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Modeling Thermal Strains with Peridynamics

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Abstract

Peridynamics, a nonlocal extension of continuum mechanics, is a natural framework for capturing constitutive response and modeling pervasive material failure. Unlike classical approaches incorporating partial derivatives, the peridynamic governing equations utilize integral expressions that remain valid in the presence of discontinuities such as cracks. The mathematical theory of peridynamics unifies the mechanics of continuous media, cracks, and discrete particles. The result is a consistent framework for capturing a wide range of constitutive responses in combination with robust material failure laws.

The effect of thermal expansion can be included in peridynamic simulations through a straightforward modification of the bond extensions. This process is described below for the *linear peridynamic solid* constitutive model. A demonstration calculation is presented in which a pre-cracked plate, fixed at opposite ends, is subjected to a uniform temperature reduction. The resulting strain energy density at the crack tip is shown to be a function of the nonlocal length scale, the peridynamic horizon.

1 Introduction to Peridynamic Theory

Peridynamics is a nonlocal extension of continuum mechanics [1, 2, 3]. In contrast to the classical approach, the balance of linear momentum is formulated as an integral equation that remains valid in the presence of material discontinuities such as cracks. In peridynamics, a material point $\mathbf{x}$ interacts directly with all neighboring material points $\mathbf{x}'$ within a finite distance, δ, termed the *horizon*. The vectors connecting the point $\mathbf{x}$ to its neighbors $\mathbf{x}'$ are referred to as *bonds*. The union of all neighbors $\mathbf{x}'$ of $\mathbf{x}$ are referred to as the *family* of $\mathbf{x}$.

The peridynamic balance of linear momentum at time t for the point $\mathbf{x}$ in the body $\mathscr{B}$ is given by

$$\rho(\mathbf{x})\ddot{\mathbf{u}}(\mathbf{x},t) = \mathbf{L}_{\mathbf{u}}(\mathbf{x},t) + \mathbf{b}(\mathbf{x},t) \qquad \forall\, \mathbf{x} \in \mathscr{B},\ \ t \geq 0, \tag{1}$$

$$\mathbf{L}_{\mathbf{u}}(\mathbf{x},t) = \int_{\mathscr{B}} \left\{ \underline{\mathbf{T}}[\mathbf{x},t]\,\langle \mathbf{x}' - \mathbf{x} \rangle - \underline{\mathbf{T}}'[\mathbf{x}',t]\,\langle \mathbf{x} - \mathbf{x}' \rangle \right\} \mathrm{d}V_{\mathbf{x}'},$$

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where ρ is the material density, $\mathbf{u}$ denotes displacement, and $\mathbf{b}$ is an external body force. The force density at point $\mathbf{x}$ due to direct interactions with neighbors $\mathbf{x}'$ is given by the term $\mathbf{L_u}(\mathbf{x}, t)$. Here, $\underline{\mathbf{T}}[\mathbf{x}, t]$ denotes the peridynamic *force state* for point $\mathbf{x}$ at time t, described below, and $\mathrm{d}V_{\mathbf{x}'}$ is the volume associated with neighbor $\mathbf{x}'$. Peridynamics is an extension of continuum mechanics in that the classical (local) equations are recovered in the limit as the horizon approaches zero, assuming the deformation field is sufficiently smooth [4].

One approach to discretizing Equation (1) is the mesh-free approach of Silling and Askari [5]. Under this approach, the strong form of the balance of linear momentum is solved numerically by dividing the body $\mathscr{B}$ into a finite number of cells, each tracked using a single node located at its center. The integral expression in Equation (1) is replaced by a summation, yielding the discrete equation

$$\rho(\mathbf{x})\ddot{\mathbf{u}}_h(\mathbf{x}, t) = \sum_{i=0}^{N} \left\{ \underline{\mathbf{T}}[\mathbf{x}, t] \langle \mathbf{x}'_i - \mathbf{x} \rangle - \underline{\mathbf{T}}'_i[\mathbf{x}'_i, t] \langle \mathbf{x} - \mathbf{x}'_i \rangle \right\} \Delta V_{\mathbf{x}'_i} + \mathbf{b}(\mathbf{x}, t), \tag{2}$$

where N is the number of cells in the neighborhood of $\mathbf{x}$, $\mathbf{x}'_i$ is the position of the node centered in cell i, and $\Delta V_{\mathbf{x}'_i}$ is the volume of cell i.

