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Detonation Modeling in Peridynamic Theory

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Abstract. Peridynamic theory is a theory of continuum mechanics that is formulated in terms of integro-differential equations without spatial derivatives. Its equations remain valid regardless of fractures or other discontinuities that may emerge in a material due to loading. This theory provides a consistent treatment of both deformation and failure of materials under dynamic loading. In bond-based peridynamics, material properties are specified through the pairwise force function. We apply the work-energy theorem to obtain the pairwise force function for a gas. With gas detonation products represented as peridynamic materials, we then use the Zeldovich, Von Neumann, and Doering detonation model and the volume-burn algorithm to formulate a detonation model in peridynamic theory. We discuss a numerical method and implementation of the detonation model, concomitant with addressing time-step stability and short-range forces. Finally, we illustrate this formulation with simulations of a cylinder-expansion test and a cylinder fragmenting under explosive loading.

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Introduction

Peridynamic theory (PD) is a theory of continuum mechanics that is formulated in terms of integro-differential equations without spatial derivatives. Its equations remain valid regardless of fractures or other discontinuities that may emerge in a material due to loading. PD provides a consistent treatment of both deformation and failure of materials under dynamic loading. In this paper, we review bond-based PD and material modeling in PD. In bond-based PD, material properties are specified through the pairwise force function (*PFF*). We discuss some properties of the *PFF*. We discuss a numerical method to solve the fundamental equation of bond-based PD and outline development of a condition for time-step stability. We apply the work-energy theorem to obtain the *PFF* for a gas. This formulation only requires knowledge of the isentrope of the gas in the pressure, specific-volume plane, and may be used with any equation of state from which the isentrope may be obtained analytically or numerically. With gas detonation products represented as PD materials, we employ the Zeldovich, Von Neumann and Doering (ZND) detonation model and the volume-burn algorithm. In PD, repulsive short-range forces act when points are sufficiently close. We discuss these forces since they provide for the transfer of momentum from an expanding gas to structures. We summarize the implementation of the detonation model. We

illustrate this formulation with simulations of a cylinder-expansion test and a cylinder fragmenting under explosive loading.

Nomenclature

CJ	Chapman-Jouguet
CMD	cumulative mass distribution
exp(x)	exponential function
JWL	Jones, Wilkins, Lee
PD	peridynamic theory or peridynamic(s)
PFF	pairwise force function
π	ratio of circumference to diameter of a circle
ZND	Zeldovich, Von Neumann, and Doering
{A: P}	set of all A with property P
×	cross product
•	dot product
|A|	magnitude of scalar or vector A

Peridynamic Theory (PD)

The version of PD introduced in 2000 is called bond-based PD[1]. A more general version, state-based PD, was introduced later[2]. Here, we will only consider bond-based PD.

Fundamental Equation of Bond-Based PD

Consider a peridynamic body that occupies a domain $\boldsymbol{R}$ as shown in Fig. 1. [a]

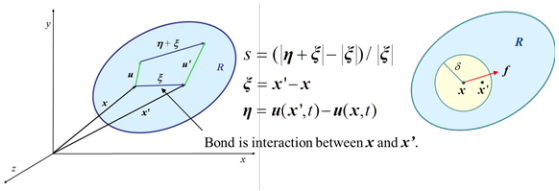

Fig. 1. A peridynamic body occupying a domain.

In Fig. 1 (left), $\boldsymbol{\xi}$ is the relative position of points $\boldsymbol{x}$ 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 of the points originally at $\boldsymbol{x}$, $\boldsymbol{x}'$ in the deformed configuration. The scalar quantity s in this figure is called the *stretch* and is a measure of relative deformation. The relative displacement in the undeformed configuration, $\boldsymbol{\xi}$, and the deformation, $\boldsymbol{\eta}$, are also defined in Fig. 1. Thus, the quantity $\boldsymbol{\eta} + \boldsymbol{\xi}$ is the relative displacement after deformation as shown in this figure. Quantities in the right graphic in Fig.1 will be discussed later.

