WARHEAD FRAGMENTATION MODELING WITH PERIDYNAMICS

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At the fundamental level, fragmentation occurs as a result of the initiation and growth of multiple, mutually interacting dynamic fractures. The statistical distributions of fragment sizes, shapes, and velocities are determined by the density of cracks and the competition between crack growth and other modes of material deformation. In this paper, we describe a three-dimensional computational model that allows spontaneous crack initiation and multiple cracks to coalesce to form fragments.

The model is based on a relatively new theory of continuum mechanics called peridynamic theory. This theory is formulated in terms of integral equations that remain valid in the presence of discontinuities in the displacement field. This feature of the theory overcomes a major obstacle in the modeling of fragmentation using the classical theory, which is based on partial differential equations that cannot be applied directly to a body containing cracks. An added benefit of the peridynamic approach is that crack growth is self-guided: there is no need for supplemental equations that govern crack initiation, velocity, growth direction, branching, and arrest. All of these features emerge directly from the equation of motion and constitutive model.

This paper outlines the basics of peridynamic theory and its implementation in a three-dimensional meshless computer code called EMU. It discusses detonation modeling and provides an application to fragmentation of an explosively loaded shell. We conclude that peridynamic theory is a physically reasonable and viable approach to modeling fragmentation phenomena and envision its use in addressing problems of design and performance of warheads.

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PERIDYNAMIC THEORY

Peridynamic theory is a theory of continuum mechanics that uses integral equations and assumes that particles in a continuum interact across a finite distance as in molecular dynamics. This theory was first published in 2000 by Silling [1]. The term "peridynamic" was taken from the Greek roots for "near" and "force".

Since peridynamic theory is relatively new compared to classical continuum mechanics, we will review the basics of peridynamic theory. In the following, we state the fundamental equation of peridynamics and introduce the pairwise force function (*PFF*). The *PFF* is the force per unit volume squared between two particles. This interaction is called a bond. Failure of a bond occurs when the stretch exceeds a value called the critical stretch. Constitutive properties of a material are given by specifying the *PFF*. Thus, in peridynamics, material response, damage, and failure are determined at the bond level. We also discuss some properties of the *PFF*, and the material models that we have used for fragmentation analysis.

The Fundamental Equation of Peridynamic Theory

Consider a peridynamic body that occupies a domain *R* as shown in Figure 1.

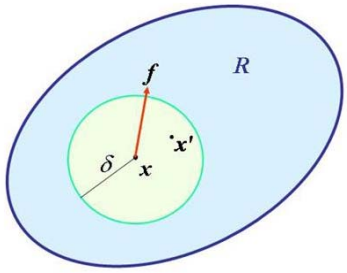

Figure. 1 A peridynamic body occupying a domain R

In peridynamics, the force density on a particle at point $\boldsymbol{x}$ and time t is assumed to be given by

$$\rho(\boldsymbol{x})\frac{d^2}{dt^2}\boldsymbol{u}(\boldsymbol{x},t) = \iiint_R \boldsymbol{f}(\boldsymbol{u}(\boldsymbol{x}',t)-\boldsymbol{u}(\boldsymbol{x},t),\boldsymbol{x}'-\boldsymbol{x})dV' + \boldsymbol{b}(\boldsymbol{x},t) \qquad (1)$$

where $\rho(\boldsymbol{x})$ is the density at $\boldsymbol{x}$, $\boldsymbol{x}$ and $\boldsymbol{x}'$ are points in the reference configuration, t is the time, $\boldsymbol{u}$ is the displacement vector, $\boldsymbol{f}$ is the *PFF*, and $\boldsymbol{b}$ is the body-force density.[1] Eq.

[1] In eq. (1) and elsewhere, bold quantities are vectors unless stated otherwise.

(1) is the fundamental equation of peridynamic theory. It is based on Newton's second law for all points within the domain of analysis. It does not contain spatial derivatives. The specific force is a functional depending on the *PFF*.

