

IMPLEMENTATION AND VALIDATION OF AN ANISOTROPIC PERIDYNAMIC INFLUENCE FUNCTION

AYLIN AHADI AND JAKOB KROCHMAL

Division of Mechanics
Lund University
PO Box 118, S-22100 Lund, Sweden
e-mail: aylin.ahadi@mek.lth.se, web page: <http://www.mek.lth.se/>

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Summary.

In this work, anisotropy is introduced in the elasto-plastic peridynamic model. The model is mathematically formulated and implemented into the source files of LAMMPS itself, extending the program in a straight-forward manner. The implemented model is tested through simulating beams loaded in compression. The model is found to severely alter the behavior of the simulations. A clear qualitative difference in behavior is shown independently of pre-existing simulation parameters. The model is shown to be internally consistent.

1 INTRODUCTION

Peridynamics is a generalized continuum theory employing a nonlocal model of force interaction. It is based on integral operators that sum internal forces on particles, separated by finite distances, thus replacing the stress-strain relationship in the classical theory of continuum mechanics. Since the integral operator is not a function of the deformation gradient, it allows for more general deformations than classical continuum theory. Peridynamics converges to the classic elastic continuum material models in the limit of infinitesimal distances between the particles, and it can be used as an alternative approach to multiscale modeling since one single model can be made valid over wide range of length scales by changing the inter-particle distances. The structure of the peridynamic models allow use of the software LAMMPS. Different peridynamic models can be implemented and added into LAMMPS. The default elasto-plastic models today are restricted to isotropic behavior of material, limiting the application of the peridynamic theory. An anisotropy extension of the elasto-plastic peridynamic model is presented below. The capabilities to represent directional dependent behavior are shown through simulating beams loaded in compression. The model is found to capture the anisotropic behavior of the beam.

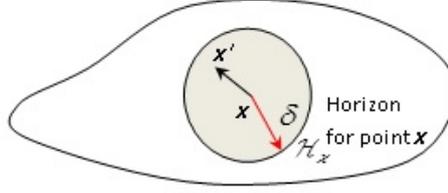


Figure 1: Schematic description of peridynamic body.

2 THEORY OF PERIDYNAMICS AND THE INFLUENCE FUNCTION

In the peridynamic theory the interactions between material points are expressed in terms of bond forces, permitting interaction between particles at a distance. The deformation at point \mathbf{x} depends collectively on all points \mathbf{x}' interacting with \mathbf{x} within the neighborhood H_x . H_x is a sphere whose center is the studied point \mathbf{x} . The radius δ is the horizon of \mathbf{x} and it is the distance limit across which a pair of material points can interact. δ can be interpreted as the length scale in the model. Internal forces within a continuous solid are thus treated as a network of non-linear pair interactions. Using the analogy of a system of springs, these pair interactions depend on the distance the material points are separated from each other. In state-based peridynamics, the equation of motion is

$$\rho(\mathbf{x})\ddot{\mathbf{u}}(\mathbf{x}, t) = \int_{H_x} \{T[\mathbf{x}, t] \langle \mathbf{x}' - \mathbf{x} \rangle - T[\mathbf{x}', t] \langle \mathbf{x} - \mathbf{x}' \rangle\} dV_{\mathbf{x}'} + \mathbf{b}(\mathbf{x}, t) \quad (1)$$

Here, T is a *force vector state field*, $\mathbf{b}(\mathbf{x}, t)$ is the external body force density field, $\rho(\mathbf{x})$ is the mass density in the reference configuration and $\mathbf{u}(\mathbf{x}, t)$ is the displacement field. As seen the equation of motion (2) contains integrals rather than differentiations and is therefore valid everywhere inside the material body regardless of any discontinuity. In the equation of motion of state-based peridynamic theory, the force vector state field T contains entirety of the constitutive model. In the Elastic-Plastic Model (EPS) model implemented in PDLAMMS the force vector state field T is split into two parts

$$T = T_i + T_d = \omega \left(-\frac{3p}{m} \mathbf{x} + \alpha(e_d - e_{dp}) \right) \quad (2)$$

where p, k, α are material constants, e_d, e_{pd} are the deviatoric and plastic extensions of the material, respective, and $\omega = \omega(\mathbf{x})$ is the influence function. The influence function regulates how the particles interact with each other. Different material properties can be simulated by having the influence function modulate the forces acting on particles in the simulation based only on their distance from each other. Such an influence function is called spherical, as forces have the same magnitude in every direction from the particle. In this work, the forces are modulated based on the direction of their relative position as seen relative to some coordinate system. A coordinate system is aligned to the model the influence function is modified to modulate the forces differently depending on what

