On the similarity of Peridynamics and Smooth-Particle Hydrodynamics

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Abstract

This paper discusses the similarity of the Peridynamic Theory and Smooth-Particle Hydrodynamics, under the condition that Peridynamics is applied to classical material models based on the deformation gradient. Specifically, we show that the discrete Peridynamic equations of motion, coincide with those of gradient-corrected Smooth-Particle Hydrodynamics in a Total-Lagrangian formulation if nodal integration is used as a discretization scheme.

Key words: meshless methods, Peridynamics, Smooth-Particle Hydrodynamics

1 Introduction

The Peridynamic theory, originally devised by Silling [1], is a nonlocal extension of classical continuum mechanics, which is based on partial differential equations. Since partial derivatives do not exist on crack surfaces and other singularities, the classical equations of continuum mechanics cannot be applied directly when such features are present. In contrast, the Peridynamic balance of linear momentum is formulated as an integral equation, which remains valid in the presence of material discontinuities. Therefore, the Peridynamic theory can be applied directly to modelling both bulk and interface properties, using the same mathematical model. Additionally, Peridynamics is readily implemented in a meshless formulation, which facilitates the simulation of large deformations when compared to the traditional mesh-based Finite-Element method used for simulating solid mechanics in the classical continuum theory [2].

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With these desirable features, Peridynamics has received considerable attention by researchers interested in numerically describing fundamental crack growth and failure effects in brittle materials [3, 4, 5, 6]. However, the scope of the original Peridynamic formulation included only so-called bond-based models [7] which were limited to a fixed Poisson ratio for linear isotropic materials and could not describe true plastic yielding. Further development of the theory led to state-based models [8], which can, in principle, describe all classic material behaviour. In particular, the state-based theory offers a route to approximating the classical deformation gradient, which can be used to obtain a classical stress tensor. The stress tensor can then be converted into nodal forces using a Peridynamic integral equation. This promising situation, i.e., the ability to use classical material models with a method that remains valid at material discontinuities, has prompted a number of studies where plastic yielding, damage, and failure was simulated using this new meshless method [9, 10].

However, no published studies are available to the best of this author’s knowledge, which compare Peridynamics to other meshless methods. While the theoretical correspondence of Peridynamics with classical elasticity theory has been established [11], no information is available on the accuracy of the discretized Peridynamic expression suitable for computer implementation. Relevant questions that need to be addressed include, but are not limit to, whether linear fields can be exactly reproduced by the discretized theory, and what the the order of convergence is when Peridynamic solutions are compared against exact results. Little is known about how common problems encountered with other meshless methods, e.g., the tensile instability [12] or the rank deficiency problem [13] affect Peridynamics.

The goal of our paper is to elucidate on some properties of Peridynamics with respect to other meshless methods. In particular, we establish that the discrete equations of the Peridynamic formulation using classical material models is identical to a very well-known meshless technique: Smooth Particle Hydrodynamics (SPH) in Total-Lagrangian formulation.

The remainder of this paper is organized as follows: we begin by deriving the fundamental expressions of the SPH approximation including the most important corrections for this method, which allow it to be used with the minimal level of accuracy required for solid mechanics simulations. Then, the essential Peridynamic expressions required for simulating classical material models are derived. Building on this foundation, the equivalence of SPH and this particular variant of Peridynamics is shown. Finally, the implications of this observation are discussed and Peridynamics (with classical material models) is characterized using the established terminology encountered in the SPH literature.
2 Total Lagrangian SPH

Smooth Particle Hydrodynamics [14] was originally devised as a Lagrangian particle method with the smoothing kernel moving with the particle, thus redefining the interaction neighbourhood for every new position the particle attains. In this sense, the kernel of the original SPH formulation has Eulerian character, as other particles move through the interaction neighbourhood. The tensile instability [12] encountered in SPH, where particles clump together under negative pressure conditions, has been found to be caused by the Eulerian kernel functions [13]. Consequently, Total Lagrangian formulations were developed [15, 16, 17], which use a constant reference configuration for defining the interaction neighborhood of the particles. Typically, the initial, undeformed configuration is taken for this purpose. In the following, this concept and the associated nomenclature is briefly explained with the limited scope of obtaining SPH expressions that are to be compared with the Peridynamic expressions. For a more detailed derivation, the reader is referred to the works cited above.