Figure 1 shows a sphere of radius δ centered at the point $\boldsymbol{x}$. It is convenient to assume that there is a distance δ such that the *PFF* function vanishes whenever $\boldsymbol{x}$ and $\boldsymbol{x'}$ are separated by a distance greater than δ in the reference configuration. The quantity δ is called the *horizon* since a particle cannot "see" any other particles beyond its horizon.

Some Properties of the Pairwise Force Function

It is convenient to express the *PFF* in terms of a new set of variables, $\boldsymbol{\xi}$ and $\boldsymbol{\eta}$, where $\boldsymbol{\xi} = \boldsymbol{x'} - \boldsymbol{x}$ and $\boldsymbol{\eta} = \boldsymbol{u}(\boldsymbol{x'},t) - \boldsymbol{u}(\boldsymbol{x},t)$. $\boldsymbol{\xi}$ is the relative position of particles at $\boldsymbol{x}$ and $\boldsymbol{x'}$ in the reference configuration and $\boldsymbol{\eta}$ is the difference in displacements at these points. Then $\boldsymbol{\eta}+\boldsymbol{\xi}$ is the relative position in the deformed configuration of the particles originally at $\boldsymbol{x}$ and $\boldsymbol{x'}$, and $\boldsymbol{f}$ is a function of $(\boldsymbol{\xi},\boldsymbol{\eta})$.

Newton's third law states that the force on a particle at $\boldsymbol{x}$ due to a particle at $\boldsymbol{x'}$ must be the negative of the force on a particle at $\boldsymbol{x'}$ due to a particle at $\boldsymbol{x}$. This law implies that $\boldsymbol{f}(\boldsymbol{\eta},\boldsymbol{\xi})$ is an odd function of $\boldsymbol{\eta}$ and of $\boldsymbol{\xi}$..

Angular momentum must be conserved in the absence of external forces To ensure conservation of angular momentum, $\boldsymbol{f}(\boldsymbol{\eta},\boldsymbol{\xi})$ must be parallel to $\boldsymbol{\eta}+\boldsymbol{\xi}$; otherwise a pair of particles would undergo angular acceleration in the absence of applied forces.

Material Models Used in Extreme Loading Analysis

A peridynamic material is said to be *micro-elastic* if and only there exists a scalar-valued function $w(\boldsymbol{\eta},\boldsymbol{\xi})$ such that

$$\boldsymbol{f}(\boldsymbol{\eta},\boldsymbol{\xi}) = \frac{\partial w}{\partial \boldsymbol{\eta}}(\boldsymbol{\eta},\boldsymbol{\xi}) . \tag{2}$$

w is called the *micro-potential*. The derivatives in eq. (2) are not the spatial derivatives that are to be avoided by using peridynamic theory. A micro-elastic material may be considered a material where each two points are connected by a spring that may be non-linear.

If a micro-elastic material is isotropic, then the magnitude of $\boldsymbol{f}$ and w depend only on the magnitudes of $\boldsymbol{\eta}+\boldsymbol{\xi}$ and $\boldsymbol{\xi}$., but not on the directions of these vectors.

For fragmentation analysis, we consider isotropic materials that have a *PFF* whose magnitude is proportional to a relative displacement called stretch. Such materials are

called *proportional* materials. The most general form of the *PFF* for proportional, micro-elastic materials is

$$\boldsymbol{f}(\boldsymbol{\eta},\boldsymbol{\xi}) = \frac{g(s,r)}{p}(\boldsymbol{\eta}+\boldsymbol{\xi}), \quad s = \frac{p-r}{r}, \quad p = |\boldsymbol{\eta}+\boldsymbol{\xi}|, \quad \text{and} \quad r = |\boldsymbol{\xi}| \tag{3}$$

where $g(s,r)$ is a piecewise linear function of the stretch s. The function g is called the *bond force* between two particles. Figure 2 shows the bond force dependence on bond stretch for proportional materials.