Equation (2) requires evaluation of the pairwise forces $\underline{\mathbf{T}}[\mathbf{x}, t] \langle \mathbf{x}' - \mathbf{x} \rangle$ and $\underline{\mathbf{T}}'[\mathbf{x}', t] \langle \mathbf{x} - \mathbf{x}' \rangle$, where the force states $\underline{\mathbf{T}}[\mathbf{x}, t]$ and $\underline{\mathbf{T}}'[\mathbf{x}', t]$ are, in general, functions of the deformations of all nodes within the neighborhoods of $\mathbf{x}$ and $\mathbf{x}'$, respectively. A constitutive model is a relation that determines the force state $\underline{\mathbf{T}}[\mathbf{x}, t]$ in terms of the *deformation state* in the neighborhood of $\mathbf{x}$ and possibly other variables as well.

1.1 Linear Peridynamic Solid Material Model

The *linear peridynamic solid* material model is one example of a peridynamic constitutive law [2]. It is a *state-based* model, meaning that the pairwise force between material points $\mathbf{x}$ and $\mathbf{x}'$ is a function of the deformations of all the material points within the neighborhoods of $\mathbf{x}$ and $\mathbf{x}'$, and possibly other variables as well [2, 6]. The linear peridynamic solid constitutive law dictates that the action of the force state at $\mathbf{x}$ on the bond $\langle \mathbf{x}' - \mathbf{x} \rangle$ is directed along the bond,

$$\underline{\mathbf{T}}[\mathbf{x}, t] \langle \mathbf{x}' - \mathbf{x} \rangle = \underline{t}\ \underline{\mathbf{M}}[\mathbf{x}, t] \langle \mathbf{x}' - \mathbf{x} \rangle, \tag{3}$$

where the magnitude is given by $\underline{t}$, and $\underline{\mathbf{M}}[\mathbf{x}, t] \langle \mathbf{x}' - \mathbf{x} \rangle$ is the unit vector pointing from the deformed position of $\mathbf{x}$ to the deformed position of $\mathbf{x}'$. Material models in which pairwise forces act in accordance with Equation (3) are termed *ordinary materials*.

In peridynamics, kinematic quantities may be defined in terms of the *bond extension*, $\underline{e}$, for each bond in a given family. Given a pair of bonded material points $\mathbf{x}$ and $\mathbf{x}'$, bond extension is defined as the difference between the length of the bond $\langle \mathbf{x}' - \mathbf{x} \rangle$ in the deformed configuration and its length in the initial configuration. A kinematic quantity appearing in the constitutive equations for the linear peridynamic solid is the peridynamic dilatation, θ,

$$\theta = \int_{\mathcal{H}} \frac{3}{m} (\underline{\omega}\, \underline{x}) \cdot \underline{e}\, dV, \tag{4}$$

where m is the weighted volume at $\mathbf{x}$, $\underline{\omega}$ is the value of the influence function between $\mathbf{x}$ and $\mathbf{x}'$, and $\underline{x}$ is the length of the bond $\langle \mathbf{x}' - \mathbf{x} \rangle$ in the undeformed configuration. The integral in Equation (4) is an integral over the volume $\mathcal{H}$ that defines the neighborhood of $\mathbf{x}$.