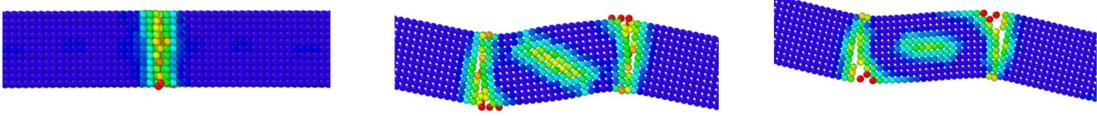


Figure 2: Deformation of the nanobeam using peridynamics, original isotropic model (left), anisotropic model with preferable direction oriented 45 (middle) and anisotropic model with preferable direction along the beam (right).

direction they have relative to this coordinate system. The default influence function in the EPS model returns the length of the incoming force vector regardless of its direction - this is equivalent to returning the distance to the edge of a sphere from the center, where the radius of the sphere is the length of the force vector. The approach taken here is to replace the sphere with an ellipsoid by setting the distance to the edge of the ellipsoid with the major semi-axis being the length of the incoming force vector and having a predefined direction, the other semi-axes having lengths some fraction of the major semi-axis. The pre-defined direction of the major semi-axis corresponds to the preferred direction of deformation of the solid being modeled. A material can have more than one preferred direction - the algorithm simulates this by storing several ellipsoids, running the scaling routine on each one and then returning the largest value.

3 RESULTS

A beam with a cross-section of 11×11 particles and a length of 100 particles was constructed in PDLAMMPS, aligned along the x axis. The beam was loaded in compression by prescribing the displacement at the two end surfaces. The tests were run for a variable amount of time steps, enough for the beam to buckle and crack. The initiation of the slip band of peridynamic nanobeam with the original isotropic model and anisotropic model with two preferable directions are seen in Fig. 2. With the isotropic model necking band is in the vertical direction, whereas when introducing anisotropic model with preferable direction, this can be controlled in the desirable direction. Fig. 3 shows result for the damage parameter runs with spherical influence functions, to use as a baseline to inspect the ellipsoid influence functions against and result with an ellipsoid influence function, where the major axis of the ellipsoid points along the loading direction, i.e. x-axis. Fig. 4 shows with an ellipsoid influence function, where the major axis of the ellipsoid points at a 45 angle from the x axis.

4 CONCLUSIONS

An anisotropic peridynamic influence function has been implemented in PDLAMMPS and validated by simulating tensile test on a beam. The model shows consistency by reproducing results accurately when given different ellipsoids with the same proportions. The beam acts qualitatively differently when there is an ellipsoid influence function present

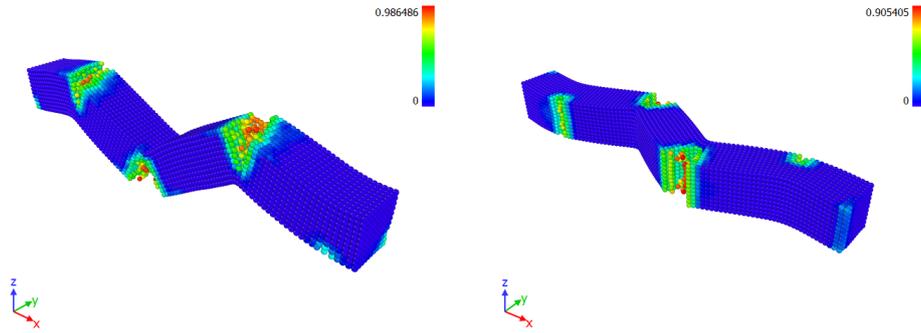


Figure 3: Deformation of the nanobeam using peridynamics, original isotropic model (left).

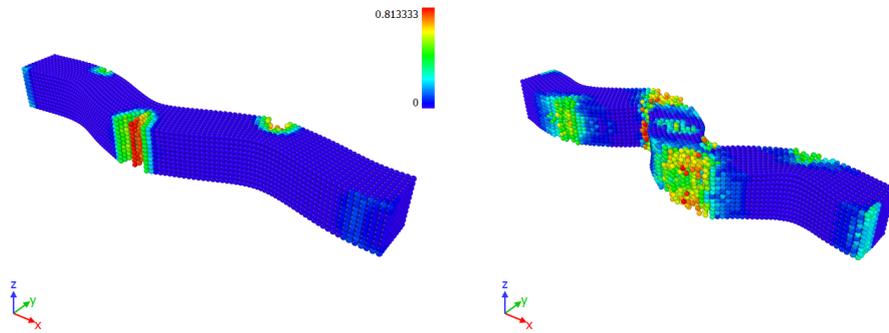


Figure 4: Deformation of the nanobeam using peridynamics, original isotropic model (left)

compared to the spherical case. With all the ellipsoid influence functions the beam bends and cracks in the x - y -plane rather than in the x - z -plane, most probably corresponding to the fact that all the ellipsoids are oriented in, and thus give rise to anisotropy in, said x - y -plane.

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