Reduction of three-dimensional axisymmetric models to two dimensions in peridynamics

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Abstract

Introduced by Silling in 2000, peridynamics provides an alternative approach to model deformations of solid materials using integral equations instead of differential equations used in the classical theory of continuum mechanics. In peridynamic simulations of material failure, cracks appear naturally and propagate as a consequence of bond-breaking between material points. In this report, we consider axisymmetric problems where the geometry, external loading, and body forces are invariant under rotation about a given axis of symmetry, resulting in axisymmetric deformation of all material points. We start with a full three-dimensional peridynamic model with a linear pairwise force function. Exploiting axisymmetry, we incorporate the contribution of out-of-plane bond forces into an effective two-dimensional pairwise force function and derive a corresponding two-dimensional model on a representative half plane passing through the axis of symmetry. This results in a significant reduction of computational cost.

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1 Introduction

Understanding how solid materials deform and fail under external loading conditions has been a long-standing area of research for scientists and engineers for centuries. The classical approach is to treat the solids as a continuum and model the displacements of material points as a solution to a differential equation. This approach works well for small deformations. However, due to the differential formulation, the classical theory fails to describe material behavior when the deformation field is non-differentiable at certain material points, for example, when a fracture is formed.

Recently, the development of peridynamics has become useful to address the limitations of classical theory of continuum mechanics. Introduced in [6], the peridynamic formulation is non-local in nature, and it assumes that every material point interacts with its neighbors via a bond force. The internal force on each material point is the resultant force exerted by all material points within its neighborhood. Since the peridynamic equation of motion is an integral equation, instead of a differential one, it can accommodate deformation fields which are discontinuous, in particular non-differentiable. Peridynamics has been used to model crack formation and crack branching [7, 3], among many other fracture problems.

2 Description of the project

In this project, we consider three-dimensional axisymmetric problems, where the geometry of the material is symmetric about an axis of symmetry and the external loading conditions are such that the deformation fields are symmetric about the same axis of symmetry. These types of problems occur naturally in various situations, such as expansion of a hollow cylinder under uniform internal pressure [5], the single-fibre pull-out test [2], formation of Hertzian cracks on impact [1], etc. Since the displacement of the material points are symmetric about the axis of symmetry, say the z-axis, it is enough to model the displacements of all points on a representative r-z plane, where r is the radial component associated with the material points relative to the axis of symmetry. However, the peridynamic neighborhood of each material point on that plane extends beyond the plane itself. Thus, we incorporate the contributions of out-of-plane bonds into the resultant force exerted on each point on the representative r-z plane, modifying the pairwise force function between any two points on the plane appropriately. In this way, we reduce a full three-dimensional peridynamic equation of motion into a two-dimensional model while effectively incorporating out-of-plane interactions. This results in significant reduction of computational cost to simulate a three-dimensional axisymmetric peridynamic problem.

2.1 Mathematical background

We start with the representation of vectors and tensors in different coordinate systems. Since the equation of motion changes depending on the choice of coordinate system, we specify the basis in which we represent each vector and tensor.

Definition 1. *Let $B = \{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ be an orthonormal basis of $\mathbb{R}^3$. For any vector $\mathbf{u} \in \mathbb{R}^3$, the representation of $\mathbf{u}$ in the basis B is defined as the column vector $[\mathbf{u}]_B = [u_1 \quad u_2 \quad u_3]^T$, where $u_i = \mathbf{u} \cdot \mathbf{e}_i$ for $i = 1,2,3$. $[\mathbf{u}]_B$ is also called the representation of $\mathbf{u}$ in the basis B. Note that $\mathbf{u} = \sum_{i=1}^{3} u_i \mathbf{e}_i$. Define $B \otimes B := \{\mathbf{e}_i \otimes \mathbf{e}_j\}_{i,j=1}^{3}$. The representation of a tensor $\mathbf{T} = \sum_{k,l=1}^{3} T_{kl} \mathbf{e}_k \otimes \mathbf{e}_l$ of order 2 with respect to the basis $B \otimes B$ is defined as the 3×3 matrix*

$$[\mathbf{T}]_{B\otimes B} = \begin{bmatrix} T_{11} & T_{12} & T_{13} \\ \vdots & \vdots & \vdots \\ T_{31} & \dots & T_{33} \end{bmatrix}.$$

In Theorem 1 below [4], we present the change of basis formula for representations of vectors and tensors.

