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Mesh sensitivity in peridynamic simulations

Steven F. Henke *, Sachin Shanbhag

Department of Scientific Computing, Florida State University, Tallahassee, FL 32306, USA

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ABSTRACT

In this work, we investigate the suitability of several meshing strategies for use with a common peridynamics solution scheme. First, we use a manufactured solution to quantify the influence of different meshes on the accuracy and conditioning of a nonlocal boundary value problem in one and two dimensions. We explore convergence behavior, the effects of model parameters, and sensitivity to perturbations. We then apply the same meshing strategies to a three-dimensional impact simulation that employs the full peridynamic mechanical theory. We present a qualitative comparison of the fracture patterns that result, and suggest best practices for generating meshes that lead to efficient, high-quality numerical simulations of peridynamic models.

1. Introduction

Peridynamics [1–3] is a generalization of the classical theory of continuum mechanics to include nonlocal force interactions. The spatial extent of these interactions provides an intrinsic length, resulting in models that exhibit a scale-dependent response to applied stimuli. Balance laws and constitutive relations are formulated using integrals (rather than spatial derivatives which are only defined on smooth fields), so the formation and evolution of discontinuities, such as cracks, boundaries, and interfaces, can be controlled by a single constitutive relation. These features enable models that reproduce many complex materials phenomena, including fracture, failure modes in composites, and phase transitions. In the same spirit of the mechanical theory, an entire nonlocal calculus is under development [4,5] for general scalar, vector, and tensor quantities.

Due to the finite nature of computing machines, peridynamic simulations are prone to subtle computational difficulties. An appreciable source of such difficulties is the computational mesh, which represents the model geometry, and in many solution schemes, is invoked as part of a quadrature rule that resolves interactions near each material point. At present, guidance on generating meshes that are appropriate for peridynamic problems is tenuous, and best practices are not established for irregular meshes, which are desirable for their versatility and efficiency in representing complex geometries. These details present sources for computation error and motivate the present study, where we systematically explore the relationship between model parameters and the underlying spatial discretization in an attempt to improve the fidelity of nonlocal simulations.

Several techniques, such as direct quadrature methods [6–9] and finite element methods [7,10,11], have been proposed for approximating solutions to this class of nonlocal models. The efficiency and accuracy of these approaches relies intimately on a discrete representation of the model geometry that tracks or captures the deformation of continuum bodies, including the location of any discontinuous features that may develop during the simulation. When present, discontinuities are constrained to follow contours of the mesh. As a result, the local resolution limits our knowledge of the position of discontinuities, and presents a restriction on the family of configurations that can be realized for that system. As a complement to mesh refinement procedures, which have been discussed by others [12,13], this work examines how irregular point placement strategies affect the accuracy of these computations and alleviates some obvious mesh dependent behaviors that have been observed. Previous studies have focused on other numerical issues in the peridynamic setting, including the performance of finite element meshes in the presence of stationary jump discontinuities [11], crack propagation and branching behavior [14], and symmetry breaking in dynamic fracture [15].

We first study mesh sensitivity in the simplified setting of a nonlocal boundary value problem (Section 2), where a manufactured solution enables a quantitative evaluation of discretization errors and conditioning. There, we identify primary error sources and examine the robustness of quadrature schemes to small

* Corresponding author. Tel.: +1 7155849882.
E-mail addresses: sfh07e@my.fsu.edu, shenke@fsu.edu (S.F. Henke), sshanbhag@fsu.edu (S. Shanbhag).

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disturbances in the placement of grid points. In addition to the widely-used tensor product grids, we demonstrate that the generators of a centroidal Voronoi tessellation (CVT) bear desirable properties for integrating peridynamic interactions. Lessons from the scalar problem are then applied (Section 3) towards understanding meshing issues in a three-dimensional impact simulation that utilizes the full peridynamic mechanical theory. Qualitative aspects of the resulting fracture patterns are discussed and explanation of the observed behavior is attempted. We conclude (Section 4) with a summary of our findings and some suggestions for future investigations.

2. Nonlocal boundary value problem

As an initial attempt at understanding mesh sensitivity in peridynamic systems, we study meshing issues in a simpler, related context: the nonlocal "elliptic" boundary value problem. Using a manufactured solution and direct quadrature method, we explore the response of the discrete system to different quadrature point positioning strategies in one and two dimensions.

2.1. Nonlocal elliptic boundary value problem

A nonlocal elliptic boundary value problem [4,5,16] is governed by the balance equation,

$$b(\boldsymbol{x}) = \int_{\Omega} \gamma\left(\boldsymbol{x}, \boldsymbol{x}'\right)\left(u(\boldsymbol{x}) - u\left(\boldsymbol{x}'\right)\right) dV_{\boldsymbol{x}'}, \quad \forall \left(\boldsymbol{x}, \boldsymbol{x}'\right) \in \Omega, \tag{1}$$

where $b(\boldsymbol{x})$ contains the known problem data, $\gamma\left(\boldsymbol{x}, \boldsymbol{x}'\right)$ is a two-point modulus function that is symmetric in its arguments (i.e., $\gamma\left(\boldsymbol{x}, \boldsymbol{x}'\right) = \gamma\left(\boldsymbol{x}', \boldsymbol{x}\right)$), $u(\boldsymbol{x})$ is the unknown scalar quantity, and $V_{\boldsymbol{x}'}$ is the volume ascribed to the material point $\boldsymbol{x}'$. This equation is termed "elliptic", because it corresponds [16] with the spatial differential operator of the classical wave and diffusion equations, and nonlocal because the behavior at any point $\boldsymbol{x}$ within the domain depends on the behavior of points $\boldsymbol{x}'$ at a finite distance. Unlike its local counterpart, a constraint domain for nonlocal problems must have a measurable volume for well-posedness. Nonlocal versions of classical boundary conditions are obtained by specifying a function value (Dirichlet) or integral flux (Neumann) over a subset of the computational domain.

