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AN IMPLICIT IMPLEMENTATION OF NON-ORDINARY STATE-BASED PERIDYNAMICS

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ABSTRACT

Peridynamics is a non-local continuum theory that was introduced by Silling. Its key advantage is its use of integral equation forms of the underlying physics, as compared to the partial differential equations in, say the finite element method and therefore does not need any extra assumptions to treat singularities. In this paper we present an implicit implementation of the non-ordinary state-based peridynamics formulation. Fracture is introduced into the peridynamic model by allowing bonds to break irreversibly. Bond breakage occurs when a damage criterion is satisfied, for instance, if the bond exceeds a critical stretch. This paper presents for the first time an implicit formulation of non-ordinary state-based peridynamic theory for finite deformation mechanics. An iterative procedure based on the Newton-Raphson method is used to solve the discretised problem.

Key Words: *peridynamics; non-local models; non-ordinary state-based formulation; fracture; implicit model*

1. Peridynamic Theory

An implicit time integration scheme allows us to perform a dynamic simulation with a larger time step for convergence and thus reduce the computational time than what would be permitted with an explicit integration scheme. However, an implicit time integration scheme can be much harder to implement. There are only a few existing examples of implicit implementations of peridynamics in the literature. A small-strain linearly elastic static implementation of the non-ordinary state-based peridynamics formulation is developed in [5, 6] and it is used to solve non-linear deformation problems for crystal plasticity simulations in [7].

In preparation for the derivation of the implicit non-ordinary state-based peridynamic scheme, a brief review of the underlying peridynamic theory is needed. In peridynamics, the problem domain is discretised by particles through bonds. The interaction between particles $\mathbf{x}$ and $\mathbf{x}'$ occurs over a finite distance defined by a given 'horizon', R. The kinematics of peridynamics theory in 2D is shown in Figure 1.

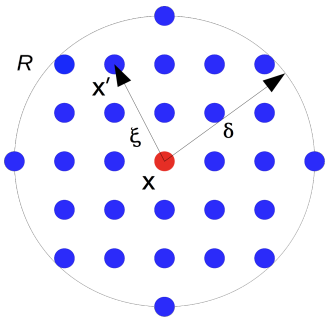

Figure 1: Particle $\mathbf{x}$ interacts with particle $\mathbf{x}'$ within a spherical neighborhood, R.

The relative position of two particles is denoted by $\boldsymbol{\xi} = \mathbf{x}' - \mathbf{x}$ and relative displacement by $\boldsymbol{\eta} = \mathbf{u}' - \mathbf{u}$ where $\mathbf{u}$ and $\mathbf{u}'$ are the displacement of particle $\mathbf{x}$ and $\mathbf{x}'$. The relationship among the variables is illustrated in Figure 2.

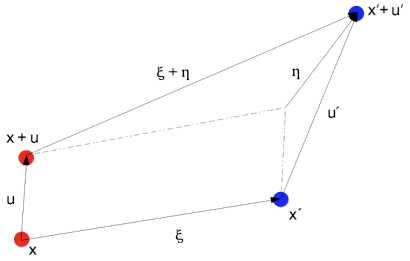

Figure 2: Reference and deformed vector states

In classical continuum mechanics, the equation of motion derived from the conservation of linear momentum and can be expressed as

$$\rho(\mathbf{x})\ddot{\mathbf{u}}(\mathbf{x},t) = \nabla \cdot \boldsymbol{\sigma} + \mathbf{b}(\mathbf{x},t), \tag{1}$$

where ρ is the mass density in the reference configuration, $\ddot{\mathbf{u}}$ denotes the acceleration, $\boldsymbol{\sigma}$ is the Cauchy stress and $\mathbf{b}$ is the prescribed body force density field [3]. However, in (1), the spatial derivative is undefined along discontinuities. In contrast, peridynamics uses an integral function of a force on particle at $\mathbf{x}$ to replace the divergence of the stress term, that is

$$\rho(\mathbf{x})\ddot{\mathbf{u}}(\mathbf{x},t) = \int_R \mathbf{f}(\eta,\xi)dV_{\mathbf{x}'} + \mathbf{b}(\mathbf{x},t), \tag{2}$$

where $\mathbf{f}$ is the pairwise peridynamic force function that the particle $\mathbf{x}'$ exerts on $\mathbf{x}$, $dV_{\mathbf{x}'}$ is volume associated with particle $\mathbf{x}'$. These basic equations can be applied anywhere in the body, so no additional theories are needed for studying fracture using the peridynamic method.

