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Modeling shockwaves and impact phenomena with Eulerian peridynamics

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ABSTRACT

Most previous development of the peridynamic theory has assumed a Lagrangian formulation, in which the material model refers to an undeformed reference configuration. In the present work, an Eulerian form of material modeling is developed, in which bond forces depend only on the positions of material points in the deformed configuration. The formulation is consistent with the thermodynamic form of the peridynamic model and is derivable from a suitable expression for the free energy of a material. It is shown that the resulting formulation of peridynamic material models can be used to simulate strong shock waves and fluid response in which very large deformations make the Lagrangian form unsuitable. The Eulerian capability is demonstrated in numerical simulations of ejecta from a wavy free surface on a metal subjected to strong shock wave loading. The Eulerian and Lagrangian contributions to bond force can be combined in a single material model, allowing strength and fracture under tensile or shear loading to be modeled consistently with high compressive stresses. This capability is demonstrated in numerical simulation of bird strike against an aircraft, in which both tensile fracture and high pressure response are important.

1. Introduction

Nearly all work on peridynamics up to now has assumed material models that are *Lagrangian*, meaning that the bond forces depend not only on the current (deformed) configuration of the body, but also on a reference (undeformed) configuration. An exception is the class of *structureless* material models that were considered in [1]. These materials have bond force densities that are independent of any reference configuration, but, due to additional assumptions in what is now called the *bond-based* peridynamic theory, the structureless materials were found to have very restrictive properties and are generally not useful in applications.

In the present work, we re-examine the possibility of peridynamic material models that depend only on the deformed configuration, but do so within the *state-based* theory. It is shown that the greater generality of the state-based theory compared with the earlier bond-based theory avoids all of the limitations of the structureless materials. When incorporated within the thermodynamic statement of peridynamics, material models in the state-based theory can use any equation of state from the standard (local) theory. Futhermore, the resulting material models, which will be called *Eulerian*, can be combined in a straightforward way with Lagrangian models. This provides a convenient way to model solids in applications that involve fracture and fragmentation under tensile or shear loading, in which a Lagrangian formulation is the natural approach, with high pressures and large deformations, in which an Eulerian model has advantages. The capabilities of the Eulerian approach to peridynamic material modeling are demonstrated with examples from shock wave physics and impact mechanics of soft materials.

In Section 2 we provide a brief overview of the peridynamic theory, including mechanics and thermodynamics. In Section 3 we introduce a peridynamic Eulerian model equipped with a Mie–Grüneisen equation-of-state. Application to shockwave ejecta in a metal subjected to a detonation wave is presented in Section 3.4, along with comparison with experiment. Combination of Eulerian and Lagrangian contributions to bond force density in a material model is discussed in Section 4. This approach is demonstrated in a problem involving comminution of a material followed by large compression in Section 4.1. Simulation of birdstrike, along with validation of the predicted centerline pressure history, is described in Section 5. It is shown that the contribution of the Lagrangian terms, even though the problem appears to be dominated by large pressures at the point of impact, significantly improve the prediction of how the projectile shape evolves.

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2. Peridynamic theory summary

Here we review key features and equations of the peridynamic theory, including the mechanical theory and thermodynamics. A more detailed discussion may be found in the review article [2]. The numerical discretization method used for all the examples in the present paper is described in the Appendix.

2.1. Mechanics

The classical momentum equation for solid mechanics in Lagrangian form is

$$\rho_0(\mathbf{x})\ddot{\mathbf{y}}(\mathbf{x},t) = \nabla\cdot\boldsymbol{\sigma}(\mathbf{x},t) + \mathbf{b}(\mathbf{x},t) \tag{1}$$

where ρ_0 is the mass density in the reference configuration, $\mathbf{x}$ is a material point in the reference configuration, $\mathbf{y}$ is the deformation map, $\nabla\cdot$ is the divergence operator, σ is the Piola stress tensor field, and $\mathbf{b}$ is the body force density field.