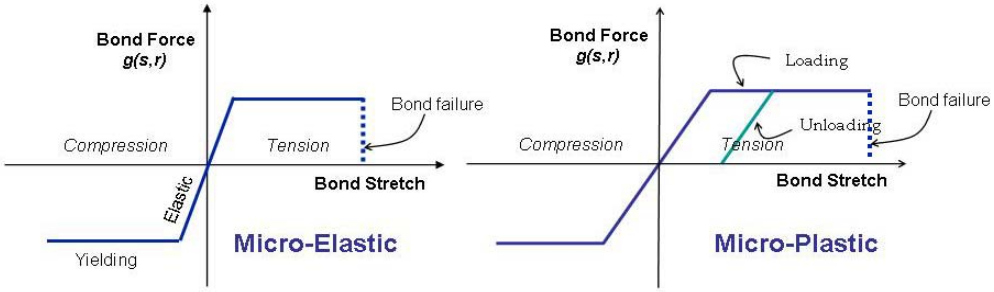

Figure 2. Bond force for micro-elastic and micro-plastic proportional materials

This figure also shows the bond force for a *micro-plastic* material. The behavior of micro-elastic and micro-plastic materials differ only on unloading. A micro-elastic material unloads reversibly back to zero stretch, while a micro-plastic material stretched beyond the elastic limit will retain some stretch when unloaded. This figure also indicates bond failure at some value of bond stretch. Peridynamic materials fail irreversibly when the stretch exceeds a value, s_c, called the *critical stretch*.

IMPLEMENTATION IN THE EMU COMPUTER CODE

EMU is the first computer code that is based on peridynamics. In the following, we review a numerical method to solve eq. (1) and summarize some important features of EMU.

Numerical Method

To solve the fundamental peridynamics equation, the computational domain is discretized into a finite set of nodes, $\{\boldsymbol{x}_i\}$. Each node has a known volume in the reference configuration. The set of nodes forms a computational grid.

The fundamental equation, eq. (1), is replaced by a finite sum, which at time t_n is

$$\rho_i \frac{d^2}{dt^2}\boldsymbol{u}_i^n = \sum_j \boldsymbol{f}(\boldsymbol{u}_j^n - \boldsymbol{u}_i^n, \boldsymbol{x}_j - \boldsymbol{x}_i)V_j + \boldsymbol{b}_i^n \tag{4}$$

where $\rho_i = \rho(\boldsymbol{x}_i)$, $\boldsymbol{u}_i^n = \boldsymbol{u}(\boldsymbol{x}_i, t_n)$, $\boldsymbol{b}_i^n = \boldsymbol{b}(\boldsymbol{x}_i, t_n)$, and V_j is the volume of node j in the reference configuration. The sum is taken over all nodes within the horizon of x_i. The acceleration term in eq. (4) is approximated by an explicit central difference.

Some Important Features of EMU

The numerical method discussed above does not use elements, and there are no geometrical objects connecting the grid points. Hence, EMU is mesh free. There is no need for a mesh generator when modeling complex structures. Only the generation of grid points is required.

EMU is Lagrangian in the sense that each node contains a fixed amount of material. A body contains multiple nodes and may undergo damage and fracture if bonds between nodes are broken. However, the mass in each node remains constant.

EMU uses explicit time integration to advance the solution to eq. (4) in time. Explicit time integration is a simple, reliable method. A stable time-step estimate was obtained by Silling and Askari [2] for a linear *PFF*.

EMU executes on parallel computers. Parallelization is performed by allowing each processor to be responsible for fixed region of space.

DETONATION MODELING IN PERIDYNAMICS

A peridynamic detonation model was developed and implemented in EMU. Since the detonation products in an explosion are gases, we first discuss modeling gases as bond-based, peridynamic materials. We then summarize the principle components of the model: input, detonation propagation, and behavior of detonation products [3].

