Accurate Prediction of Dynamic Fracture with Peridynamics

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Dynamic fracture and fragmentation processes exhibit several striking characteristic phenomena. Numerical simulations, using any of a variety of methods, have had only limited success in replicating any of these characteristic phenomena. A fundamental impediment for numerical simulations of fracture that are based on traditional solid mechanics theory is that the governing equations are expressed as partial differential equations and the derivatives they entail ***do not exist*** *at discontinuities. To remedy this inherent limitation, Silling proposed peridynamics as an enhancement of traditional solid mechanics theory. In the peridynamic continuum theory, momentum and energy conservation are expressed as integral equations that apply, without modification, to all types of material response; no auxiliary laws or rules are needed to treat crack initiation or growth. Hallmarks of the theory are nonlocal force interactions between material points; direct use of force and displacement in preference to stress and strain; representation of actual displacement rather than a local gradient approximation; and a numerical implementation that yields a mesh-free method. We show that the resulting simulation capability is able to accurately represent a wide variety of characteristic dynamic fracture phenomena, making peridynamics exceptional among numerical solid mechanics methods. Moreover, the method is* ***predictive*** *in that these phenomena are not "programmed" into the simulations in any way, but emerge from the combination of system geometry, initial and boundary conditions, and the chosen material force density constitutive model.*

Introduction

Material cracking and fracture are technologically important phenomena whose understanding remains a grand challenge in materials physics and engineering mechanics. The aims in managing cracking and fracture range from preventing them completely, to mitigating their effects on a body or structure, to guiding them to produce favorable fragmentation. The discipline of fracture mechanics can be partitioned into the study of quasi-static or stable cracking and dynamic fracture. The former includes fatigue cracking and slow crack growth; the latter encompasses situations where inertial effects influence cracking. The onset of defect or crack growth is the best understood aspect of fracture and can be accurately predicted by existing theories. In contrast, methods for predicting crack growth speed and direction, as well as whether and where branching occurs, are few and severely unreliable. In addition to predicting crack growth direction, a successful theory or simulation capability for dynamic fracture must be able to reproduce and provide insight into the following phenomena and experimental observations that are uniquely characteristic of dynamic fracture:

1. A steady, limiting crack speed;
2. Energy dissipation in dynamic crack growth (e.g., Charpy test);
3. The Mirror, Mist, Hackle sequence of textures on the fracture surface;
4. The transition from stable to unstable crack growth;
5. Arrest of unstable crack growth;
6. The specific angle of cracking the Kalthoff-Winkler notched plate impact experiment [1];
7. Transonic interface crack speeds [2];
8. Crack branching;
9. Fragment size distribution;

10. Membrane bursting;
11. The multiple, unstable cracking modes of fiber-reinforced composites;
12. Peeling and tearing of thin sheets.

Method

Until recently, no numerical simulation method was able to reproduce all these dynamic fracture phenomena, even qualitatively, let alone with quantitative accuracy. To address this deficiency, over the past decade, Silling and coworkers have developed peridynamics, which is a well-founded, new theory of continuum mechanics that is enabling unprecedented simulations of dynamic fracture in homogeneous and highly heterogeneous materials [3-7].

By representing the source terms of the conservation laws with integral equations, peridynamics avoids the problem inherent to traditional solid mechanics that the derivatives contained in the equations of motion, represented by partial differential equations, are not defined at material discontinuities. Instead, in peridynamics, fracture evolves from the deformation according to the equations of motion and the constitutive model. Consequently, simulation of fracture within peridynamics *does not require* supplemental kinetic relations that, in traditional fracture mechanics, would be needed to specify crack initiation, growth velocity, direction, arrest, and branching. In place of the traditional divergence of a stress field, peridynamics computes the force density that accelerates any material point using a functional of the displacement field within a spherical neighborhood of the point. The radius of the neighborhood is called the "horizon," which is a material parameter. The resulting nonlocality of the interaction forces in peridynamics allows it to model complex material behavior possessing an intrinsic length-scale, which is represented by the horizon parameter.

An early version of peridynamics, called "bond-based" theory, was limited to the special case of forces, called "bonds," between pairs of material points such that each bond responds independently of the others [3]. Damage and fracture are then easily treated at the bond level by allowing bonds between material points to break when they are stretched beyond some limit; a broken bond no longer contributes to the net force acting on its endpoints. The onset of bond breakage leads to local material softening, which can cause damage to accumulate, with broken bonds coalescing into a surface that becomes a fracture. Only bonds that exist in the initial state are considered during a simulation; no new bonds form as a result of deformation. Once a bond is broken, it does not heal. The result is a history dependent theory in which crack initiation and growth, and all associated phenomena, *emerge spontaneously*, in an unguided fashion, simply from the choice of system geometry, initial and boundary conditions, and the constitutive model.