The strength of the interaction modulus typically decays with distance, so it is customary to truncate nonlocal interactions outside a finite region $\mathcal{H}_{\boldsymbol{x}} \subset \Omega$ surrounding each material point $\boldsymbol{x}$. That is,

$$\gamma\left(\boldsymbol{x}, \boldsymbol{x}'\right) = 0 \quad \forall \boldsymbol{x}' \notin \mathcal{H}_{\boldsymbol{x}}. \tag{2}$$

This choice reduces the number of interactions that must be processed in simulating models, and supports a banded matrix structure in the discrete case. In this work, we assume that such a neighborhood exists, and is a ball,

$$\mathcal{H}_{\boldsymbol{x}} = \left\{\boldsymbol{x}' \in \Omega : \left\|\boldsymbol{x} - \boldsymbol{x}'\right\| \leq \delta\right\}, \tag{3}$$

parameterized by its radius δ, termed the peridynamic horizon. The local limit of δ provides correspondence with classical theories [5], and facilitates determining parameters in the modulus function. Changes to the horizon modify the relationship between these parameters (through a process called scaling [12,13]), and generally alters the dispersive properties of a medium [17]. Consequently, the cut-off radius is viewed as a constitutive parameter rather than a computational convenience. For more on physical and computational aspects involving the horizon see Refs. [6,11,17–19].

On the interior of the nonlocal region, we make the constitutive assumption that the modulus function is given by,

$$\gamma\left(\boldsymbol{x}, \boldsymbol{x}'\right) = \left\|\boldsymbol{x}' - \boldsymbol{x}\right\|^{-P} \quad \forall \boldsymbol{x}' \in \mathcal{H}_{\boldsymbol{x}}, \tag{4}$$

where the nonlocal exponent P controls the strength profile of nonlocal interactions and affects the amount of smoothing [4] the integral operator imparts on the problem data. The form of Eq. (4) subsumes modulus functions found in a variety of settings, including micromechanics [1,2] ($P = 1$), mass and heat transport [20,21] ($P = 2$), and the fractional Laplacian [16,22] ($P = d + 2s$, where d is the spatial dimension and the parameter $0 < s < 1$). In problems where the domain is stationary, changing the value of P is equivalent to convolution of the integral operator with a spherical influence function [2,23].

2.2. Problem setup

For the computational experiments, we select a smooth manufactured solution that also appears in Ref. [11], and generalize it for multiple dimensions,

$$\hat{u}(\boldsymbol{x}) = R^2 - \|\boldsymbol{x}\|^2, \quad \forall \boldsymbol{x} \in \Omega \cup \Gamma, \tag{5}$$

where Ω is the solution domain and Γ the constraint domain. Direct substitution can be used to determine the forcing term that corresponds to this manufactured solution,

$$\hat{b}(\boldsymbol{x}) = \begin{cases} 2\delta^{3-P}/(3-P) & d = 1, P < 3 \\ 2\pi\delta^{4-P}/(4-P) & d = 2, P < 4, \end{cases} \tag{6}$$

which depends on the number of spatial dimensions d, nonlocal horizon δ, and nonlocal exponent P.

To facilitate a comparison with the impact problem that appears later in this paper, the solution domain Ω is chosen to be the ball-shaped region,

$$\Omega := \{\boldsymbol{x} : \|\boldsymbol{x}\| \leq r\}, \tag{7}$$

that is enclosed by a constraint domain Γ, shaped like a spherical shell,

$$\Gamma := \{\boldsymbol{x} : r < \|\boldsymbol{x}\| \leq R\}. \tag{8}$$

These domains are parameterized by an inner radius r and outer radius R, such that $r + \delta \leq R$. Throughout the volume of the constraint region, we augment the governing equation with nonlocal Dirichlet data by enforcing the values,

$$u(\boldsymbol{x}) = \hat{u}(\boldsymbol{x}), \quad \forall \boldsymbol{x} \in \Gamma. \tag{9}$$

This setup effectively removes all boundaries and their associated difficulties (see [10,13,15]) from this research.

2.3. Solution method

Approximation of the governing equation (1) by a composite quadrature rule yields the discretization,

$$b(\boldsymbol{x}_i) \approx \sum_{j \neq i} \gamma\left(\boldsymbol{x}_i, \boldsymbol{x}_j\right)\left(u(\boldsymbol{x}_i) - u\left(\boldsymbol{x}_j\right)\right) V_j, \tag{10}$$

where all points positioned inside the computational domain are assigned an equal fraction of the region's analytical volume. This can be written as a linear system of equations,

$$\left[A\left(\boldsymbol{x}_i, \boldsymbol{x}_j\right)\right]\left[u\left(\boldsymbol{x}_j\right)\right] = \left[b(\boldsymbol{x}_i)\right], \tag{11}$$

where the entries of the system matrix are given by,

$$\left[A\left(\boldsymbol{x}_i, \boldsymbol{x}_j\right)\right] = \begin{cases} \sum_{j \neq i} \gamma\left(\boldsymbol{x}_i, \boldsymbol{x}_j\right) V_j & i = j \\ -\gamma\left(\boldsymbol{x}_i, \boldsymbol{x}_j\right) V_j & i \neq j. \end{cases} \tag{12}$$