Gases as Peridynamic Materials

The micro-potential has units of energy per unit volume squared and represents the internal energy density associated with a bond. To obtain an expression for the *PFF*, let all the bonds be held fixed except for bond k. Then, the change in energy density when bond k is stretched dp_k is

$$dW = \frac{1}{2} f_k dp_k \Delta V_k = \frac{dW}{dX}\frac{\partial X}{\partial p_k} dp_k \text{ , which implies } \quad f_k = \frac{2}{\Delta V_k}\frac{dW}{dX}\frac{\partial X}{\partial p_k} \tag{5}$$

where f_k, is the *PFF* for this bond, ΔV_k is the reference volume of node k, $X = \rho_0/\rho$ is the expansion, and ρ and ρ_0 are the respective deformed and reference densities. The one half is present in eq. (5) since each node owns half the energy of the bond.

Eq. (5) implies that the *PFF* of a gas depends on how the internal energy per unit volume of the gas changes with the expansion of the gas (X). There are many ways to approximate the expansion. We approximate X as

$$X = \left[\frac{1}{V} \sum_j \left(\frac{p_j}{r_j} \right)^{-m} \Delta V_j \right]^{-3/m}, \quad V = \sum_k \Delta V_k \tag{6}$$

where the sum is taken over the nodes inside the horizon of the given node, $p_j = |\boldsymbol{\eta}_j + \boldsymbol{\xi}_j|$, and $r_j = |\boldsymbol{\xi}_j|$. A value of $m = 1$ is used in the current version of EMU.

The expansion of the gas is generally represented as an isentropic process. Since the derivative of the internal energy with respect to specific volume at constant entropy is minus the pressure (P) [4], the expression for f_k in eq. (5) and eq. (6) imply that

$$f_k = -\frac{6P}{r_k V} \left(\frac{p_k}{r_k} \right)^{-m-1} X^{1+m/3}. \tag{7}$$

Implementation of (7) requires knowledge of P as a function of X for an isentropic process. In the initial implementation, we consider gases to be ideal gases. Then, the pressure is $P = P_0 X^{\gamma}$, where P_0 is the initial pressure and γ is the ratio of specific heats.

Peridynamic Detonation Model

For each explosive material, the user provides the location of the detonation point and time of detonation initiation along with the density of the unreacted explosive and the detonation speed. The user may also specify the temperature, Chapman-Jouguet (CJ) pressure (P_{CJ}) and the ratio of molar specific heats of the detonation gases (γ).

The detonation times at the explosive material nodes are calculated using program burn. In program burn, detonation times are calculated during input processing using a Huygen's construction procedure. In this procedure, the detonation propagates from the initial detonation point spherically at the specified detonation speed. This construction permits detonations to propagate around obstacles.

When detonation occurs, the gas expands adiabatically from one half the CJ pressure. The initial pressure is set to this pressure to obtain the correct energy in the ideal-gas reaction products from the detonation process. The peridynamic force on each gas node is obtained from this pressure and eq. (7).

FRAGMENTATION OF AN EXPLOSIVELY-LOADED SHELL

Consider an explosively-loaded shell with cross section depicted in Figure 3. We performed an EMU simulation of the system's motion for about 89 ms after detonation. For the simulation, the shell is considered a micro-plastic peridynamic material with density 8000 kg/m^3, sound speed 4000 m/s, yield strength 400 MPa, and critical stretch 0.3, and the explosive is considered a peridynamic explosive material with an unreacted density 1785 kg/m^3, detonation speed 8747 m/s, detonation pressure 31.66 GPa, and γ = 3.3.