The force density at $\boldsymbol{x}$ at time t in bond-based PD, is given by

$$\rho(\boldsymbol{x})\,\frac{d^2}{dt^2}\,\boldsymbol{u}(\boldsymbol{x},t) = \iiint_{\boldsymbol{R}} \boldsymbol{f}(\boldsymbol{\eta},\boldsymbol{\xi})dV' + \boldsymbol{b}(\boldsymbol{x},t) \quad (1)$$

where $\boldsymbol{x}$ is a point in the reference configuration, t is the time, $\rho(\boldsymbol{x})$ is the density at $\boldsymbol{x}$, $\boldsymbol{u}$ is the displacement vector, $\boldsymbol{R}$ is the domain of the body, $\boldsymbol{f}$ is the pairwise force function (*PFF*), $\boldsymbol{\eta}$ and $\boldsymbol{\xi}$ are defined in Fig. 1, and $\boldsymbol{b}$ is the body-force density. The integral in (1) is taken over the volume occupied by $\boldsymbol{R}$. All functions are assumed to be sufficiently well behaved that the integral exists.

(1) is based on Newton's second law for all points within the domain of analysis and does not contain any spatial derivatives. The *PFF* gives the force per unit volume squared on a point at $\boldsymbol{x}$ due to the point at $\boldsymbol{x}'$. In conventional continuum-mechanics theory, this functional is replaced by the divergence of the stress tensor. All constitutive properties of a material in bond-based PD are given by specifying the *PFF*.

Fig. 1 (right) shows a sphere of radius δ centered at the point $\boldsymbol{x}$, $S_\delta(\boldsymbol{x}) = \{\boldsymbol{x_i}: |\boldsymbol{x_i} - \boldsymbol{x}| < \delta\}$. It is assumed that there is a distance δ such that the *PFF* function vanishes outside $S_\delta(\boldsymbol{x})$ for each point $\boldsymbol{x}$ in the domain of analysis. The quantity δ is called the *horizon* since a point cannot "see" a force beyond its horizon. All points within $S_\delta(\boldsymbol{x})$ are said to belong to the *family* of $\boldsymbol{x}$. The appropriate value of δ depends on the physical nature of the application. However, in numerical modeling at the macroscale, typically δ is chosen to be three times the grid spacing.

Properties of the Pairwise Force Function

Newton's laws not only lead to the fundamental equation of peridynamics, but also imply properties of the *PFF*. Newton's third law states that the force at $\boldsymbol{x}$ due to point $\boldsymbol{x}'$ must be the negative of the force at $\boldsymbol{x}'$ due to point $\boldsymbol{x}$. Therefore

[a] In this figure and elsewhere, bold quantities are vectors unless stated otherwise.

for (1) to satisfy Newton's third law, $\boldsymbol{f}(\boldsymbol{\eta},\boldsymbol{\xi})$ must satisfy

$$\boldsymbol{f}(-\boldsymbol{\eta},-\boldsymbol{\xi}) = -\boldsymbol{f}(\boldsymbol{\eta},\boldsymbol{\xi}) \text{ for all } \boldsymbol{\eta},\boldsymbol{\xi} \quad (2)$$

Thus, $\boldsymbol{f}(\boldsymbol{\eta},\boldsymbol{\xi})$ is an odd function of $(\boldsymbol{\eta},\boldsymbol{\xi})$.

Another property of the *PFF* follows from the requirement to conserve angular momentum in the absence of external forces. If angular momentum were not conserved, then two points initially at rest would move even in the absence of external torques. Thus, to insure conservation of angular momentum, $\boldsymbol{f}(\boldsymbol{\eta},\boldsymbol{\xi})$ must satisfy

$$(\boldsymbol{\eta}+\boldsymbol{\xi}) \times \boldsymbol{f}(\boldsymbol{\eta},\boldsymbol{\xi}) = 0 \quad (3)$$

where "×" is the cross product. This expression implies that the force between any two points in the continuum must be parallel to their current relative position. Therefore, (3) implies that $\boldsymbol{f}(\boldsymbol{\eta},\boldsymbol{\xi})$ must have the functional form

