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Peridynamics, Fracture, and Nonlocal Continuum Models

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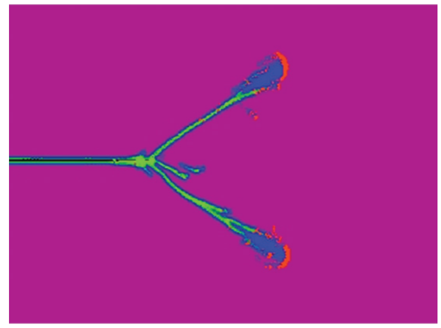

Figure 1. *Peridynamic simulation of dynamic fracture starting from a short edge crack. Areas where damage has occurred are shown in blue and green. The active process zones where damage is increasing are shown in red. Because the plate is stretched at a constant rate, the cracks see a higher and higher strain field ahead of them as they grow.*

Most physical processes are the result of collective interactions across disparate length and time scales. The dynamic fracture of brittle solids is a particularly interesting collective interaction connecting large and small length scales. With the application of enough stress or strain to a sample of brittle material, atomistic-scale bonds will eventually snap, leading to fracture of the macroscopic specimen.

The classic theory of dynamic fracture [7, 10] is based on the notion of a deformable continuum containing a crack. The crack is mathematically modeled as a branch cut that begins to move when an infinitesimal extension of the crack releases more energy than needed to create a fracture surface. Classic fracture theory, together with experiment, has been enormously successful in characterizing and measuring the resistance of materials to crack growth—and thereby enabling engineering design. However, the capability to quantitatively predict the dynamics of multiple propagating cracks that are free to nucleate, change course, bifurcate, and, indeed, stop if they choose lies completely outside the classic approach.

Armed with supercomputers, contemporary science is engaged in the quest for a multiscale framework for quantitatively predicting the dynamics of multiple cracks that freely propagate and interact. Investigators realize the importance of quantifying the influence of macroscopic forces on the dynamics at the length scales at which atomic bonds are broken. Bottom-up approaches, recognizing the inherent discreteness of fracture through lattice models, have provided penetrating insight into the dynamics of the fracture processes [2,12,13,20]. Nevertheless, numerical simulations of fine-grained atomistic models, while offering important and necessary insight into the fracture process, do not scale up to finite-size samples with multiple freely propagating cracks.

Complementary to the bottom-up approaches are top-down computational approaches that use cohesive zone elements [9, 22]. More recently, cohesive zones have been applied within the extended finite element method [1] to minimize the effects of mesh dependence on free crack paths. Current challenges facing these methods (indeed, all computational methods) include multiple growing cracks interacting in complex patterns.

What remains elusive is an underlying continuum model that can seamlessly evolve both smooth and discontinuous deformation in a way that is useful for predicting free crack propagation. To be applicable, a model must be able to deliver quantifiable results and recover the classic results of fracture mechanics in situations in which it is known to hold.

The peridynamic continuum model [17,18], a spatially nonlocal continuum theory, was introduced recently to fill this gap. Each material point interacts through short-range forces with other points inside a horizon of prescribed diameter δ. The short-range forces depend on the relative displacement between material points and are derived from a peridynamic potential specifying a kinematic constitutive relation. Within the recently developed nonlocal vector calculus framework [4], peridynamics can be viewed as nonlocal balance laws involving nonlocal fluxes defined between material domains that might not have a common boundary. This provides an alternative to standard approaches for circumventing the technicalities associated with the lack of sufficient regularity in local balance laws; by avoiding the explicit use of spatial derivatives, the approach allows for both smooth and discontinuous deformations. For short-range forces akin to elastic bonds that break when stretched beyond a critical point, the peridynamic formulation delivers remarkable simulations, capturing both crack branching (Figure 1) and multiple crack interactions (Figure 2).