Theorem 1. *Let $B = \{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ and $R = \{\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3\}$ be two orthonormal bases of $\mathbb{R}^3$. Let $[\mathbf{v}]_B = [v_1 \quad v_2 \quad v_3]^T$ and $[\mathbf{v}]_R = [\bar{v}_1 \quad \bar{v}_2 \quad \bar{v}_3]^T$. Then, $[\mathbf{v}]_R = \mathbf{Q}[\mathbf{v}]_B$, where $\mathbf{r}_k = \sum_{j=1}^{3} Q_{kj}\mathbf{e}_j$, for $k = 1,2,3$. Let $\mathbf{C}$ be a tensor of order n with $\mathbf{C} = \sum_{i_1,\dots,i_n=1}^{3} C_{i_1\dots i_n}\mathbf{e}_{i_1} \otimes \cdots \otimes \mathbf{e}_{i_n} = \sum_{i_1,\dots,i_n=1}^{3} D_{i_1\dots i_n}\mathbf{r}_{i_1} \otimes \cdots \otimes \mathbf{r}_{i_n}$. Then, $C_{i_1\dots i_n} = \sum_{i_1,\dots,i_n=1}^{3} Q_{j_1 i_1} Q_{j_2 i_2} \cdots Q_{j_n i_n} D_{j_1\dots j_n}$ for $i_1,\dots,i_n = 1,2,3$.*

2.2 Classical theory

Now, we briefly review the theory of classical linear elasticity. From now on, we shall assume that $B = \{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ is the Euclidean basis of $\mathbb{R}^3$ and $\Omega \in \mathbb{R}^3$ is a homogeneous *isotropic* body (i.e., the material properties are invariant under any orthogonal change of basis) with mass density ρ. By $\partial\Omega$, we denote the boundary of the body. Let $\mathbf{b}$ be a prescribed body force density and $\boldsymbol{\sigma}$ be a stress tensor. For a small deformation $\mathbf{u} = \sum_{i=1}^{3} u_i\mathbf{e}_i \in \mathbb{R}^3$, the equation of motion in classical linear elasticity, also known as Cauchy momentum equation, can be written as

$$\rho\frac{\partial^2 u_i}{\partial t^2} = \frac{\partial \sigma_{i1}}{\partial x_1} + \frac{\partial \sigma_{i2}}{\partial x_2} + \frac{\partial \sigma_{i3}}{\partial x_3} + b_i, \quad i = 1,2,3,$$

where the stress-strain relation from the *generalized Hooke's law* is given by

$$\begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{12} \\ \sigma_{23} \\ \sigma_{31} \end{bmatrix} = \begin{bmatrix} \lambda+2\mu & \lambda & \lambda & 0 & 0 & 0 \\ \lambda & \lambda+2\mu & \lambda & 0 & 0 & 0 \\ \lambda & \lambda & \lambda+2\mu & 0 & 0 & 0 \\ 0 & 0 & 0 & \mu & 0 & 0 \\ 0 & 0 & 0 & 0 & \mu & 0 \\ 0 & 0 & 0 & 0 & 0 & \mu \end{bmatrix} \begin{bmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ 2\varepsilon_{12} \\ 2\varepsilon_{23} \\ 2\varepsilon_{31} \end{bmatrix}$$

and the components of infinitesimal strain tensor $\boldsymbol{\varepsilon}$ are given by

$$\varepsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right),$$

where λ and μ are known as the *Lamé constants* of the material.

2.3 Cylindrical coordinate system

The cylindrical coordinate system is a natural choice for objects that have rotational symmetry about some axis. Without loss of generality, we consider the z-axis as the axis of symmetry. In the cylindrical coordinate system, vectors and tensors are represented in a local basis at each point of the body. For every point $\mathbf{x} = \sum_{i=1}^{3} x_i \mathbf{e}_i \in \Omega$, we define a local basis given by the unit vectors $\mathbf{e}_{r(\mathbf{x})}, \mathbf{e}_{\theta(\mathbf{x})}$ and $\mathbf{e}_{z(\mathbf{x})}$ associated with the radial, angular, and vertical directions, respectively. The vector $\mathbf{e}_{r(\mathbf{x})}$ points in the direction of $\mathbf{x}$ from the z-axis, the vector $\mathbf{e}_{\theta(\mathbf{x})}$ is a rotation of $\mathbf{e}_{r(\mathbf{x})}$ in the counterclockwise direction about the z-axis by $\frac{\pi}{2}$, and the vector $\mathbf{e}_{z(\mathbf{x})}$ points in the z-direction. More precisely,

