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SPECIAL ISSUE

PERIDYNAMICS AND MULTISCALE MODELING

Guest Editors

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PREFACE

Dynamic processes that involve fracture and damage inherently involve multiple scales as atomic bonds break and elastic waves propagate and reflect from the boundaries influencing the evolution of the fracture processes. Recently, with the advent of multiscale approaches, it has been debated whether continuum methods can ever, alone, be developed to predict dynamic fracture and damage and whether atomistic-to-continuum, or possibly quantum mechanical, multiscale models are the only possible solutions (outside of modeling an entire structure by molecular dynamics) for accurately simulating dynamic fracture events. Currently, and for the foreseeable future, purely atomistic simulations of dynamic fracture in materials with macroscopic dimensions are not possible. At the same time, atomistic-to-continuum couplings cannot reproduce many of the experimentally observed characteristics of dynamic crack propagation, especially in brittle materials. The likely reason for this failure is the limited length and time scales such simulations are capable of spanning, and the difficulties of mixing two “immiscible” models: the discrete and the continuum models. Very promising recent results on dynamic fracture obtained with peridynamics indicate that this nonlocal *continuum model* can offer an improvement over existing multiscale techniques that rely on the standard (local) formulation of solid mechanics.

Stewart Silling published the first paper on peridynamics a little over a decade ago (Silling, 2000). The theory can be viewed as an extension of the classical continuum mechanics as it permits modeling dynamic phenomena in which the primary variables (displacements, for example) are, or become, discontinuous functions. This nonlocal formulation also introduces damage models at the microscale that lead naturally to initiation and autonomous propagation of cracks at the macroscale. From its original 2000 version, peridynamics has known a landmark generalization in 2007 by Silling and coworkers (state-based peridynamics), it has enabled unprecedented simulations of dynamic fracture in homogeneous and heterogeneous materials, and it has reached well beyond solid mechanics, gradually evolving into a general theory for modeling of various physical phenomena (Silling et al., 2007).

The papers in this special issue address aspects related to the natural connections between peridynamics and multiscale modeling. Even in its simplest form, the original bond-based peridynamics, the theory, at its core, links the bond elasticity and bond damage microscale properties with the macroscale behavior and measurable quantities. The contributors to the present issue provide a balanced treatment between novel theoretical results and applications. The *theoretical developments* focus on the following: a coarsening method to represent a complex microstructure with a reduced number of degrees of freedom; the connection between phonon dispersion properties and the nonlocal constitutive model; a new energy-based criterion for modeling ductile fracture in peridynamics; the connection between anomalous diffusion, fractional diffusion, and a peridynamic model for diffusion; a variational formulation for nonlocal diffusion; the effect of the influence function on the dynamic response of a peridynamic material; and a formulation for modeling anisotropic elastic and damage material response in unidirectional fiber-reinforced laminas. The applications provide numerical solutions for some challenging problems: multiscale analysis of a defect in a ho-

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mogenized bar; dynamic elasto-plastic fracture and damage; Hertzian fracture generated by impact on a brittle target; adaptive refinement in peridynamics; and dynamic splitting in unidirectional fiber-reinforced composite materials.

The papers in this issue cover topics on the current state-of-the-art in peridynamics and point to some of the research directions of interest in the near future. The following is a brief discussion of the articles contained in this issue:

Stewart Silling opens this issue with a paper on coarsening in peridynamics, which refers to the process of deriving a simplified model from a fully detailed model. An important aspect of a multiscale method is the problem of how to represent a complex microstructure with a reduced number of degrees of freedom. Silling introduces a rigorous and mathematically consistent technique for deriving peridynamic material models for a sequence of increasingly coarsened descriptions of a body, starting from a known detailed, small-scale linearized state-based peridynamic description. Each successively coarsened model excludes some of the material present in the previous model, and the length scale increases accordingly. Interestingly, the excluded material, while not present explicitly in the coarsened model, is nevertheless taken into account implicitly through its effect on the forces in the coarsened material. Numerical examples demonstrate that the method accurately reproduces the effective elastic properties of a composite as well as the effect of a small defect in a homogeneous medium.