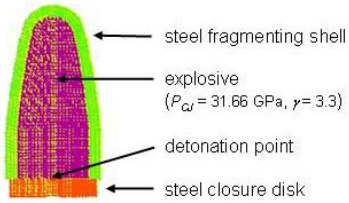

Figure 3. Cross section view of an explosively-loaded shell

Figure 4 compares simulation results with radiographic images from a test. The radiographic image is shown on the left and steel material from the EMU simulation is shown at the closest corresponding times, about 27.3 ms and 45.1 ms. This figure shows very good agreement between the image and the EMU results.

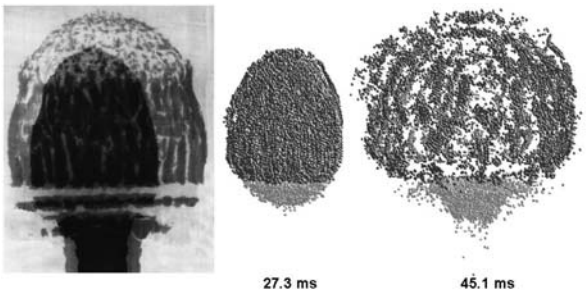

Figure 4. Comparison of radiographic image (left) and EMU simulation results

Since a grid of any significant size may form a large number of fragments that are difficult to comprehend on the basis of plots, some statistical tools have been developed to help in the interpretation of results. These tools include cumulative distributions of volume, size, and mass of fragments and velocity distributions of fragments.

Figure 5 shows a velocity distribution at about 50 ms. Each fragment is plotted on the (θ, ϕ) plane as a circle. The location of the center of the circle gives the direction of

the fragment's velocity vector in terms of these angles. The radius of the circle is proportional to the kinetic energy of the fragment.

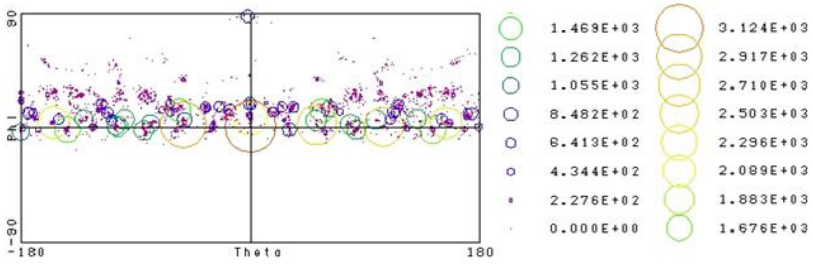

Figure 5. Velocity distribution at about 50 ms

Two tests that collected fragments were performed for the shell shown in Figure 3. We performed simulations to determine the sensitivity of fragmentation to critical stretch and other EMU inputs. Figure 6 compares the calculated mass cumulative distributions with data for five values of the critical stretch ranging from 0.05 to 0.4. The results for a critical stretch of 0.1 agree well with the data.

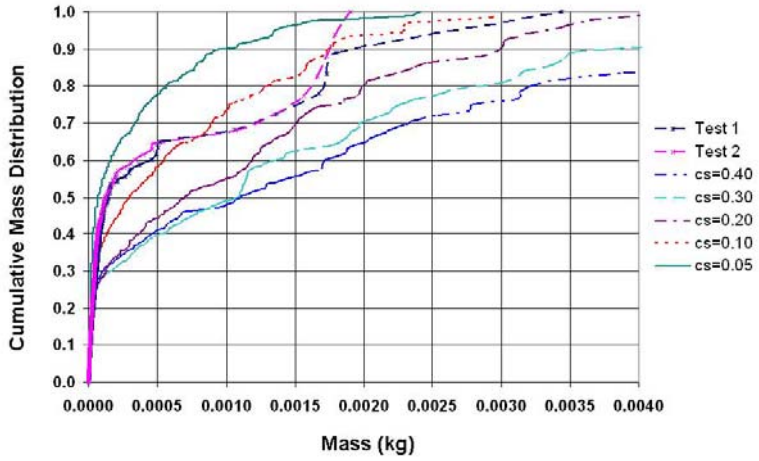

Figure 6. Sensitivity of fragmentation to critical stretch

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