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A multiscale method for nonlocal mechanics and diffusion and for the approximation of discontinuous functions

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Abstract

A multiscale implementation of hybrid continuous/discontinuous finite element discretizations of nonlocal models for mechanics and diffusion in two dimensions is developed. The implementation features adaptive mesh refinement based on the detection of defects and results in an abrupt transition between refined elements that contain defects and unrefined elements free of defects. An additional difficulty overcome in the implementation is the design of accurate quadrature rules for stiffness matrix construction that are valid for any combination of the grid size and horizon parameter, the latter being the extent of nonlocal interactions. As a result, the methodology developed can attain optimal accuracy at very modest additional costs relative to situations for which the solution is smooth. Portions of the methodology can also be used for the optimal approximation, by piecewise linear polynomials, of given functions containing discontinuities. Several numerical examples are provided to illustrate the efficacy of the multiscale methodology.

Keywords: Peridynamics; Multiscale methods; Nonlocal models; Anomalous diffusion; Finite element methods; Discontinuous displacements

1. Introduction

Classical partial differential mechanics models for solid mechanics feature local interactions, i.e., a point only interacts with points within an infinitesimal distance. In contrast, in the peridynamics (PD) model, points interact with points within a finite influence horizon δ. This nonlocal approach has significant advantages for studying defects such as the nucleation and propagation of cracks [1–6], problems for which the classical approach breaks down because the necessary derivatives do not exist.

The peridynamics model admits a variational formulation that in turn suggests the construction of a discretized model via a finite element method (FEM). For problems with smooth data, FEMs have well-understood convergence behavior with respect to the typical element size h. This allows for the efficient solution of complex systems. However,

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in cases in which discontinuities are expected, the rapid convergence of FEMs may be lost unless suitable precautions are taken. Such precautions might involve careful adjustments of the mesh or the use of a discontinuous basis functions. For these remedies to help, it must also be possible to determine, to reasonable accuracy, the location and extent of the discontinuities.

In [7], a one-dimensional PD model was considered, using a piecewise linear polynomial basis for which a problem with smooth data would typically have an L^2 convergence rate of $O(h^2)$. When discontinuous solutions were considered, the convergence rate deteriorated to $O(h^{1/2})$. However, the optimal rate was recovered by adjusting the mesh to bracket the discontinuity by a single tiny element whose characteristic length was $O(h^4)$, whereas the remaining mesh was essentially unchanged. In [7], the locations of the discontinuities were assumed to be explicitly available to the algorithm; this made it easy to tailor the mesh or element choice in the optimal way. In practical problems, however, the detection of discontinuities and the estimation of their extent and severity are not simple tasks. An adaptive approach must be taken which is able to repeatedly adjust the size, shape, and element type of a local portion of the mesh, based on some computable numerical error indicators.

Whereas some regions of a solid may contain singularities, there may also exist large regions of smoothness and regularity, a behavior that is well and efficiently handled by classical partial differential equations (PDEs) approaches. A multiscale implementation of the peridynamics model in one dimension was developed in [8]; the solution interval was divided according to the observed behavior, and then a PDE model was applied in subintervals in which the displacement was detected to be smooth, and an PD model was applied only in the vicinity of discontinuities of the displacement. The application of the PD model was further divided into the use of discontinuous Galerkin (DG) discretizations in the elements containing the discontinuity and continuous Galerkin (CG) discretization in immediately neighboring elements. Thus, elements of the PD-CG type would form an intermediate layer between the PDE regions of smoothness and the PD-DG regions of sharp local discontinuity. The flexibility rendered by using multiple models in this way requires, however, a strategy for correctly coupling them over transition regions.

The work in [7] and [8] was restricted to the one-dimensional case. It is the purpose of this paper to consider the issues involved in implementing a multiscale PD model in two-dimensional regions. We assume that there are some curves across which the displacement is discontinuous and which are separated by relative large regions within which the displacement is smooth. The goal is to implement a finite element discretization that accurately and efficiently approximates the solution with, if possible, a convergence rate that is comparable to the optimal convergence rate observed when there are no discontinuities present.

As often occurs when moving from one to two dimensions, the proper treatment of the geometry becomes significantly more difficult. The most obvious change is that adaptive remeshing becomes much more complicated, and requires attention to element shape (no small angles) and element connectivity (no hanging nodes).

Another geometric issue involves the treatment of discontinuities. In one dimension, a local discontinuity occurs at a single point, and isolating that point just requires determining a very small element that contains it. A discontinuity in two dimensions might, however, constitute a point, a curve intersecting the boundary, or a closed curve contained within the region. Depending on the geometric complexity and curvature of the discontinuity, the technique of "covering" by a very small element may become unfeasible.

A third geometric issue arises because the PD model seeks to integrate interactions over a local circular region defined by the horizon δ. An FEM model approximates such integrals using numerical quadrature over the collection of triangles that form the mesh. However, an effect of the horizon is to render the integrand not smooth across the horizon circumference, resulting in possibly disastrous failures of standard quadrature methods in triangles that intersect the horizon circumference.

In this paper, we consider how to handle these and several other obstacles. Our goal is to implement a multiscale PD finite element method in two dimensions for a problem in which discontinuities are likely to occur but whose locations are not known. We concentrate on the response necessary for a multiscale PD implementation to adapt to the discovery of a discontinuity. This response will include local refinement, remodeling, remeshing, new quadrature rules, and a seamless transition from the nonlocal PD model to a local PDE one. Our goal is an accurate and efficient computation of approximate solution despite the presence of discontinuities.

Clarification about what is meant by *multiscale* is perhaps needed. In this paper, multiscale features of solutions, i.e., large regions over which solutions are smooth vs. small regions over which solutions suffer defects, are resolved by using grid sizes that are large (small) with respect to the horizon for the former (latter). Thus, our approach is