$$\boldsymbol{f}(\boldsymbol{\eta},\boldsymbol{\xi}) = F(\boldsymbol{\eta},\boldsymbol{\xi})(\boldsymbol{\eta}+\boldsymbol{\xi}) \text{ for all } \boldsymbol{\eta},\boldsymbol{\xi} \quad (4)$$

where F is a scalar-valued function. Since $\boldsymbol{f}(\boldsymbol{\eta},\boldsymbol{\xi})$ is an odd function of $(\boldsymbol{\eta},\boldsymbol{\xi})$, $F(\boldsymbol{\eta},\boldsymbol{\xi})$ must be an even function of $(\boldsymbol{\eta},\boldsymbol{\xi})$.

Material Modeling in Peridynamic Theory

All constitutive properties of a material are given by specifying the *PFF*. Here we summarize only aspects of material modeling that are needed for understanding the solid models used in the examples and gases as PD materials.

The Micro-Potential

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

$$\boldsymbol{f}(\boldsymbol{\eta},\boldsymbol{\xi}) = \frac{\partial w(\boldsymbol{\eta},\boldsymbol{\xi})}{\partial \boldsymbol{\eta}} \quad (5)$$

The function w is called the *micro-potential*. It is important to realize that the derivatives in (5) are not the spatial derivatives that are to be avoided by using PD.

The micro-potential has units of energy per unit volume squared. It represents potential energy density associated with a bond. We may define a functional that for a displacement $\boldsymbol{u}$ is the *local displacement energy density*,

$$W_u(\boldsymbol{x},t) = \frac{1}{2}\iiint_R w(\boldsymbol{\eta},\boldsymbol{\xi})dV' \quad (6)$$

(6) is the energy density at the point $\boldsymbol{x}$ and time t associated with a displacement $\boldsymbol{u}$ of all the points in domain R. The factor of 1/2 is present since only half the energy is associated with each endpoint of the bond. Integration of (6) over the body yields the *total macroscopic energy* functional.

Proportional Materials

A class of *PFF*'s that is useful for modeling solid materials is called proportional materials. Such materials are a further development of the idea that micro-elastic materials may be considered materials in which two points are connected by a spring that, in general, may be non-linear. The *PFF* for a proportional material has a magnitude proportional to the stretch s, where

$$s = \frac{p-r}{r}, p = |\boldsymbol{\eta}+\boldsymbol{\xi}|, r = |\boldsymbol{\xi}|. \quad (7)$$

The most general form of the *PFF* for this material is

$$\boldsymbol{f}(\boldsymbol{\eta},\boldsymbol{\xi}) = \frac{g(s,r)}{p}(\boldsymbol{\eta}+\boldsymbol{\xi}) \quad (8)$$

where $g(s,r)$ is a piecewise linear function of the stretch s. The function g is called the *bond force* between two points for a proportional PD material.

Material Failure in Peridynamic Theory

A bond in a PD material fails irreversibly when the stretch s exceeds a value, s_c, called the *critical stretch*. Not only does the critical stretch define failure of a material, but it also assures the existence of a horizon for proportional materials.

Numerical Method

To solve the fundamental PD equation of motion, (1), the domain is discretized into a set of nodes, $\{\boldsymbol{x}_i\}$, as depicted in Fig. 3. Each node has a known volume in the reference configuration. The nodes form a computational grid.

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

$$\rho_i \frac{d^2}{dt^2}\boldsymbol{u}_i^n = \sum_j \boldsymbol{f}\left(\boldsymbol{u}_j^n - \boldsymbol{u}_i^n, \boldsymbol{x}_j - \boldsymbol{x}_i\right)V_j + \boldsymbol{b}_i^n \quad (9)$$

where $\rho_i = \rho(x_i)$, $\boldsymbol{u}_i^n = \boldsymbol{u}(\boldsymbol{x}_i,t_n)$, $b_i^n = \boldsymbol{b}(\boldsymbol{x}_i,t_n)$, and V_j is the volume of node j. The sum is taken over all nodes within the horizon δ of x_i .