$$
\begin{aligned}
\mathbf{e}_{r(\mathbf{x})} &= \frac{1}{r(\mathbf{x})}\left(x_1\mathbf{e}_1 + x_2\mathbf{e}_2\right),\\
\mathbf{e}_{\theta(\mathbf{x})} &= \frac{1}{r(\mathbf{x})}\left(-x_2\mathbf{e}_1 + x_1\mathbf{e}_2\right),\\
\mathbf{e}_{z(\mathbf{x})} &= \mathbf{e}_3,
\end{aligned}
$$

where $r(\mathbf{x}) = \sqrt{x_1^2 + x_2^2}$. Note that, for every $\mathbf{x}$, the set $L(\mathbf{x}) = \left\{e_{r(\mathbf{x})}, e_{\theta(\mathbf{x})}, e_{z(\mathbf{x})}\right\}$ is an orthonormal basis at $\mathbf{x}$ in the local cylindrical coordinate system. For isotropic materials, the Cauchy momentum equation in the cylindrical coordinate system for axisymmetry reduces to

$$
\begin{aligned}
\rho\frac{\partial^2 u_r(\mathbf{x},t)}{\partial t^2} &= (\lambda+\mu)\frac{\partial}{\partial r}\left(\frac{1}{r}\frac{\partial}{\partial r}(r u_r(\mathbf{x},t)) + \frac{\partial u_z(\mathbf{x},t)}{\partial z}\right) + \mu\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial u_r(\mathbf{x},t)}{\partial r}\right) + \frac{\partial^2 u_r(\mathbf{x},t)}{\partial z^2} - \frac{u_r(\mathbf{x},t)}{r^2}\right)\\
&\quad + b_r(\mathbf{x},t),\\
\rho\frac{\partial^2 u_z(\mathbf{x},t)}{\partial t^2} &= (\lambda+\mu)\frac{\partial}{\partial z}\left(\frac{1}{r}\frac{\partial}{\partial r}(r u_r(\mathbf{x},t)) + \frac{\partial u_z(\mathbf{x},t)}{\partial z}\right) + \mu\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial u_z(\mathbf{x},t)}{\partial r}\right) + \frac{\partial^2 u_z(\mathbf{x},t)}{\partial z^2}\right) + b_z(\mathbf{x},t),
\end{aligned}
$$

and

$$\rho\frac{\partial^2 u_\theta(\mathbf{x},t)}{\partial t^2} = \mu\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial u_\theta(\mathbf{x},t)}{\partial r}\right) + \frac{\partial^2 u_\theta(\mathbf{x},t)}{\partial z^2} - \frac{u_\theta(\mathbf{x},t)}{r}\right) + b_\theta(\mathbf{x},t),$$

where $[\mathbf{u}]_{L(\mathbf{x})} = [u_r \quad u_\theta \quad u_z]^T$.

2.4 Peridynamic model

The equation of motion for a point $\mathbf{x} \in \Omega$ at time $t \geqslant 0$ in bond-based peridynamics [6] is given by

$$\rho\frac{\partial^2 \mathbf{u}}{\partial t^2}(\mathbf{x},t) = \int_{H_\mathbf{x}} \mathbf{f}(\mathbf{u}(\mathbf{x},t),\mathbf{u}(\mathbf{x}',t),\mathbf{x},\mathbf{x}',t)d\mathbf{x}' + \mathbf{b}(\mathbf{x},t), \tag{1}$$

where $H_\mathbf{x}$ is the peridynamic neighborhood given by $H_\mathbf{x} = B_\delta(\mathbf{x}) \cap \Omega$, where $B_\delta(\mathbf{x}) = \{\mathbf{x}' \in \mathbb{R}^3 : \|\mathbf{x}' - \mathbf{x}\| \leqslant \delta\}$ is the ball of radius δ centered at $\mathbf{x}$. In (1), $\mathbf{f}$ is the pairwise force function that describes the nonlocal interaction between the point $\mathbf{x}$ and any other point $\mathbf{x}' \in H_\mathbf{x}$. In this work, we consider a linear bond-based peridynamic model given by

$$\mathbf{f}(\mathbf{u}(\mathbf{x},t),\mathbf{u}(\mathbf{x}',t),\mathbf{x},\mathbf{x}',t) = \lambda(\|\mathbf{x}' - \mathbf{x}\|)((\mathbf{x}' - \mathbf{x}) \otimes (\mathbf{x}' - \mathbf{x}))(\mathbf{u}(\mathbf{x}',t) - \mathbf{u}(\mathbf{x},t)),$$

where $\lambda(\|\mathbf{x}' - \mathbf{x}\|)$ is the micro-modulus function which is based on the material properties.