The value of $\underline{t}$ in a linear peridynamic solid is given by

$$\underline{t} = \frac{3k\theta}{m}\underline{\omega}\,\underline{x} + \frac{15\mu}{m}\underline{\omega}\,\underline{e}^d, \tag{5}$$

where μ and k are the shear modulus and bulk modulus, respectively, and $\underline{e}^d$ is the deviatoric part of the extension,

$$\underline{e}^d = \underline{e} - \frac{\theta\,\underline{x}}{3}. \tag{6}$$

1.2 Incorporating Thermal Strains

Thermal strains may be incorporated into the linear peridynamic solid through a straightforward modification of the bond extension. Let $\underline{x}$ denote the length of the bond $\langle \mathbf{x}' - \mathbf{x} \rangle$ in the undeformed configuration, and $\underline{y}$ the length of the bond $\langle \mathbf{x}' - \mathbf{x} \rangle$ in the deformed configuration. The bond extension, $\underline{e}$, is then given by

$$\underline{e} = \underline{y} - \underline{x}. \tag{7}$$

The portion of bond extension resulting from a change in temperature may be modeled as

$$\underline{e}^{\text{thermal}} = \alpha\,\Delta T\,\underline{x}, \tag{8}$$

where α is the coefficient of thermal expansion and ΔT is the change in temperature. The portion of the bond extension contributing to the force state is then

$$\underline{e}^* = \underline{e} - \underline{e}^{\text{thermal}} = \underline{e} - \alpha\,\Delta T\,\underline{x}. \tag{9}$$

Incorporating thermal strains into the expression for the dilatation, given by Equation (4), yields

$$\theta^* = \int_{\mathcal{H}} \frac{3}{m}\,(\underline{\omega}\,\underline{x}) \cdot \underline{e}^*\,dV. \tag{10}$$

Likewise, the deviatoric part of the bond extension given by Equation (6) becomes

$$\underline{e}^{*d} = \underline{e}^* - \frac{\theta^*\,\underline{x}}{3}. \tag{11}$$

Inclusion of thermal strains in the expression for $\underline{t}$, Equation (5), yields

$$\underline{t}^* = \frac{3k\theta^*}{m}\underline{\omega}\,\underline{x} + \frac{15\mu}{m}\underline{\omega}\,\underline{e}^{*d}. \tag{12}$$

1.3 Modeling Crack Propagation

Peridynamics includes a natural mechanism for modeling fracture through the breaking of peridynamic bonds. In an undamaged material, bonds connect a given material point $\mathbf{x}$ to each material point $\mathbf{x}'$ within its neighborhood in the reference configuration. A damage law dictates the conditions under which individual bonds are broken. Material discontinuities, such as cracks, form as a result of the accumulation of broken bonds.

The critical stretch damage model is one example of a peridynamic bond failure law [5]. The critical stretch model assigns a damage value of zero (unbroken) or one (broken) as a function of the maximum stretch

obtained by a bond and a critical stretch material parameter, $\underline{s}_{\text{crit}}$. The damage value, ϕ, is given by the relation

$$\phi = \begin{cases} 0 & \text{for} \quad \underline{s}_{\max} < \underline{s}_{\text{crit}} \\ 1 & \text{for} \quad \underline{s}_{\max} \geq \underline{s}_{\text{crit}}, \end{cases} \tag{13}$$

where $\underline{s}_{\max}$ is the maximum stretch,

$$\underline{s}_{\max} = \frac{\underline{e}_{\max}}{\underline{x}}. \tag{14}$$

Here, $\underline{e}_{\max}$ is the maximum extension between the bonded material points $\mathbf{x}$ and $\mathbf{x}'$ achieved over the duration of the simulation. The use of the maximum extension, $\underline{e}_{\max}$, ensures that the breaking of bonds is irreversible.

Modification of Equations (13) and (14) to include thermal strains yields

$$\phi = \begin{cases} 0 & \text{for} \quad \underline{s}^*_{\max} < \underline{s}_{\text{crit}} \\ 1 & \text{for} \quad \underline{s}^*_{\max} \geq \underline{s}_{\text{crit}}, \end{cases} \tag{15}$$

where

$$\underline{s}^*_{\max} = \frac{\underline{e}^*_{\max}}{\underline{x}}. \tag{16}$$

2 Example Simulation: Plate with a Pre-crack

The modified linear peridynamic solid constitutive law, described above, was applied to model the response of a pre-cracked plate subjected to a change in temperature. Simulations were carried out using the open-source computational peridynamics code *Peridigm* [7, 8].

