferent elastic energy density will assign this deformation the same energy as the identity deformation.

# 5 Concluding Remarks

We have proposed a new approach to incorporate classical local strain energy responses into peridynamics. Unlike correspondence methods that aim to achieve the similar goal but have issues such as linear instabilities, our approach is stable to linear perturbations if the underlying local strain energy is stable. In contrast to other stabilization methods, namely [TR14, Sil17] which handle interpenetration and linear instabilities respectively, our approach handles both these settings in a single framework. In addition, we do not introduce additional penalty parameters but instead work exclusively through the given local large-deformation elastic energy functions. The final equations of motion are written in terms of the stress response function, and can form the starting point when a strain energy function is not available as in inelasticity.

The two key elements of our approach are the definition of a bond-level deformation gradient, and the subsequent use of this quantity as the argument in a classical local strain energy density that is then averaged to obtain the

peridynamic energy density. Roughly, the correspondence model first averages and then evaluates the energy, whereas the bond-level deformation gradient model first evaluates the energy and then averages. These operations do not commute for standard small- and large-deformation energy density functions. We examine this further in Appendix A where we also present a simpler version of the bond-level deformation gradient model. A related perspective on this issue is to notice that the deformation gradient is a 1-form in the notation of differential geometry [MH94]. Volume and area averages of 1-forms generally do not provide meaningful physical quantities; rather, they are objects that are naturally integrated along curves, e.g. [AD15].

The bond-level deformation gradient model is more expensive than the usual correspondence models. In the discretized setting, the usual correspondence models require one integration at each node to find the average deformation gradient field, and then a further integration at each node to sum over the stresses to find the force density. The bond-level deformation gradient model requires three such integrations at each node: once to find the average deformation gradient field, and two more as can be immediately seen in (3.9). We also note that the linearly-stabilized model proposed in [Sil17] has a similar level of effort: one integration to find the average deformation gradient in his (14), a second integration to find the stabilizing stress in his (54), and finally a third integration at each node to find the force density in his (2). However, we also note that integration is a linear operation, and corresponds to matrix-vector multiplication operations in a discretized setting. In a uniform discretization, the quadrature weights are the same at every node and therefore one can store a single, dense but relatively small, matrix that corresponds to this operation and use it to perform the integrations rapidly.

We notice that sets of zero measure do not contribute to the energy. Loosely speaking, if a single infinitesimal bond collapses to zero stretch or an infinitesimal material point drifts away from the body, there will be no contribution to the integral measures of energy. This issue occurs generically in peridynamics and not just in the bond-level deformation gradient model in this paper. While this is also true in the classical local elasticity setting, the choice of appropriate standard function spaces for the solution prevents such deformations from occurring there. However, peridynamics aims to have solutions with reduced smoothness that can model fracture, and then the appropriate function space that allows fracture but not these more complex and seemingly-unphysical deformations must be used. Characterizing this and related issues is the focus of much current activity, e.g. [JL17, MD15, BMC14, RTT].

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## A A Simplified Bond-Level Deformation Gradient Model

We discuss here a slightly simplified version of the bond-level deformation gradient model. While it has the advantage of simplicity over the version discussed in the main body of the paper, a minor point is that it does not precisely fit within the framework of standard correspondence models.

Below, we use the superscript $s$ to denote the simplified redefinition of quantities that have already been introduced.

We begin by redefining the average deformation gradient as

$$\boldsymbol{F}^s_{ave}(\boldsymbol{x}) = 3\int_{\mathring{\boldsymbol{x}}\in\Omega} \alpha(\boldsymbol{x}-\mathring{\boldsymbol{x}})\frac{\mathring{\boldsymbol{y}}-\boldsymbol{y}}{\left|\mathring{\boldsymbol{x}}-\boldsymbol{x}\right|}\otimes\widehat{\mathring{\boldsymbol{x}}-\boldsymbol{x}}\,dV_{\mathring{\boldsymbol{x}}} \tag{A.1}$$