While the bond-based peridynamic theory results in a mesh-free numerical implementation [6] that yields qualitatively accurate simulations of dynamic fracture in heterogeneous brittle materials, such as reinforced concrete and fiber-reinforced, laminated composites, it suffers two serious limitations. First, because peridynamics uses the more fundamental quantities of force and displacement in preference to the theoretical continuum quantities of stress and strain, the bond-based theory cannot apply material constitutive models of classical solid mechanics. Second, the elastic portion of a material's response is restricted to that of a Cauchy solid, resulting in a Poisson's ratio of 0.25 for any linear isotropic solid. These limitations of the bond-based theory were remedied with the "state-based" peridynamic theory [4]. The formal structure of the momentum conservation equation is unchanged; the force density remains an integral over the neighborhood of a material point of a difference in force states. However, the pairwise force function of the bond-based theory is replaced with a more general functional of the displacement field within the horizon. This effectively makes the bond forces on a material point additionally dependent on deformations of other bonds within the horizon.

Bond-based peridynamics is a special case of the state-based theory [4]. Another special case of this theory allows the force on a material point to be computed through a classical 'stress-strain" constitutive model: Within the horizon, the strain tensor is approximated from the deformation and the resulting stress tensor is then mapped onto a distribution of bond forces.

A fundamental difference from classical solid mechanics theory is that the peridynamic functionals are formulated directly in terms of the displacement field, rather than the spatial derivatives of displacement. Since the classical assumption of smoothness is not required, an initially spherical volume can deform into a highly distorted, non-smooth region, not only into an ellipsoid. Constitutive models in peridynamics can, correspondingly, represent a wider range of material phenomena than can the stress-strain-based models of classical solid mechanics. Characterization of the range of material behaviors accessible in peridynamics and their usefulness are largely unexplored areas of investigation. In this regard, it is of interest that a formal mapping exists from interatomic potentials to peridynamic force density functions [9]. Indeed, peridynamic theory shares the same formal structure as molecular dynamics (MD) [10a] and can be regarded as a continuum version of MD [10b].

State-based peridynamic is consistent with classical elasticity in the range of applicability of the latter: It converges to classical elasticity in the appropriate limit as the horizon shrinks to zero, assuming that the underlying deformation is sufficiently smooth [5]. Additionally, because peridynamics avoids any assumption of smoothness of the deformation field and treats the exact kinematics, it is well aligned with the kinematic assumptions of molecular dynamics. These features illustrate ways in which peridynamics is a generalization of the classical theory.

Results and Discussion

Figure 1 illustrates that the peridynamic state theory enables use of traditional stress-strain based material models. Figure 1a shows well-behaved simulation results for a uniaxial tension test on an aluminum bar represented by a standard visco-plasticity constitutive model [8]. The calculation remains stable with decreasing load (Figure 1b). Figure 1c shows the results of a Taylor impact test using the same constitutive model for aluminum [8]. The final shape is seen to agree well with the experimental observation [11].

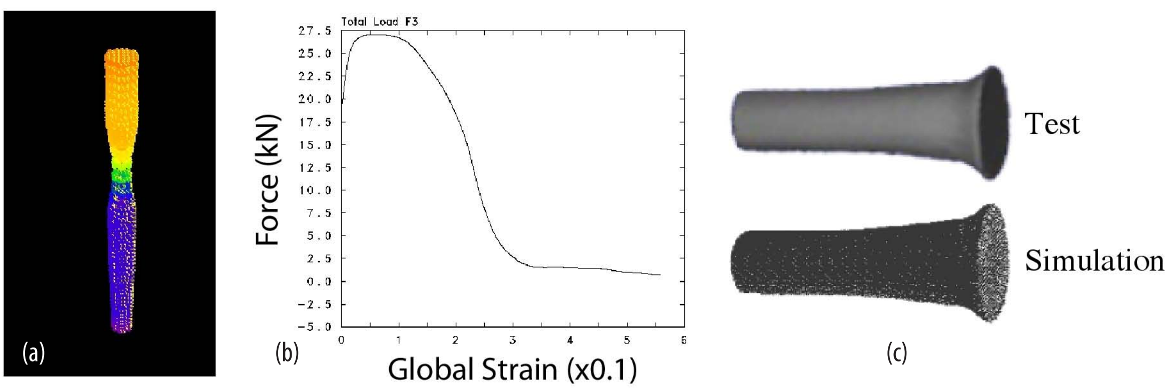

Figure 1. Employing conventional material models in state-based peridynamics. (a) Necking in a smooth bar loaded in uniaxial tension. Colors denote axial velocity. (b) Force-strain curve. (c) Experimental [11] and simulated images of a Taylor impact test on 6061 T-6 Aluminum [8].