However, the original "bond-based" theory proposed in [1] and defined in Equation (2) places limitations on the choice of the material properties. For this reason, a "state-based" formulation was developed in [2] to allow arbitrary constitutive relations to be implemented within the peridynamics framework. The equation of motion in the state-based Peridynamics can be expressed as

$$\rho(\mathbf{x})\ddot{\mathbf{u}}(\mathbf{x},t) = \int_R \underline{\mathbf{T}}\,[\mathbf{x},t]\langle\mathbf{x}'-\mathbf{x}\rangle - \underline{\mathbf{T}}\,[\mathbf{x}',t]\langle\mathbf{x}-\mathbf{x}'\rangle dV_{x'} + \mathbf{b}(\mathbf{x},t), \quad \forall\mathbf{x}' \in R \tag{3}$$

where $\underline{\mathbf{T}}\,[\mathbf{x},t]\langle\mathbf{x}'-\mathbf{x}\rangle$ and $\underline{\mathbf{T}}\,[\mathbf{x}',t]\langle\mathbf{x}-\mathbf{x}'\rangle$ are the force-vector states [2]. $\underline{\mathbf{T}}$ depends on the deformations of all bonds connected from particle $\mathbf{x}$ and $\mathbf{x}'$. The model is called ordinary when the force exerted by a bond between particles is in the same direction as the deformed bond. However, there is no requirement that force states be in the same direction as their deformation states, and models in which they are not in the same direction are called non-ordinary.

2. Non-ordinary peridynamic numerical implementation

Dividing the body R into a number of cells, each represented by a particle, the integral expressions in (3) can be approximated with a finite sum as in [4], i.e.

$$\rho(\mathbf{x}_i)\ddot{\mathbf{u}}(\mathbf{x}_i,t) = \sum_{j=1}^{m} \underline{\mathbf{T}}\,[\mathbf{x}_i,t]\langle\mathbf{x}_j-\mathbf{x}_i\rangle - \underline{\mathbf{T}}\,[\mathbf{x}_j,t]\langle\mathbf{x}_i-\mathbf{x}_j\rangle V_j + \mathbf{b}(\mathbf{x}_i,t). \tag{4}$$

Some specific states that are used in the peridynamic concept are:

$$\text{reference position vector state} : \underline{\mathbf{X}}\langle\boldsymbol{\xi}\rangle = \boldsymbol{\xi} = \mathbf{x}' - \mathbf{x} \tag{5}$$

$$\text{displacement vector state} : \underline{\mathbf{U}}\langle\boldsymbol{\xi}\rangle = \boldsymbol{\eta} = \mathbf{u}' - \mathbf{u} \tag{6}$$

$$\text{deformation vector state} : \underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle = \boldsymbol{\eta} + \boldsymbol{\xi} = (\mathbf{u}' + \mathbf{x}') - (\mathbf{u} - \mathbf{x}) \tag{7}$$

where $\mathbf{u}'$ and $\mathbf{u}$ are located at $\mathbf{x}'$ and $\mathbf{x}$, respectively, in the reference configuration. The non-local deformation gradient at $\mathbf{x}$ can be expressed as

$$\mathbf{F}(\mathbf{x}) = \left[\int_R \omega\langle\boldsymbol{\xi}\rangle(\underline{\mathbf{Y}}(\boldsymbol{\xi}) \otimes \boldsymbol{\xi}) dV_{\boldsymbol{\xi}} \right] \cdot \mathbf{B}(\mathbf{x}) \tag{8}$$

and the shape tensor $\mathbf{B}(\mathbf{x})$ as

$$\mathbf{B}(\mathbf{x}) = \left[\int_R \omega\langle\boldsymbol{\xi}\rangle(\boldsymbol{\xi} \otimes \boldsymbol{\xi}) dV_{\boldsymbol{\xi}} \right]^{-1}. \tag{9}$$

where $\otimes$ denotes the tensor product of two vectors and $\omega\langle\boldsymbol{\xi}\rangle$ is a constant non-negative weighting function that defines the horizon in which the force relationship between particles is nonzero and all particles $\mathbf{x}'$ have equal influence on $\mathbf{x}$ [5]. The ideal value of constant weighing function is still under investigation and is currently taken to be unity [4] . For a discrete system, the non-local deformation gradient (8) at a particle i can be expressed as [4]

$$\mathbf{F}(\mathbf{x}_i) = \begin{bmatrix} \sum_{j=1}^{m} \omega\langle\boldsymbol{\xi}\rangle(\underline{Y}(\xi_x) \cdot \xi_x) V_j & \sum_{j=1}^{m} \omega\langle\boldsymbol{\xi}\rangle(\underline{Y}(\xi_x) \cdot \xi_y) V_j \\ \sum_{j=1}^{m} \omega\langle\boldsymbol{\xi}\rangle(\underline{Y}(\xi_y) \cdot \xi_x) V_j & \sum_{j=1}^{m} \omega\langle\boldsymbol{\xi}\rangle(\underline{Y}(\xi_y) \cdot \xi_y) V_j \end{bmatrix} \cdot \mathbf{B}(\mathbf{x}_i), \tag{10}$$

and shape tensor (9) as

$$\mathbf{B}(\mathbf{x}_i) = \begin{bmatrix} \sum_{j=1}^{m} \omega\langle\boldsymbol{\xi}\rangle(\xi_x \cdot \xi_x) V_j & \sum_{j=1}^{m} \omega\langle\boldsymbol{\xi}\rangle(\xi_x \cdot \xi_y) V_j \\ \sum_{j=1}^{m} \omega\langle\boldsymbol{\xi}\rangle(\xi_y \cdot \xi_x) V_j & \sum_{j=1}^{m} \omega\langle\boldsymbol{\xi}\rangle(\xi_y \cdot \xi_y) V_j \end{bmatrix}^{-1}. \tag{11}$$