Comparing with (2.3), we notice the following differences between $\boldsymbol{F}^s_{ave}$ and $\boldsymbol{F}_{ave}$: first, the integrand has been normalized in $\boldsymbol{F}^s_{ave}$; second, there is a leading factor of 3 corresponding to the 3D setting, which must be replaced by 2 for the 2D setting, see (1.1); and third, the tensor $\boldsymbol{K}$ accounts for these dimensional factors in the standard correspondence models but plays no role in this formula, and consequently does not appear at all in the simplified model[5]. Also, when the deformation is uniform and given by $\boldsymbol{y}=\boldsymbol{F}_0\cdot\boldsymbol{x}$, we have that $\boldsymbol{F}^s_{ave}=\boldsymbol{F}_{ave}=\boldsymbol{F}_0$. Further, the formula above could alternatively be posed as a redefinition of $\alpha$ to extract factors of $\left|\mathring{\boldsymbol{x}}-\boldsymbol{x}\right|$.

We now redefine the bond-level deformation gradient by using precisely the formula in (3.2), but replacing $\boldsymbol{F}^s_{ave}$ for $\boldsymbol{F}_{ave}$:

$$\boldsymbol{F}^s_{bond}(\boldsymbol{x},\breve{\boldsymbol{x}}) = \boldsymbol{F}^s_{ave}(\boldsymbol{x})\left(\boldsymbol{I}-\widehat{\breve{\boldsymbol{x}}-\boldsymbol{x}}\otimes\widehat{\breve{\boldsymbol{x}}-\boldsymbol{x}}\right)+\frac{\breve{\boldsymbol{y}}-\boldsymbol{y}}{|\breve{\boldsymbol{x}}-\boldsymbol{x}|}\otimes\widehat{\breve{\boldsymbol{x}}-\boldsymbol{x}} \tag{A.2}$$

These simplified redefinitions give us the satisfying relation that averaging $\boldsymbol{F}^s_{bond}(\boldsymbol{x},\breve{\boldsymbol{x}})$ over $\breve{\boldsymbol{x}}\in\Omega$ gives $\boldsymbol{F}^s_{ave}(\boldsymbol{x})$:

$$\begin{aligned}
&\int_{\breve{\boldsymbol{x}}\in\Omega}\alpha(\boldsymbol{x}-\breve{\boldsymbol{x}})\boldsymbol{F}^s_{bond}(\boldsymbol{x},\breve{\boldsymbol{x}})\,dV_{\breve{\boldsymbol{x}}}\\
&=\boldsymbol{F}^s_{ave}(\boldsymbol{x})\int_{\breve{\boldsymbol{x}}\in\Omega}\alpha(\boldsymbol{x}-\breve{\boldsymbol{x}})\,dV_{\breve{\boldsymbol{x}}}-\boldsymbol{F}^s_{ave}(\boldsymbol{x})\cdot\int_{\breve{\boldsymbol{x}}\in\Omega}\alpha(\boldsymbol{x}-\breve{\boldsymbol{x}})\widehat{\breve{\boldsymbol{x}}-\boldsymbol{x}}\otimes\widehat{\breve{\boldsymbol{x}}-\boldsymbol{x}}\,dV_{\breve{\boldsymbol{x}}}+\int_{\breve{\boldsymbol{x}}\in\Omega}\alpha(\boldsymbol{x}-\breve{\boldsymbol{x}})\frac{\breve{\boldsymbol{y}}-\boldsymbol{y}}{|\breve{\boldsymbol{x}}-\boldsymbol{x}|}\otimes\widehat{\breve{\boldsymbol{x}}-\boldsymbol{x}}\,dV_{\breve{\boldsymbol{x}}}\\
&=\boldsymbol{F}^s_{ave}(\boldsymbol{x})-\boldsymbol{F}^s_{ave}(\boldsymbol{x})\cdot\frac{\boldsymbol{I}}{3}+\frac{1}{3}\boldsymbol{F}^s_{ave}(\boldsymbol{x})=\boldsymbol{F}^s_{ave}(\boldsymbol{x})
\end{aligned} \tag{A.3}$$

To arrive at the result above, we have used the properties of $\alpha$ from (1.1) corresponding to 3D; in 2D, the factors of $1/3$ are replaced by factors of $1/2$ giving the same final result.