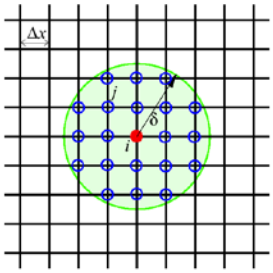

Fig. 2. Computational grid.

The acceleration term in (9) is approximated by an explicit central difference

$$\frac{d^2}{dt^2}\boldsymbol{u}_i^n = \frac{\boldsymbol{u}_i^{n+1} - 2\boldsymbol{u}_i^n + \boldsymbol{u}_i^{n-1}}{(\Delta t)^2} \qquad (10)$$

where Δt is the time step.

(9) and (10) are solved to obtain the displacements $\boldsymbol{u}_i^{n+1}$. The error in (10) is well known to be second order in time.[3]

Gases as Peridynamic Materials

Since the detonation products in an explosion are gases, we must determine how to model gases as PD materials. In this section, we develop a general expression for the *PFF* of a gas. This development generalizes the development that is documented in Demmie and Silling[4].

Pairwise Force Function for a Gas

The *PFF* for a gas can be determined from the change in internal energy per unit volume of the gas and expressed in terms of the expansion of the gas, X, where

$$X = \frac{v}{v_0} = \frac{\rho_0}{\rho} \qquad (11)$$

v and v_0 are the deformed and reference specific volumes of the gas, ρ and ρ_0 are the deformed and reference densities, respectively. Implementation of a gas model requires computing the expansion at a node from the undeformed and deformed bond lengths between this node and all gas nodes in its family.

To derive a general expression for the *PFF* of a gas, consider (5) and (6). From (5), the micro-potential, w, may be written as

$$w(\boldsymbol{x},t) = \int_{\boldsymbol{\eta}_0}^{\boldsymbol{\eta}(\boldsymbol{x},t)} \boldsymbol{f}(\boldsymbol{\eta},\boldsymbol{\xi}) \bullet d\boldsymbol{\eta} \qquad (12)$$

where $\boldsymbol{\eta}_0$ is some fiducial state of stretch. Since the integral (6) vanishes outside the horizon of $\boldsymbol{x}$, $H(\boldsymbol{x})$, (6) may be written using (12) as

$$W_u(\boldsymbol{x},t) = \frac{1}{2}\iiint_{H(\boldsymbol{x})} \left[\int_{\boldsymbol{\eta}_0}^{\boldsymbol{\eta}(\boldsymbol{x},t)} \boldsymbol{f}(\boldsymbol{\eta},\boldsymbol{\xi}) \bullet d\boldsymbol{\eta}\right] dV_{\boldsymbol{\xi}} \qquad (13)$$

Let all the bonds be held fixed except for bond k at a given value of $\boldsymbol{\xi}$. Then, for an incremental stretch dp_k in bond k, (13) becomes dW, where

$$\begin{aligned} dW &= \frac{1}{2}\boldsymbol{f} \bullet \boldsymbol{\eta}\, dV_{\boldsymbol{\xi}} = \frac{1}{2}\boldsymbol{f} \bullet (\boldsymbol{\eta} + \boldsymbol{\xi})\, dV_{\boldsymbol{\xi}} \\ &= \frac{1}{2} f_k dp_k V_k \end{aligned} \qquad (14)$$

In (14), f_k is the magnitude of the *PFF* at bond k due to this incremental stretch dp_k in this bond, and V_ξ and V_k are volume elements associated with bond k. The latter two equalities follow since $\boldsymbol{\xi}$ is fixed under the stretch and $\boldsymbol{f}$ is parallel to $\boldsymbol{\eta}+\boldsymbol{\xi}$ as stated in (4).

The quantity f_k in (14) is the *PFF* for a gas. This quantity can be expressed in terms of the expansion X as follows.