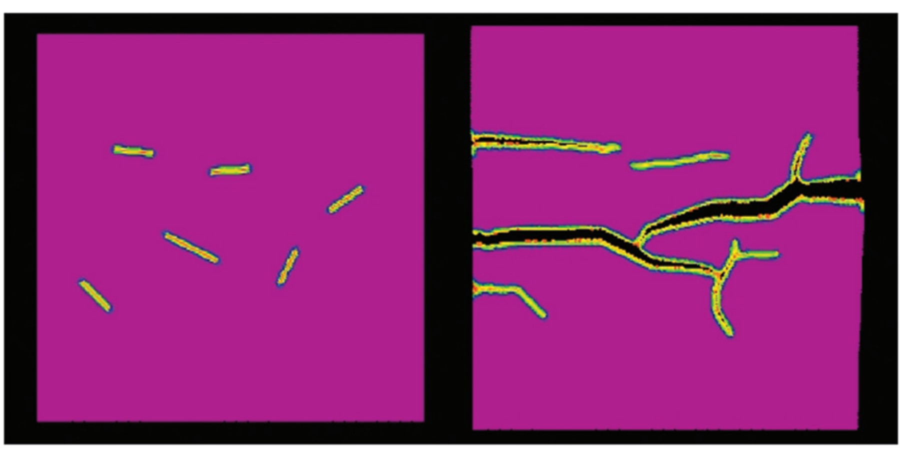

Figure 2. *Simulation of the interaction of defects in a brittle plate stretched at a constant rate in the vertical direction. Left: initial defects. Right: growth and merging of defects, leading to macroscopic failure.*

To test the theory of the peridynamic model, investigators have developed new mathematical results on its well-posedness and have assessed its connection to accepted continuum field theories. In a recent study, for linear elastic short-range forces and up-scaled linear peridynamics, which sent the peridynamic horizon δ to zero, the macroscopic limit of peridynamics was found to satisfy the classic equations of linear elasticity, with the macroscopic elastic moduli given by moments of the peridynamic nonlocal interaction kernel. Such relations can be established formally for smooth functions via simple Taylor expansions [6,19] and more rigorously in functional-analytic settings for solutions with minimal regularity [5,14].

Progress has also been made in developing a nonlocal calculus of variations for the analysis of variational and time-dependent problems subject to various nonlocal boundary conditions or, more precisely, conditions constraining the solutions on sets of nonzero measure. These results also make possible numerical analysis of discretizations of various types, and offer insight into the convergence and compatibility of numerical approximations in both nonlocal regimes and local limits under minimal regularity assumptions [21]. This, in turn, has influenced the development of robust and efficient numerical simulation tools for peridynamics, such as EMU, PDLAMMPS, and Peridigm [15,16].

Peridynamics provides a new tool for understanding the multiscale and nonlocal features of crack propagation. In a recent development, the peridynamic formulation was used to connect the dynamics associated with bond-breaking at small length scales to dynamic free crack propagation inside a brittle material as observed at macroscopic length scales [11]. Motivated by the short-range forces associated with simulations (Figures 1 and 2), a nonlinear peridynamic medium was considered with short-range forces that are initially elastic and soften beyond a critical relative displacement [11]. The peridynamic model was up-scaled to identify the macroscopic dynamics. It was shown rigorously [11] that the limiting macroscopic evolution has bounded energy given by the bulk and surface energies of classic brittle fracture mechanics. The macroscopic free crack evolution corresponds to the simultaneous evolution of the fracture surface and linear elastic displacement away from the crack set. The elastic moduli, wave speed, and energy release rate for the macroscopic evolution are explicitly determined by moments of the peridynamic potential energy. This delivers an interesting new connection between nonlocal short-range forces acting over small length scales and dynamic free crack evolution inside a brittle medium at the macroscopic scale. It also provides a second theoretical test of peridynamics and mathematically demonstrates that energies for nonlinear peridynamics converge to those of classic elastic fracture mechanics in the macroscopic limit. An unexpected twist in this investigation is that tools from the theory of image segmentation [8] can be brought to bear on this problem.

The latter typifies many interesting instances in which investigation of nonlocal peridynamics can cross over into other subject areas. For example, one can not only draw the analogy of nonlocal vector calculus with the traditional calculus, but also find similarities and connections with fractional calculus, discrete calculus, and calculus on graphs developed for subjects like the anomalous diffusion [3]. Indeed, nonlocality is ubiquitous in nature. By encoding spatial nonlocality explicitly at the continuum level while maintaining consistency to traditional local continuum equations when local models are well defined, nonlocal continuum models like peridynamics show much promise as effective alternatives to local convectional models.

Signs of growing research activity in the area include recent workshops at Oberwolfach, the Statistical and Applied Mathematical Sciences Institute, Brown University, and the University of Texas at San Antonio; various minisymposia at national meetings of SIAM and other organizations; and the new MURI center for material failure predictions through peridynamics funded by the Air Force Office of Scientific Research. The study of peridynamics is inspiring new mathematics and offers a valuable opportunity for applied mathematicians to team up with materials scientists and engineers to take a crack at developing new modeling and simulation capabilities for fracture and other interesting problems.

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