The primary motivations for development of the peridynamic theory arise from the inapplicability of the PDE (1) at cracks or crack tips due to the nonexistence of the necessary spatial derivatives on these singularities, and the inability of this equation to include long-range forces. Since (1) cannot be applied directly on discontinuites, special techniques such as XFEM [3] have been proposed to insert cracks into discretized regions that are assumed to undergo smooth deformation elsewhere. Although these special techniques have achieved many successes, they require additional complexity, including supplemental equations that dictate the crack growth velocity and direction.

In contrast, the peridynamic theory of solid mechanics is based on integral equations, for which discontinuous solutions present no difficulty [1,4]. In peridynamics, cracks nucleate, grow, branch, merge, and arrest when and where it is energetically favorable for them to do so according to the basic field equations and material model. This capability for *autonomous crack growth* avoids the need for the special techniques of fracture mechanics. See [5] for a comparison of peridynamics with cohesive zone methods and XFEM. Peridynamics has been successfully applied to model fracture in polycrystals [6], failure and fracture in composites [7], dynamic brittle fracture in glass [8], and failure in electronic packages due to drop-shock [9], among other applications. As a multiscale material model, peridynamics has been demonstrated to be an upscaling of molecular dynamics [10]. It has been implemented within a massively parallel open-source molecular dynamics code [11], demonstrating scalable computational performance on a computer with 65,000 processors.

In the peridynamic model, any material point $\mathbf{x}$ interacts through the material model with its neighbors $\mathbf{q}$ within a prescribed distance δ of itself in the reference configuration. This maximum interaction distance δ is called the *horizon*, and the material within the horizon of $\mathbf{x}$ in the reference configuration is called the *family* of $\mathbf{x}$, denoted $\mathcal{H}_\mathbf{x}$. The vector between $\mathbf{x}$ and any point $\mathbf{q}$ in its family is called a *bond*, denoted $\mathbf{q}-\mathbf{x}$. Fig. 1 illustrates the horizon and family of $\mathbf{x}$. Associated with each bond is a *pairwise bond force density vector* (force per unit volume squared) that $\mathbf{q}$ exerts on $\mathbf{x}$, denoted $\mathbf{f}(\mathbf{q},\mathbf{x},t)$. The peridynamic equation of motion is

$$\rho_0(\mathbf{x})\ddot{\mathbf{y}}(\mathbf{x},t) = \int_{\mathcal{H}_\mathbf{x}} \mathbf{f}(\mathbf{q},\mathbf{x},t)\, dV_\mathbf{q} + \mathbf{b}(\mathbf{x},t). \tag{2}$$

The pairwise bond force density function is antisymmetric:

$$\mathbf{f}(\mathbf{x},\mathbf{q},t) = -\mathbf{f}(\mathbf{q},\mathbf{x},t), \tag{3}$$

which ensures that linear momentum is globally balanced.

The bond forces are determined jointly by the collective deformation of $\mathcal{H}_\mathbf{x}$ and the collective deformation of $\mathcal{H}_\mathbf{q}$. To precisely describe these collective deformations, a mathematical formalism involving

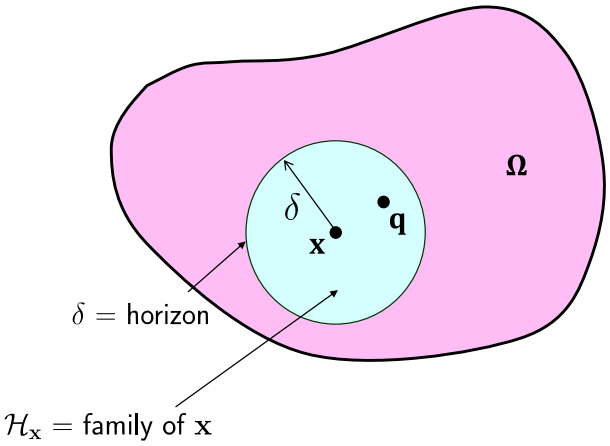

Fig. 1. A typical material point $\mathbf{x}$ interacts with its neighbors $\mathbf{q}$ within its horizon.