Using the deformation gradient (8), the left Cauchy-Green strain matrix $\mathbf{C}(\mathbf{x})$ and logarithmic strain ϵ can be calculated as

$$\mathbf{C}(\mathbf{x}) = \mathbf{F}(\mathbf{x})\mathbf{F}(\mathbf{x})^{\mathbf{T}} \tag{12}$$

$$\boldsymbol{\epsilon} = \frac{1}{2} \ln \mathbf{C}(\mathbf{x}). \tag{13}$$

For 2D plane strain deformation, the Cauchy stress, $\boldsymbol{\sigma}(\boldsymbol{x})$ can be written as

$$\begin{bmatrix} \boldsymbol{\sigma}_{11} \\ \boldsymbol{\sigma}_{22} \\ \boldsymbol{\sigma}_{12} \end{bmatrix} = \frac{E}{(1+\nu)(1-2\nu)} \begin{bmatrix} 1-\nu & \nu & 0 \\ \nu & 1-\nu & 0 \\ 0 & 0 & \frac{1-2\nu}{2} \end{bmatrix} \begin{bmatrix} \boldsymbol{\epsilon}_{11} \\ \boldsymbol{\epsilon}_{22} \\ 2\boldsymbol{\epsilon}_{12} \end{bmatrix} \tag{14}$$

and the first Piola-Kirchoff stress tensor is expressed as

$$\boldsymbol{P} = J\boldsymbol{\sigma}(\boldsymbol{x})\mathbf{F}(\mathbf{x})^{-T} \tag{15}$$

where $J = \det \mathbf{F}(\mathbf{x})$. The force state of a bond with the bond vector $\boldsymbol{\xi}$ in terms of stress tensor $\boldsymbol{\sigma}$, takes the form [4]

$$\underline{\mathbf{T}}\langle\boldsymbol{\xi}\rangle = \omega(|\boldsymbol{\xi}|)[\boldsymbol{P}(\mathbf{F})]^T \cdot \mathbf{B}(\mathbf{x}) \cdot \boldsymbol{\xi} \tag{16}$$

and the derivative of $\underline{\mathbf{T}}$ with respect to the displacements can be written using (16) as:

$$\frac{\partial \underline{\mathbf{T}}\langle\boldsymbol{\xi}\rangle}{\partial \mathbf{u}} = \frac{\partial \underline{\mathbf{T}}\langle\boldsymbol{\xi}\rangle}{\partial \mathbf{F}} \frac{\partial \mathbf{F}}{\mathbf{u}} = \omega(|\boldsymbol{\xi}|) \frac{\partial \mathbf{P}}{\partial \mathbf{F}} \frac{\partial \mathbf{F}}{\partial \mathbf{u}} \cdot \mathbf{B}(\mathbf{x}) \cdot \boldsymbol{\xi}. \tag{17}$$

The stiffness matrix can be written as:

$$\mathbf{K}(\mathbf{x}) = \sum_{i=1}^{m} \left(\frac{\partial \underline{\mathbf{T}}\,[\mathbf{x}]\langle\mathbf{x}'_i - \mathbf{x}\rangle}{\partial \mathbf{u}} - \frac{\partial \underline{\mathbf{T}}\,[\mathbf{x}'_i]\langle\mathbf{x} - \mathbf{x}'_i\rangle}{\partial \mathbf{u}} \right) V_{\mathbf{x}'_i} \tag{18}$$

where m is the number of neighbour particles of $\mathbf{x}$ and $V\mathbf{x}'_i$ is the volume occupied by each neighbour particles. For a 2D problem, the global matrix is 2N $\times$ 2N where N is the total number of particles in the simulation.

3. Future work

The capability of the explicit implementation of non-ordinary state-based peridynamic problems has been successfully illustrated in numerous studies [4]. Therefore, it is planned to extend the implicit implementation to a comparison of fracture predictions using different damage criteria and compare the results with reference solutions found in the literature. [2, 4].

4. Conclusions

This paper offers for the first time an implicit implementation of non-ordinary state-based peridynamic theory for finite deformation mechanics. Newton-Raphson implementation of the peridynamic method developed here to allow the solution procedure extended towards solving non-linear deformation problems. and therefore, to a range of damage criteria.

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