The possibility of extracting the parameters in a peridynamic model from fitting to wave dispersion curves data has been noted from the original paper in 2000. The work by Weckner and Silling in this issue demonstrates how to utilize experimentally measurable wave speeds in order to determine nonlocal constitutive equations. The authors perform ab initio lattice dynamics calculations for silicon using density functional pertubation theory. They determine the phonon dispersion relation along paths of high symmetry directions in the first Brillouin zone. Results are compared to experimental data obtained using neutron scattering. The proposed technique then establishes a rigorous correlation between the strongly nonlocal constitutive equation and the measured material properties at “small” length scales. Coarsening techniques would allow applying these results to “larger” length scales.

Bobaru and Ha show how a peridynamic model behaves when one desires to change the size of the nonlocal interaction (the peridynamic horizon), and implicitly refining the grid spacing. Since the horizon induces a length scale, such a formulation is effectively a multiple-scale model. The results show that, unlike atomistic-to-continuum coupling methods in which the transition between a discrete formulation to a continuum one results in ghost or spurious forces, a direct coupling between two peridynamic continua (with different horizons/length scales) does not result in such forces. A varying horizon size is necessary to efficiently perform adaptive refinement, which is a required step in any concurrent multiscale model.

The peridynamic ideas are not limited to modeling mechanical behavior and models for heat transfer and mass diffusion have been recently published. An obvious benefit of using peridynamics in this situation is the case of modeling “anomalous” diffusion through heterogeneous, cracked, or porous media. Burch and Lehoucq present boundary value problems for nonlocal diffusion on bounded domains. The contribution includes a variational formulation that leads to a conforming finite-element method using piecewise discontinuous shape functions. The authors demonstrate that nonlocal diffusion is a model for anomalous diffusion applicable when Fick’s law represents an inaccurate model. A generalization of Fick’s law in terms of a nonlocal flux holds, and the relationship between nonlocal and fractional diffusion is explained. The numerical examples show that numerical solutions of boundary value problems in which the order of the fractional Laplacian lies in the interval $(0; 2]$ is possible.

A common misconception about peridynamics was that it can only be used to model fracture in brittle materials. Foster, Silling, and Chen use their recently published rate-dependent elasto-viscoplastic state-based peridynamic model and introduce a novel energy-based failure criterion for modeling dynamic crack propagation in ductile materials. The damage model is set to match the measured mode I dynamic fracture toughness for a sample steel material. The peridynamic simulations of dynamic crack propagation in the steel samples match exceptionally well the evolution of the crack in experimental results obtained also by the authors using high-speed camera imaging.

Hertzian cracks are a characteristic type of damage that takes place at the impact between a penetrator and a brittle three-dimensional (3D) target. Peridynamics has been shown to predict the formation of such cracks. The role of the influence function used in the peridynamic theory on these types of cracks and on wave propagation is analyzed by Seleson and Parks. Their contribution begins by showing how a bond-based peridynamic model can be directly obtained from the more general state-based model. Dispersion relations are analyzed with respect to the localization effect induced by modulating the influence function. The 3D numerical examples use a recent implementation of peridynamics in the molecular dynamics code LAMMPS (named PDLAMMPS) by Parks and co-authors.

Hu, Ha, and Bobaru introduce a homogenized multiscale peridynamic model for simulating fracture in a unidirectional fiber-reinforced composite lamina. Analytical expressions for the micromodulus function and the critical relative elongation are obtained by calibrating to measurable material properties of the lamina. A certain scaling of the micromodulus function is necessary for the discrete model so that the strain energy density remains the same under grid refinement. The splitting fracture mode is predicted without any special criteria for this type of failure. The maximum crack propagation speed from the peridynamic simulations approaches the analytical solution for a steady-state dynamic debonding crack. Convergence studies under uniform grid refinement for a fixed horizon size (m-convergence) and under decreasing the peridynamic horizon (while keeping the number of nodes cover by a horizon fixed) are performed.

In closing, the guest editor wishes to express his gratitude to the Editor in Chief of the *International Journal for Multiscale Computational Engineering*, Professor Jacob Fish, for suggesting the special issue and expertly and patiently guiding us along the process. Special thanks are due to the reviewers who have responded promptly and provided expert reviews of the papers in this issue. The funding agencies (Sandia National Laboratories, DOE, Boeing, ARO, ARL) were instrumental in providing support for the work on peridynamics, including some of the articles contained in this issue. Last, but not least, the guest editor dedicates his work for this special issue to the creator of peridynamics, Dr. Stewart A. Silling, and wishes to thank him for his guidance and unlimited generosity and kindness.

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