When $\mathbf{x}$ is in the bulk of the body, i.e. more than δ distance away from the boundary of Ω, the neighborhood $H_\mathbf{x} = B_\delta(\mathbf{x})$. Defining $\boldsymbol{\xi} = \mathbf{x}' - \mathbf{x}$ and $\boldsymbol{\eta} = \mathbf{u}(\mathbf{x}',t) - \mathbf{u}(\mathbf{x},t)$, we can express (1) for the linear bond-based peridynamic model as

$$\rho\frac{\partial^2 \mathbf{u}}{\partial t^2}(\mathbf{x},t) = \int_{B_\delta(\mathbf{x})} \lambda(\|\boldsymbol{\xi}\|)(\boldsymbol{\xi} \otimes \boldsymbol{\xi})\boldsymbol{\eta}\, d\mathbf{x}' + \mathbf{b}(\mathbf{x},t). \tag{2}$$

For isotropic materials, in the cylindrical coordinate system for axisymmetry, when the material point $\mathbf{x}$ is δ distant away from the z-axis, (2) reduces to

$$\begin{aligned}
\rho \ddot{u}_r(r,z) = \int\limits_{B_\delta^2(r,z)} & \left[-r\left(r'u_r(r',z')+ru_r(r,z)+\left(u_z(r',z')-u_z(r,z)\right)\left(z'-z\right)\right)\lambda_{0,0}^{\alpha}\right. \\
& +\left(u_r(r',z')\left(r^2+r'^2\right)+2rr'u_r(r,z)+r'\left(z'-z\right)\left(u_z(r',z')-u_z(r,z)\right)\right)\lambda_{1,0}^{\alpha} \\
& \left. -\left(rr'u_r(r',z')+r'^2u_r(r,z)\right)\lambda_{2,0}^{\alpha}\right]r'dA(r',z')+b_r(r,z), \\
\rho \ddot{u}_z(r,z) = \int\limits_{B_\delta^2(r,z)} & \left[\left(z'-z\right)\left(r'u_r(r',z')+ru_r(r,z)+\left(z'-z\right)\left(u_z(r',z')-u_z(r,z)\right)\right)\lambda_{0,0}^{\alpha}\right. \\
& \left. -\left(z'-z\right)\left(ru_r(r',z')+r'u_r(r,z)\right)\lambda_{1,0}^{\alpha}\right]r'dA(r',z')+b_z(r,z),
\end{aligned}$$

where $\lambda_{m,n}^{\alpha} = \int\limits_{-\alpha}^{\alpha} \lambda(\|\xi\|)\cos^m(\varphi)\sin^n(\varphi)d\varphi$ for integers m and n, and $\alpha = \cos^{-1}\left(\frac{\delta^2-(z'-z)^2-r'^2-r^2}{-2rr'}\right)$. $B_\delta^2(r,z)$ is the two-dimensional disk of radius δ centered at $\mathbf{x}$.

In the case when the material point $\mathbf{x}$ is not δ distant away from the z-axis, to get the equations of motion in the r-z plane, $\int\limits_{B_\delta^2(r,z)} \lambda_{m,n}^{\alpha}(\cdot)dA$ is replaced by $\int\limits_{B_\delta^2(-r,z)\cap\{r'>0\}} \lambda_{m,n}^{\pi}(\cdot)dA + \int\limits_{B_\delta^2(r,z)\setminus B_\delta^2(-r,z)} (\cdot)\lambda_{m,n}^{\alpha}dA$ (see Figure 1)

3 Contributions made to the project

My contribution to the project was to derive the theorerical model, as well as to implement the model numerically. I rigorously defined the notion of axisymmetry in terms of the local coordinate system at each material point and derived the final axisymmetric peridynamic equation using cylindrical coordinate transform. Using Matlab, I implemented a framework to simulate the dynamics of both the classical and the peridynamic equations and computed the error between them at each time step. During my internship, I met with the members of my group and presented my progress on a weekly basis. I also prepared a poster and presented it in the "Summer 2019 Poster Session Opportunity with ORPA Research Symposium".