Changes in the energy per unit volume, dW, result from the stretch dp_k. Therefore, using the definition of dW and the chain rule, (14) may be written as

$$dW = \frac{\partial W}{\partial p_k} dp_k = \frac{\partial W}{\partial X}\frac{\partial X}{\partial p_k} dp_k \qquad (15)$$

since W depends on p_k through its dependence on X.

Equating (14) and (15) and solving for f_k yields a general expression for the *PFF* of a gas

$$f_k = \frac{2}{V_k}\frac{\partial W}{\partial X}\frac{\partial X}{\partial p_k} \qquad (16)$$

The *PFF* can be obtained from (16) once the energy per unit volume, W, is known as a function of the expansion X, and X is known as a function of the incremental stretches for all gas bonds within the horizon of a node.

There are many possible ways to approximate the expansion X. We now describe the method currently implemented. Consider the ratio of the

reference density to the deformed density. This ratio is X. We approximate X at a given node by

$$X = \left[\frac{1}{V}\sum_j \left(\frac{r_j}{p_j}\right) V_j\right]^{-3}, V = \sum_k V_k \qquad (17)$$

where the sum is taken over the nodes inside the horizon of the given node, $p_j = |\boldsymbol{\eta}_j + \boldsymbol{\xi}_j|$, $r_j = |\boldsymbol{\xi}_j|$, and V_j is the reference volume of node j. We refer to the nodes inside the horizon of a given node as its family. Hence, V is the total reference volume of the family of the given node.

Calculating the derivatives in (16) using (17), we obtain

$$f_k = \frac{6}{r_k V}\frac{\partial W}{\partial X}\left(\frac{r_k}{p_k}\right)^2 X^{4/3} \qquad (18)$$

If we identify W with the internal energy per unit volume of the gas, then (18) and knowledge of the dependence of W on the expansion X yield an expression for the *PFF* at node k.

From the standard axiomatic formulation of thermodynamics[5], the pressure is an intensive variable defined as minus the partial derivative of the internal energy with respect to specific volume at constant entropy. Therefore, the derivative in (18) is the negative pressure, P, which implies that the magnitude of the *PFF* for node k in a gas is

$$f_k = -\frac{6P}{r_k V}\left(\frac{r_k}{p_k}\right)^2 X^{4/3} \qquad (19)$$

Implementation of (19) requires knowledge of the pressure P as a function of the expansion X on an isentrope. The negative sign indicates that the force is repulsive.

Volume Burn Algorithm

Implementation of the *PFF* for gases given by (18) requires knowledge of P as a function of X along an isentrope. To determine the isentrope to use, we employ the ZND model[6] and the volume burn algorithm.

Fig. 2 depicts the pertinent features of the ZND model[b] and shows the integral that states the volume burn algorithm. This figure shows an initial state of specific volume v_0 and pressure P_0 and the Rayleigh line $R(v)$ emanating from this point. The Chapman-Jouguet (CJ) point is shown with specific volume v_{CJ} and pressure P_{CJ}. This point is defined as the point where the Rayleigh line and Hugoniot for the detonation products are tangent. The isentrope for the detonation products is also tangent to the Rayleigh line at the CJ point..

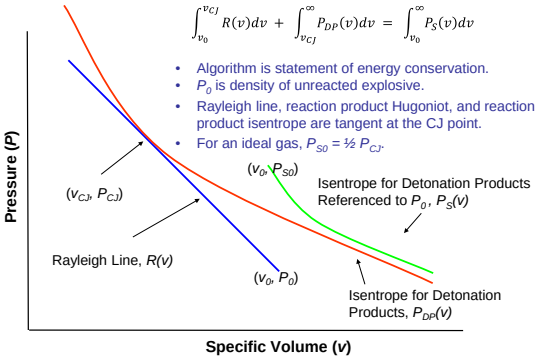

Fig. 3. Detonation Process.