Figure 2 shows that peridynamics recovers the characteristic structure of the "mirror, mist, hackle" surface produced by dynamic fracture. The fracture surface varies from being mirror-smooth near the onset of fracture, to cloudy further along the crack's progression, until it becoming very rough. The roughening of the fracture surface results from microscopic crack branching. Eventually, this can lead to macroscopic crack branching with further propagation of the fracture [12]. In the two-dimensional simulation shown, a crack is propagated from an initial notch at the left edge in a sheet of brittle material. The horizontal edges are initially displaced vertically and then held fixed, resulting in an initial tensile stress field. The fracture surface exhibits the characteristic progression from the smooth, mirror region, to the rougher mist region, to the very rough hackle region. Comparison of the damage (2a) with the fracture surface (2b) reveals that the roughening arises from arrested micro-branches along the fracture surface.

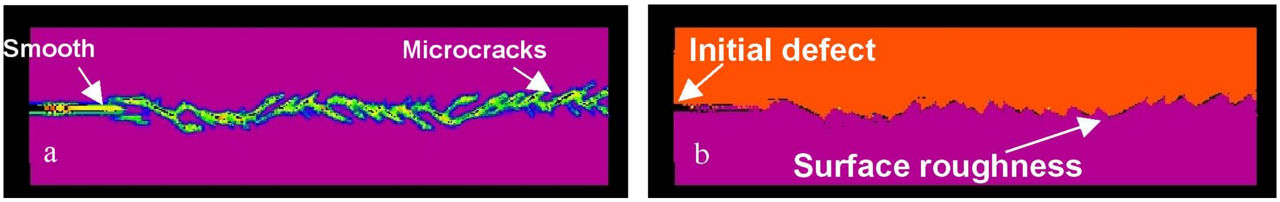

Figure 2. (a) Material damage (bond breaking) from dynamic cracking produced by lateral tension applied to an initially notched thin plate. (b) Fracture surface created by dynamic cracking simulation of Figure 2a.

Figure 3 shows the crack velocity history from this simulation. The initially unsteady speed is seen to reach a relatively stable limiting value that is substantially below the theoretical limiting wave speed. This result is in good agreement with experimental observations [12].

A simulation of the Kalthoff-Winkler experiment is shown in Figure 4. In this experiment a metal plate with two notches is struck on edge by an impactor [1]. The resulting cracks emanate from the notches at reproducible angles that depend on the impactor speed. For the chosen impactor speed, cracks are observed to make a 70° angle to the initial notch direction, which is well reproduced by the peridynamic simulation. Note, in addition, that the transition from mode II to mode I fracture naturally evolves without intervention by the analyst.

Under high stress intensity levels, branches can be emitted from a crack tip. With increasing stress level, the branching point moves closer to the starting defect. Figure 5 illustrates that both branching and the trend in branching point location can emerge from peridynamic simulations [13]. The cracks emanate from initial notches at the left edge. The only parameters specified for these simulations were constant values of density, Young's modulus, and energy release rate; no kinetic relation was used to guide the branching.

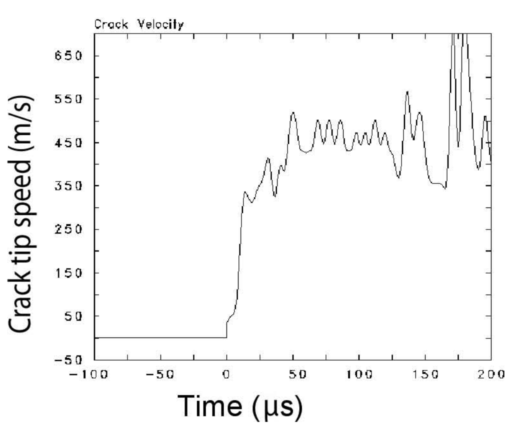

Figure 3. Crack velocity history for the simulation of Figure 2.