2.1 Total Lagrangian formulation

In the total Lagrangian formulation, conservation and constitutive equations are expressed in terms of the material coordinates $X$, which are taken to be the coordinates of the initial, undeformed reference configuration. A mapping between the current coordinates, and the reference coordinates describes the body motion at time $t$:

$$x = \phi(X, t),$$

(1)

Here, $x$ are the current, deformed coordinates and $X$ the reference (Lagrangian) coordinates. The displacement $u$ is given by

$$u = x - X,$$  

(2)

The conservation equations for mass, impulse, and energy in the total Lagrangian formulation are given by

$$\rho J = \rho_0 J_0$$  

(3)

$$\ddot{u} = \frac{1}{\rho_0} \nabla_0 \cdot \mathbf{P}$$  

(4)

$$\dot{e} = \frac{1}{\rho_0} \dot{\mathbf{F}} : \mathbf{P}^T,$$  

(5)

where $J$ and $J_0$ are the current and initial Jacobian determinants, $\rho$ is the current mass density and $\rho_0$ is the initial mass density, $\mathbf{P}$ is the nominal stress tensor (the transpose of the first Piola-Kirchhoff stress tensor), $e$ is the

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internal energy, \(\nabla_0\) is the gradient or divergence operator expressed in the material coordinates, and \(F\) denotes the deformation gradient,

\[
F = \frac{d\mathbf{x}}{d\mathbf{X}} = \frac{d\mathbf{u}}{d\mathbf{X}} + I,
\]

\(2.2\) The SPH Approximation

The SPH approximation for a scalar function \(f\) in terms of the Lagrangian coordinates can be written as

\[
f(\mathbf{X}_i) = \sum_{j \in S} V_j^0 f(\mathbf{X}_j) W_i(X_{ij})
\]

(7)

The sum extends over all particles within the range of a scalar weight function \(W_i\), which is centered at position \(\mathbf{X}_i\) and depends on the distance between coordinates \(\mathbf{X}_i\) and \(\mathbf{X}_j\), \(X_{ij} = \|\mathbf{X}_j - \mathbf{X}_i\|\). \(V^0\) is the volume associated with a particle in the reference configuration. The weight function is typically chosen to be radially symmetric and have compact support, i.e., it includes only neighbors within a certain radial distance. This domain of influence is denoted \(S\).

The SPH approximation of a derivative of \(f\) is obtained by operating directly with the gradient operator on the kernel functions,

\[
\nabla f(\mathbf{X}_i) = \sum_{j \in S} V_j^0 f(\mathbf{X}_j) \nabla W_i(X_{ij}),
\]

(8)

where the gradient of the kernel function is defined as follows:

\[
\nabla W_i(X_{ij}) = \left(\frac{dW(X_{ij})}{dX_{ij}}\right) \frac{\mathbf{X}_j - \mathbf{X}_i}{X_{ij}}
\]

(9)

The conditions for the zeroth- and first-order completeness of the SPH approximation are stated as follows:

\[
\sum_{j \in S} V_j^0 W_i(X_{ij}) = 1
\]

(10)

\[
\sum_{j \in S} V_j^0 \nabla W_i(X_{ij}) = 0
\]

(11)

In the simple form as stated here, neither of the completeness conditions are fulfilled by the SPH approximation. An ad-hoc improvement consists in adding eqn. (11) to eqn. 8, such that a symmetrized approximation for the derivative of a function is obtained,
The symmetrization does not result in first-order completeness, however, it yields zeroth-order completeness for the derivatives of a function.

2.3 Restoring First-Order Completeness

In order to fulfill first-order completeness, the SPH approximation has to reproduce the constant gradient of a linear field. A number of correction techniques [18, 19, 20] exploit this condition as the basis for correcting the gradient of the SPH weight function,

$$\sum_{j \in S} V_j^0 (X_j - X_i) \otimes \nabla W_j(X_{ij}) = I,$$  \hspace{1cm} (13)

where \( I \) is the diagonal unit matrix. Based on this expression, a corrected kernel gradient can be defined:

$$\tilde{\nabla} W_i(X_{ij}) = L_i^{-1} \nabla W_i(X_{ij}),$$  \hspace{1cm} (14)

which uses the correction matrix \( L \), defined as:

$$L_i = \sum_{j \in S} V_j^0 \nabla W_i(X_{ij}) \otimes (X_j - X_i).$$  \hspace{1cm} (15)

By construction, the corrected kernel gradient now satisfies eqn. (13),

$$\sum_{j \in S} V_j^0 (X_j - X_i) \otimes L_i^{-1} \nabla W_i(X_{ij}) = I,$$  \hspace{1cm} (16)

2.4 Corrected SPH expressions for Solid Mechanics

For calculating the internal forces of a solid body subjected to a deformation, expressions are required for (i) the deformation gradient, (ii) a constitutive equation which provides a stress tensor as function of the deformation gradient, and (iii) an expression for transforming the stresses into forces acting on the nodes which serve as the discrete representation of the body.