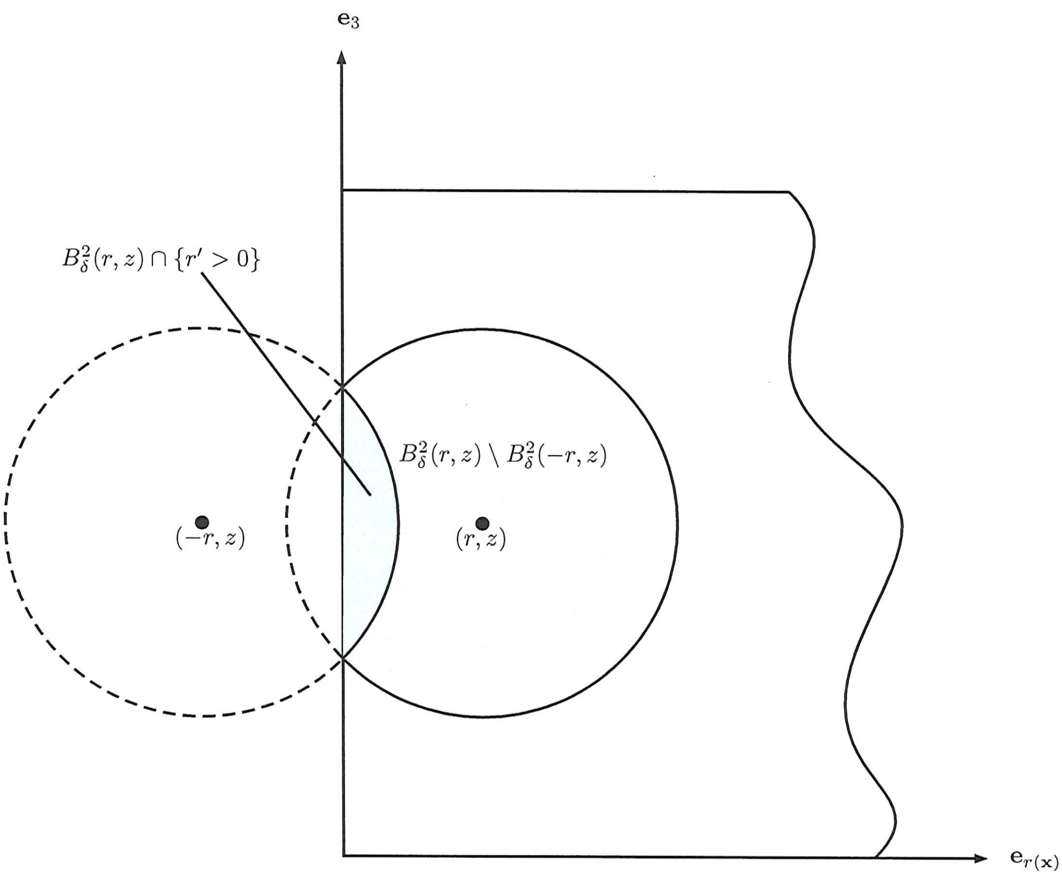

Figure 1: The region of integration in the r-z plane, when the horizontal cross-section of $B_\delta(\mathbf{x})$ intersects the z-axis.

4 What new skills and knowledge did you gain?

To handle tedious symbolic computations, I learned and used the open source software Sage and its cloud-based implementation CoCalc, which was new to me. While implementing the axisymmetric model in Matlab, I learned several tricks to efficiently generate meshes, to improve computational speed by vectorizing certain operations, and to manage memory efficiently. To understand the theory of classical linear elasticity better, I read several books on tensor calculus, which strengthened my mathematical understanding.

5 Experience Impact on My Academic/Career Planning

In my study of partial differential equations as a Ph.D. student, non-local models play an important role. My project for the internship was a direct application of non-local models to engineering-related problems, linking theory to real-world situations. While working with the research group at the lab, I was introduced to new and exciting problems in the field of solid mechanics. Throughout the internship, I gained valuable coding experience that will help me simulate mathematical models with ease. Overall, the internship helped me become a well-rounded mathematician with experience in diverse mathematical fields and motivated me to take up a research career.

6 Relevance to the mission of NSF

The study of deformation of solid materials is useful in many fields of science and engineering, resulting in better design of equipments, products, and structures. This will in turn lead to innovations that will improve the lives of people, advancing their health, prosperity, and welfare, while promoting scientific progres. Thus, my project is important and it relates to the NSF mission.

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