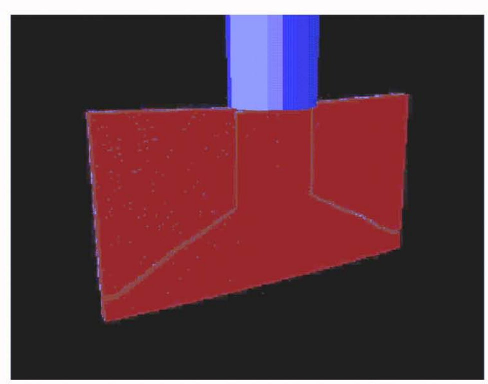

Figure 4. Kalthoff-Winkler Experiment. Peridynamics simulation of impact on a pre-notched plate.

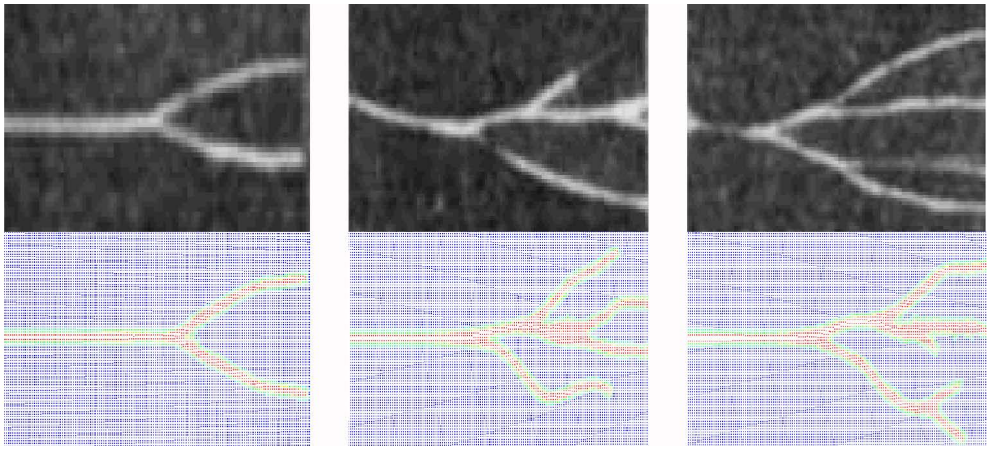

Figure 5. Cascading crack branching in glass under progressively higher applied stresses, left to right. Top row - Experimental results for soda-lime glass [14]. Bottom row - Simulations of Duran 50 glass [13]. Boundary conditions differed slightly in the experiment and simulation.

As a mesh-free method, peridynamics is well suited for simulating highly heterogeneous materials. Figure 6 shows the varying cracking modes that develop in laminated, fiber reinforced composites having differing lay-ups. All specimens have an initial horizontal center notch and are pulled in uniaxial tension. The figure illustrates variations of cracking mode with distribution of composite fiber directions that are comparable to those observed in laboratory tests.

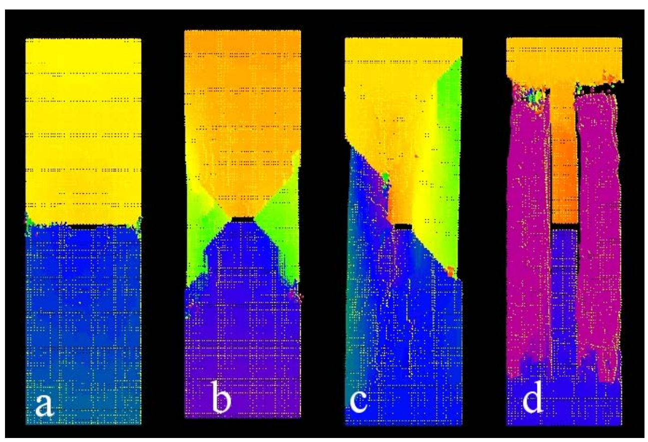

Figure 6. Variation in cracking modes in a notched laminate composite bar under vertically applied tension: (a) Quasi-isotropic sample; (b) All +/- 45º plies; (c) +/- 45º plies and Ø° plies; (d) Mostly Ø° plies (along length of bar). Images are colored by vertical displacement.

For the seven remaining characteristic phenomena of the 12 listed above, peridynamic simulation results for each agree very well with experiments, except for arrest of unstable crack growth, which has not yet been simulated.

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