The plate, illustrated in Figure 1, has dimensions of 0.50 by 0.25 by 0.05 inches. The pre-crack, also illustrated in Figure 1, runs from the left-hand side of the plate into the plate at an angle of 45 degrees. The material parameters assigned to the plate are given in Table 1.

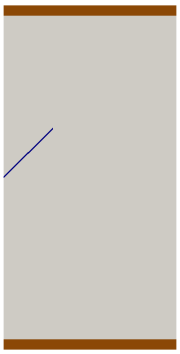


Figure 1: Plate with a pre-crack. The pre-crack is shown in blue. The sections at the top and bottom of the plate, colored brown, denote the volumes over which boundary conditions are applied.

Table 1: Material Model Parameters.

Young's Modulus	3.0e7 $\frac{lbf}{in^2}$
Poisson's Ratio	0.3
Density	7.25e-4 $\frac{lb \cdot s^2}{in^4}$
Thermal Expansion Coefficient	6.3e-6 $\frac{in}{in \cdot ^\circ \mathrm{F}}$
Peridynamic Horizon	1.26e-2 in

A quasi-static simulation was carried out in which the ends of the plate, as illustrated in Figure 1, where held fixed and the plate was subjected to a 158.73 degree decrease in temperature, from 1000 degrees to 841.27 degrees Fahrenheit. For the purpose of comparison, an initial simulation using classical finite-element analysis was carried out using *Ansys*. Results from the *Ansys* simulation are presented in Figure 2.

Peridynamic simulation results are presented in Figure 3 for two different discretizations. Figure 3(a) contains results for an uniformly-spaced discretization, whereas Figure 3(b) contains results obtained using a discretization created with the *Cubit* meshing tool. In both cases, a concentration of strain energy is present in the vicinity of the crack tip and the strain-energy contours are in qualitative agreement with those obtained using classical finite element analysis.

An important distinction between the peridynamic solution and the classical (local) solution stems from the nonlocal length scale present in the peridynamic model. This length scale is provided by the peridynamic horizon and dictates the nonlocal region over which the integral operator in Equation (1) acts. This length scale is independent of the discretization and strongly influences the distribution of strain energy in the vicinity of the crack tip. In contrast, the distribution of strain energy in the classical finite-element solution is determined largely by the size of the elements at the crack tip.

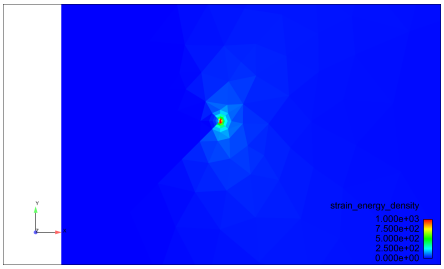
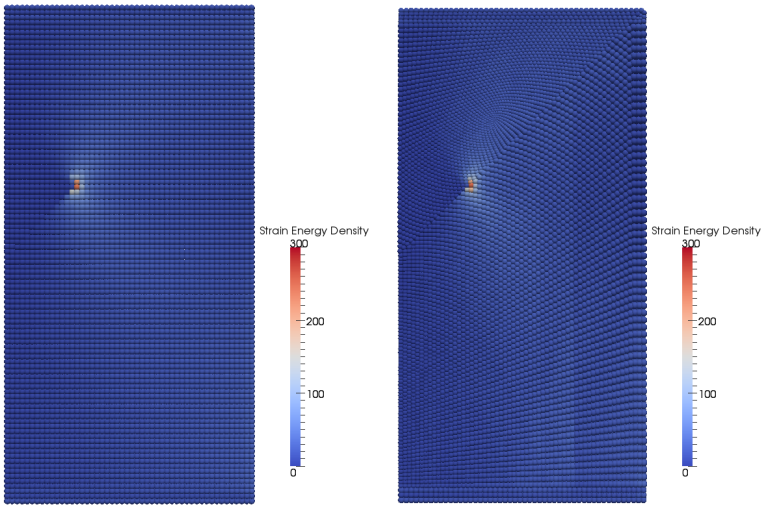


Figure 2: Classical finite-element solution using *Ansys*. Strain energy density is shown in the vicinity of the crack tip.