The volume burn algorithm,

$$\int_{v_0}^{v_{CJ}} R(v)dv + \int_{v_{CJ}}^{\infty} P_{DP}(v)dv = \int_{v_{S0}}^{\infty} P_S(v)dv\,, \qquad (20)$$

is a statement of conservation of energy for the detonation products. Given the isentrope for the detonation-product gases and the Rayleigh line[7],

$$R(v) - P_0 = \frac{U^2}{v_0} - \frac{U^2}{v_0^2}v, \qquad (21)$$

where U is the detonation speed. (20) is solved to determine the reference pressure, P_{S0}, to be used in this isentrope for the detonation products in (18). For an ideal gas this procedure yields a reference pressure half the CJ pressure.

Time-Step Stability

It is possible to obtain a stability condition for the linearized equations for one-dimensional motion with a *PFF*

$$f(\eta, \xi) = C(\xi)\eta, \qquad C(\xi) = \frac{\partial f}{\partial \eta}(0, \xi) \qquad (22)$$

Applying the standard assumption for a von Neumann stability analysis[8]

$$u_i^n = \zeta^n exp\left(\kappa i\sqrt{-1}\right) \qquad (23)$$

[b] The Hugoniot for the unreacted explosive and the Von Neumann spike are not shown in Fig. 3.

where κ is a positive real number and ζ is a complex number, we obtain the stability condition[3]

$$\Delta t < \min \sqrt{\frac{2\rho}{\sum_k V_k C_{ik}}} \text{ for all } i \qquad (24)$$

where $C_{ik} = C(x_k - x_i)$.

To insure stability, it is essential to use the density, ρ, in (24) given by (11), i.e.,

$$\rho = \frac{\rho_0}{X} \qquad (25)$$

where ρ_0 is the initial density of the unreacted explosive and X is the expansion. For an explosive, it is essential that ρ_0 is the initial, unreacted value and X be the expansion given by (17). Otherwise the solution process is not stable and unrealistic fragmentation will occur under explosive loading. For solids under reasonable loadings, the expansion is about one and $\rho \sim \rho_0$. However, if X is given by some model, especially for high-impulse loading, (25) is used with ρ_0 the initial density.

For nonlinear material models, including (19), the form of the stability condition used is

$$C(\xi) = \left|\frac{\partial f}{\partial p}(0, \xi)\right| \qquad (26)$$

In this case, we apply a safety factor to the estimate in (24) to account for possible nonlinear material response that would make the estimated stable time step based on (24) too large.

Short-Range Forces

In bond-based PD, repulsive short-range forces act when nodes are sufficiently close. These forces prevent bonds from compressing indefinitely and violating non-impenetrability of matter. They are responsible for loading a solid material with an expanding gas. Without these forces, a container with a detonating explosive would not expand and fragment. The expanding gas would simply diffuse through the container.

When two nodes, i and j, are sufficiently close, the repulsive force, f_{ij}^{SR}, between them is given by

$$f_{ij}^{SR} = F_{SR} k_{PD} V_i V_j (p - p_{contact}) \qquad (27)$$

where F_{SR} is a force factor input by the user, k_{PD} is the PD spring constant for the bond connecting nodes i and j, p is the separation given in (7), $p_{contact}$ is the separation where short-range forces begin to act, and V_i and V_j are the respective volumes of nodes i and j. Short-range forces are included in the estimate of a stable time step.

The quantity $p_{contact}$ is calculated from the input parameters by the user for the material and short-range forces. Since (27) is only applied when $p < p_{contact}$, the force is negative and repulsive.

The PD spring constant in (27) is given by

$$k_{PD} = \frac{18K}{\pi \delta^4} \qquad (28)$$

where K is the bulk modulus and δ is the horizon.

Peridynamic Detonation Model

In this section, we discuss propagation of the detonation, EOSs for the detonation products, and summarize the implementation of our detonation model.

Propagation of Detonation (Program Burn)

The detonation times must be determined at each node containing an explosive. These times are calculated during input processing using a Huygen's construction procedure. This method is called *program burn*.