With these redefinitions, the energy densities per unit volume in the correspondence approach and the bond-level deformation gradient model are therefore given respectively by:

$$\underbrace{W(\boldsymbol{x})=\tilde{W}_{loc}\left(\int_{\breve{\boldsymbol{x}}\in\Omega}\alpha(\boldsymbol{x}-\breve{\boldsymbol{x}})\boldsymbol{F}^s_{bond}(\boldsymbol{x},\breve{\boldsymbol{x}})\,dV_{\breve{\boldsymbol{x}}}\right)}_{\text{correspondence model}}\text{ compared to }\underbrace{W(\boldsymbol{x})=\int_{\breve{\boldsymbol{x}}\in\Omega}\alpha(\boldsymbol{x}-\breve{\boldsymbol{x}})\tilde{W}_{loc}\left(\boldsymbol{F}^s_{bond}(\boldsymbol{x},\breve{\boldsymbol{x}})\right)\,dV_{\breve{\boldsymbol{x}}}}_{\text{bond-level deformation gradient model}} \tag{A.4}$$

That is, the correspondence model first averages and then evaluates the energy, whereas the bond-level deformation gradient approach first evaluates the energy and then averages. As noted elsewhere in this manuscript, these operations do not commute for standard small- and large-deformation energy density functions.

The equation of motion in the simplified bond-level deformation gradient model is given by:

$$\begin{aligned}
\rho\ddot{y}_i =& b_i+\int_{\breve{\boldsymbol{x}}\in\Omega}\alpha(\breve{\boldsymbol{x}}-\boldsymbol{x})\frac{\partial\tilde{W}_{loc}}{\partial(y-\breve{y})_i}\,dV_{\breve{\boldsymbol{x}}}+\int_{\breve{\boldsymbol{x}}\in\Omega}\frac{\alpha(\breve{\boldsymbol{x}}-\boldsymbol{x})}{|\breve{\boldsymbol{x}}-\boldsymbol{x}|}\frac{1}{2}\left(T^s_{bond}(\boldsymbol{x},\breve{\boldsymbol{x}})+T^s_{bond}(\breve{\boldsymbol{x}},\boldsymbol{x})\right)_{ij}\left(\widehat{\breve{x}-x}\right)_j\,dV_{\breve{\boldsymbol{x}}}\\
&+\frac{1}{2}\int_{\breve{\boldsymbol{x}}\in\Omega}\int_{\mathring{\boldsymbol{x}}\in\Omega}\alpha(\breve{\boldsymbol{x}}-\mathring{\boldsymbol{x}})\frac{\alpha(\boldsymbol{x}-\mathring{\boldsymbol{x}})}{\left|\boldsymbol{x}-\mathring{\boldsymbol{x}}\right|}(T^s_{bond}(\mathring{\boldsymbol{x}},\breve{\boldsymbol{x}}))_{ij}\left(\widehat{\breve{x}-\mathring{x}}\right)_j\left(1-\left(\widehat{\breve{x}-\mathring{x}}\right)_k\left(\widehat{x-\mathring{x}}\right)_k\right)\,dV_{\mathring{\boldsymbol{x}}}\,dV_{\breve{\boldsymbol{x}}}
\end{aligned} \tag{A.5}$$

[5]While the use of $\boldsymbol{K}$ would make the current discussion cumbersome, the normalization by $\boldsymbol{K}$ in fact makes it much simpler to deal with boundaries generally.

This can be compared with the version in (3.9). Note that $\boldsymbol{T}^s_{bond}(\boldsymbol{x},\hat{\boldsymbol{x}}) = \left.\dfrac{\partial \tilde{W}_{loc}}{\partial \boldsymbol{F}}(\boldsymbol{F})\right|_{\boldsymbol{F}=\boldsymbol{F}^s_{bond}(\boldsymbol{x},\hat{\boldsymbol{x}})}$.

We note that various integrands contain $\dfrac{1}{|\boldsymbol{x}-\breve{\boldsymbol{x}}|}$ and similar quantities. The weight function $\alpha$ must be appropriately chosen to for these integrals to converge in principle and be computable efficiently in practice. However, this issue also arises in the model described in the body of the paper and not just this simplified version.

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