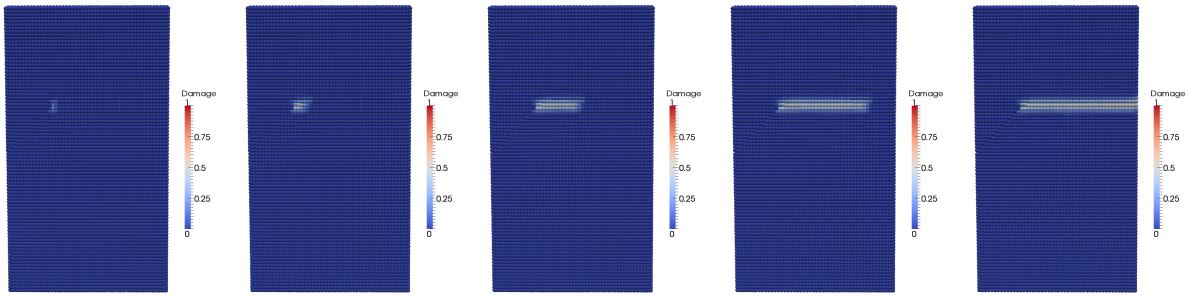
(a) Equally-spaced grid. (b) Cubit-generated mesh.

Figure 3: Comparison of *Peridigm* simulations using a uniformly-spaced mesh (49999 elements) and a Cubit-generated mesh (62020 element). In both cases, the peridynamic horizon is 0.0126 in.

2.1 Modeling Crack Propagation

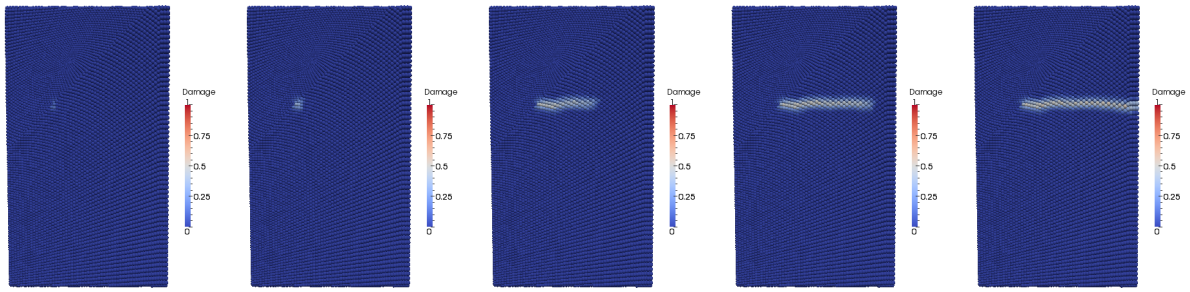
A set of calculations was carried out to demonstrate peridynamics as a means to model crack propagation. The pre-cracked plate, described above, was held fixed at its ends and subjected to a reduction in temperature. Material failure was modeling using the critical stretch bond failure law, described in Section 1.3. The simulations were carried out via explicit transient dynamics in *Peridigm*.

Crack initiation and propagation resulting from thermally-induced material constriction is presented in Figures 4 and 5. Figure 4 contains results for a uniformly-spaced mesh, and Figure 5 contains results for a mesh generated with *Cubit*. In both cases, the crack initiates at the tip of the pre-crack and propagates in a direction roughly perpendicular to the direction of maximum strain. The results show a weak mesh dependence, which can be further reduced with mesh refinement.



(a) (b) (c) (d) (e)

Figure 4: Dynamic crack propagation through a uniformly-distributed mesh.



(a) (b) (c) (d) (e)

Figure 5: Dynamic crack propagation through a mesh generated with *Cubit*.

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