Program burn proceeds as follows. There are a set of nodes whose detonation times are specified user in the input. Initial detonation times at the other nodes are initially set to a large number. The construction proceeds by sweeping through the grid and examining at each node the detonation times of the nodes in a spherical neighborhood of this node. The detonation time at this node is the smallest time for a detonation to propagate from any detonated node in this neighborhood to this node. This process continues until detonation times are computed for all nodes. This Huygen's construction procedure insures that detonations propagate around obstacles and isolated regions of explosive material do not detonate. However, if there are no obstructions or isolated regions of explosive, a detonation radius may be specified. In this case, the detonation time at a particular node is the minimum of the times for the detonation to propagate along a straight line from the initially detonating nodes to this node.

Equations of State for Detonation Products

In our implementation of the PD detonation

model, two EOSs are available, an ideal gas and the Jones, Wilkins, Lee (JWL) model.

For an ideal gas, the pressure, P_S, along an isentrope is given as a function of the expansion, X, is given by[9]

$$P_S(X) = P_{S0}\left(\frac{V_0}{V}\right)^{\gamma} = P_{S0}X^{-\gamma} \qquad (29)$$

where P_{S0} is the reference pressure in Fig. 2 and γ is the ratio of molar specific heat at constant pressure to the molar specific heat at constant volume.

In the JWL model, this pressure is given by[10]

$$P_S(X) = \sum_{i=1}^{2} A_i exp(-R_i X) + CX^{-(\omega+1)} \qquad (30)$$

where the A_i, R_i, C, and ω are parameters determined for explosives by cylinder-expansion tests.

A Detonation Model for Peridynamic Theory

Fig. 4 summarizes the implementation of our PD detonation model. This figure shows three aspects of the implementation – the inputs, the determination of detonation times during input processing, and the treatment of reaction products after detonation.

- **Detonation model inputs:**
  - Location of detonation points and initial detonation times, density of explosive, and detonation speed.
  - Parameters for equation of state (ideal gas or JWL).
- **Program burn model for detonation times.**
  - Detonation times computed prior to time advancement using Huygen's construction.
  - Detonations can propagate around obstacles.
- **Upon detonation:**
  - Detonation products are treated as ideal or JWL gas undergoing an adiabatic expansion.
  - Energy is conserved using volume-burn algorithm.
  - The PD interactions between nodes are given by (19).
  - Interactions with solids given by short-range forces (28)

Figure 4. Implementation of PD detonation model.

The user specifies inputs listed in this figure for the explosive-material. These inputs are the locations of the detonation points and their respective detonation times, the detonation speed, the density of the explosive, and the equation of state (EOS) for the detonation products. We use the ideal gas and the JWL EOSs.

From the explosive-material input, the detonation times for all explosive nodes are computed prior to time advancement. Once the explosive in a node has detonated, the detonation products are treated as ideal or JWL gases undergoing an adiabatic expansion from the reference state shown in Fig. 3. The energy of the detonation products is conserved using the volume-burn algorithm. The PD interactions between explosive-material nodes are given by (18). Interactions with non-explosive material nodes are given by the short-range forces in (26).

Examples

The PD detonation model was implemented in a computer code. In this section, we provide two example simulations to illustrate the application of this model – a cylinder expansion and a fragmentation test. Both tests use a hollow cylindrical tube with open ends. These tubes were filled with explosive that was detonated.

Cylinder-Expansion Test

Fig. 5 compares displacement versus time for a cylinder-expansion test using a cylinder made of copper (Cu) filled with explosive and a simulation of this test.

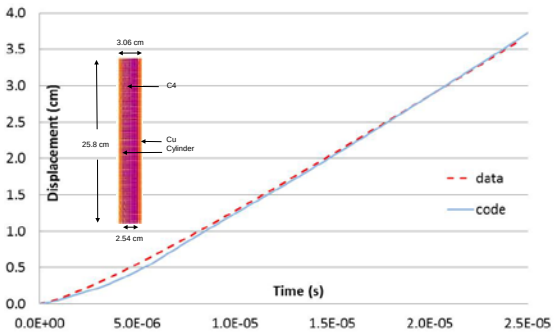

Fig. 5. Comparisons of displacements versus time for an exploding Cu cylinder test.