objects called *states* is used. States are operators that act on bonds. For present purposes, states are vector valued, that is, if $\underline{\mathbf{A}}$ is a state, then $\underline{\mathbf{A}}\langle\mathbf{q}-\mathbf{x}\rangle$ is a vector. The inner product of any two states $\underline{\mathbf{A}}$ and $\underline{\mathbf{B}}$ is defined by

$$\underline{\mathbf{A}}\bullet\underline{\mathbf{B}} = \int_{\mathcal{H}_\mathbf{x}} \underline{\mathbf{A}}\langle\mathbf{q}-\mathbf{x}\rangle\cdot\underline{\mathbf{B}}\langle\mathbf{q}-\mathbf{x}\rangle\, dV_\mathbf{q}.$$

States are the nonlinear analogues of second order tensors in linear algebra, which are linear transformations that map vectors to vectors. For functions of states, Fréchet derivatives are used instead of tensor gradients. To define the Fréchet derivative, let Ψ be a scalar-valued function of a vector state $\underline{\mathbf{A}}$. Suppose there is a state denoted $\Psi_{\underline{\mathbf{A}}}$ such that for any increment $\Delta\underline{\mathbf{A}}$,

$$\Psi(\underline{\mathbf{A}}+\Delta\underline{\mathbf{A}}) = \Psi(\underline{\mathbf{A}}) + \Psi_{\underline{\mathbf{A}}}\bullet\Delta\underline{\mathbf{A}} + o(\|\Delta\underline{\mathbf{A}}\|) \tag{4}$$

where

$$\|\Delta\underline{\mathbf{A}}\| = \sqrt{\Delta\underline{\mathbf{A}}\bullet\Delta\underline{\mathbf{A}}}.$$

Then $\Psi_{\underline{\mathbf{A}}}$ is the Fréchet derivative of Ψ. For a more complete discussion of states, see [4].

For purposes of material modeling, the basic kinematical quantity is the *deformation state* $\underline{\mathbf{Y}}$, defined at any $[\mathbf{x},t]$ by

$$\underline{\mathbf{Y}}[\mathbf{x},t]\langle\mathbf{q}-\mathbf{x}\rangle = \mathbf{y}(\mathbf{q},t)-\mathbf{y}(\mathbf{x},t). \tag{5}$$

The deformation state maps bonds onto their images under the deformation and is analogous to the deformation gradient tensor in the classical theory.

Pairwise bond force densities are assigned through the *force state* $\underline{\mathbf{T}}$:

$$\mathbf{f}(\mathbf{q},\mathbf{x},t) = \underline{\mathbf{T}}[\mathbf{x},t]\langle\mathbf{q}-\mathbf{x}\rangle - \underline{\mathbf{T}}[\mathbf{q},t]\langle\mathbf{x}-\mathbf{q}\rangle.$$

In this equation, there are contributions from the force states at both endpoints of the bond $\mathbf{q}-\mathbf{x}$. Clearly this expression for $\mathbf{f}$ satisfies the required antisymmetry (3). The material model $\hat{\underline{\mathbf{T}}}$ prescribes the force state as a function of the deformation state:

$$\underline{\mathbf{T}}[\mathbf{x},t] = \hat{\underline{\mathbf{T}}}(\underline{\mathbf{Y}}[\mathbf{x},t]), \qquad \underline{\mathbf{T}}[\mathbf{q},t] = \hat{\underline{\mathbf{T}}}(\underline{\mathbf{Y}}[\mathbf{q},t]). \tag{6}$$

Eq. (6) show the main motivation for using the state formalism: instead of a material model that gives a tensor-valued function of a tensor, in peridynamics we have a state-valued function of a state. The material model may include dependencies on other variables such as temperature or the time derivative of $\underline{\mathbf{Y}}$. A particularly useful material model is the *elastic* material:

$$\underline{\mathbf{T}} = \hat{\underline{\mathbf{T}}}(\underline{\mathbf{Y}}) = W_{\underline{\mathbf{Y}}}(\underline{\mathbf{Y}})$$