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Computational Materials Modeling with Peridynamics

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We provide an overview and introduction to peridynamics, proposed in [1] as a nonlocal extension of classical solid mechanics. Peridynamics is suitable for modeling the failure and fracture of engineering materials.

The classical theory of continuum mechanics is based on partial differential equations. These equations do not hold on crack surfaces and other singularities, as partial derivatives are not defined at discontinuities. In the classical theory, cracks are regarded as a pathological solution requiring special treatment. In contrast, the peridynamic theory is based on integral equations, for which discontinuous functions present no difficulty [1,2]. By utilizing integral equations, the peridynamic theory avoids the need for the special techniques of fracture mechanics. In peridynamics, cracks are just another kind of solution and require no special treatment.

In peridynamics, each point in a body interacts directly and nonlocally with all points in a nearby region. Consequently, peridynamics has been called a "continuum formulation of molecular dynamics." Not surprisingly, a particular discretization of peridynamics has the same computational structure as classical molecular dynamics [3]. This computational structure has been leveraged to implement peridynamics within a massively parallel open-source molecular dynamics code [4].

Peridynamics has been successfully applied to model fracture in polycrystals [5], failure and fracture in composites [6], failure in nanofiber networks [7], and dynamic brittle fracture in glass [8], among other applications. As a representative example, Figure 1 shows a peridynamic simulation of a brittle disk after impact by a hard projectile [4]. As a multiscale material model, peridynamics has been demonstrated to be an upscaling of molecular dynamics [9].

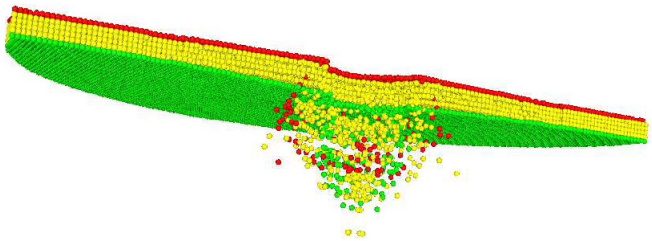

Figure 1a, Cut view of disk showing debris cloud after impact by projectile. Top and bottom monolayers of disk have been colored to show final particle positions.

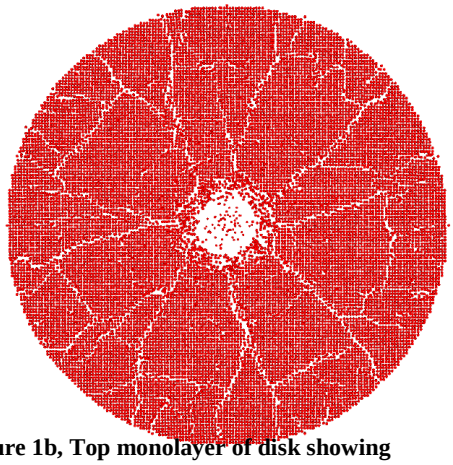

Figure 1b, Top monolayer of disk showing fragmentation after impact.

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