This figure also shows a schematic of the Cu tube. Initially, it was 25.8 cm long, had an inside diameter of 2.54 cm, and had 0.26-cm thick walls.

The material model used for Cu is the proportional model given by (8). The parameters that must be specified for this model are the material density, bulk sound speed, which is the square root of the bulk modulus divided by the density, the yield strength, and the critical stretch.

The respective values used for this simulation are 8930 kg/m^3, 3602 m/s, 324 MPa, and 2.0. The JWL model was used for the explosive.

The agreement between the simulation and data is excellent. The small deviations early in the test should be well within any experimental errors and uncertainties in the simulation.

Fragmenting-Cylinder Test

Fig. 6 compares cumulative mass distributions (CMD) from a fragmentation test using a cylinder made of steel filled with explosive and a simulation of this test. Initially, it was 4.25 in. long, had an inside diameter of 1.0 in., and had 1/8th thick walls. This test was performed at a facility that can capture 99% of the fragments from an exploding object.

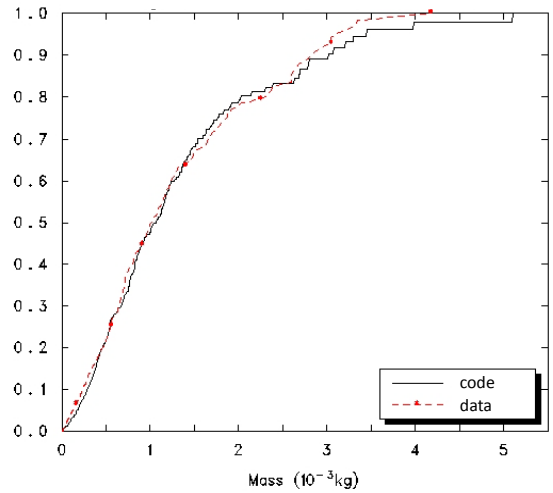

Figure 6. Comparisons of CMDs for a fragmenting steel cylinder test.

The steel was modeled as a proportional, micro-plastic material. A micro-plastic material uses (8), but differs from the micro-elastic model only on unloading. In the code implementation, a micro-elastic material unloads reversibly, but a micro-plastic material does not. The values for the steel density, bulk sound speed, yield strength, and critical stretch[c] are 7850 kg/m^3, 3212 m/s, 750 MPa, and 0.11, respectively. The JWL parameters model was used for the explosive.

The agreement between the simulation and data is excellent. The main disparities are for large mass fragments, which may caused by interactions with the capture media (sawdust) or the container walls which are not represented in the simulation.

Summary and Conclusions

In this paper, we described a detonation model for peridynamic theory (PD). After a concise discussion of the aspects of bond-based PD and numerical method needed for completeness, we showed how to represent gases as PD materials by deriving a pairwise force function (*PFF*) for a gas. This derivation was based on the work-energy theorem. The volume burn algorithm was then discussed. This algorithm is a statement of conservation of energy for the detonation products and provides a reference pressure to use in the pressure isentropes needed in the gas *PFF*. This algorithm is based on the ZND detonation model. Time-step stability was addressed since it is essential to obtain solutions to the PD equation for explosive loadings. The stability condition obtained is needed to provide for solutions as the explosive material changes from a solid to a gas which undergoes expansion. We discussed short-range forces. These forces prevent bonds from compressing indefinitely and violating non-impenetrability of matter. They are responsible for loading a solid material with an expanding gas. Without these forces, an expanding gas would simply diffuse through the solid. We provided an outline of the details of implementing our PD detonation model in a computer code. Finally, we showed comparisons of simulations with expanding-cylinder and fragmenting-cylinder tests. The simulation results are in excellent agreement with the data. We conclude that the PD with the detonation model described in this paper is a viable technology for studying explosive loading.

[c] Damage stretch coefficient and minimum stretch coefficient models were used for the steel. These models increase the critical as damage increases or in compression, respectively.

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