The deformation gradient is obtained by calculating the derivative of the displacement field, i.e., by using the symmetrized SPH derivative approximation, eqn. (12), for eqn. (6):
\[ F_i^{SPH} = \sum_{j \in S} V_j^0 (u_j - u_i) \otimes L_i^{-1} \nabla W_i(X_{ij}) + I. \]  

Note that in the above equation, the corrected kernel gradient has been introduced via the matrix \( L_i^{-1} \). The SPH approximation of the stress divergence, eqn. (4), is not so clear. Depending on how it is performed, several different approximations can be obtained [21]. The most frequently used form, which is variationally consistent with respect to an energy minimization principle [19], is the following:

\[ f_i = \sum_{j \in S} V_i^0 V_j^0 (P_j + P_i) \nabla W_i(X_{ij}). \]  

For a radially symmetric kernel which depends only on distance, the antisymmetry property \( \nabla W_i(X_{ij}) = -\nabla W_j(X_{ji}) \) holds. Therefore, the above force expression will conserve linear momentum exactly, as \( f_{ij} = -f_{ji} \). We use the antisymmetry property of the kernel gradient to rewrite the force approximation as follows:

\[ f_i = \sum_{j \in S} V_i^0 V_j^0 (P_i \nabla W_i(X_{ij}) + P_j \nabla W_i(X_{ij})) \]
\[ = \sum_{j \in S} V_i^0 V_j^0 (P_i \nabla W_i(X_{ij}) - P_j \nabla W_j(X_{ji})). \]

Replacing the uncorrected kernel gradient with the corrected gradient (c.f. eqn. (14), the following expression is obtained:

\[ f_i = \sum_{j \in S} V_i^0 V_j^0 (P_i L_i^{-1} \nabla W_i(X_{ij}) - P_j L_j^{-1} \nabla W_j(X_{ji})). \]

This corrected force evaluation conserves linear momentum due to its antisymmetry with respect to interchange of the particle indices \( i \) and \( j \), i.e., \( f_{ij} = -f_{ji} \). The here constructed antisymmetric force expression is usually not seen in the literature. In contrast, it seems to be customary [18, 19, 20] to directly insert the corrected kernel gradient into eqn. (18), which destroys the local conservation of linear momentum. We note that the above construction of the SPH expression that conserves linear momentum is arbitrary, and in similar spirit to the \textit{ad-hoc} symmetrization procedure encountered in eqn. (12).

3 Peridynamics for classical material models

This section provides a concise derivation of the Peridynamic approximation of the deformation gradient and the forces acting on particles. In contrast
to the preceding section, where this quantities have been derived for SPH, we employ a different nomenclature here, which is consistent with the most relevant Peridynamic literature. In Peridynamics, each particle defines the origin of an influence domain, termed neighborhood $H$, of radius $\delta$. Within this neighborhood, vectors $\xi$ from the origin to any point in $H$ exist, see the following figure.

![Figure 1](image)

Fig. 1 In the meshless Peridynamic method, particle interactions are defined in a reference configuration which is shown here. A region of influence termed $H$ is defined by a radial cutoff $\delta$ around a particle $i$. Bonds exist between $i$ and all particles $j$ within $H$. These bonds are denoted here by $\xi_{ij}$, of which only one is shown above. Note that this representation already employs discrete particle locations whereas the Peridynamic theory assumes a continuum of points.

### 3.1 Vector states

Central to the state-based Peridynamic theory is the concept of *states*. States are functions that act on vectors. This is written in the following way,

$$ A \langle \xi \rangle = \xi', $$

(22)

where the state $A$ has acted on the vector $\xi$ to produce a different vector $\xi'$. Angular brackets indicate which vector the state acts upon. The mapping results produce tensors of different order, depending on the nature of the state. *Vector states* of order one map a vector to a different vector. *Scalar states* of order zero produce a scalar for every vector they act on. For the purpose of this paper we only need to be concerned with the following states:

The *reference position vector state* $X$ returns the original bond vector.
The deformation state $\mathbf{Y}$ returns the deformed image of the original bond vector. Let the original vector go from $\mathbf{X}$ to $\mathbf{X}'$, i.e., $\xi = \mathbf{X}' - \mathbf{X}$. Upon deformation, the coordinates of these two points change to $\mathbf{x}$ and $\mathbf{x}'$. The deformation state vector returns the deformed image of the original vector, i.e.,

$$\mathbf{Y}(\xi) = \mathbf{x}' - \mathbf{x}$$

(24)

The influence function $\omega$ is a scalar state that returns a number $w$ that depends only on the magnitude of $\xi$:

$$\omega(\xi) = w \in \mathbb{R}^+$$

(25)

Vector and scalar states can be combined using the usual mathematical operations addition, subtraction, multiplication, etc. The conventions are detailed in [8]. Here, we only need the definition of the tensor product between two vector states $\mathbf{A}$ and $\mathbf{B}$,

$$\mathbf{A} \ast \mathbf{B} = \int_H \omega(\xi) \mathbf{A}(\xi) \otimes \mathbf{B}(\xi) \, dV_\xi$$

(26)

This tensor product is required for the following Peridynamic concepts. Firstly, the shape tensor is defined:

$$\mathbf{K} = \mathbf{X} \ast \mathbf{X} = \int_H \omega(\xi) \xi \otimes \xi \, dV_\xi$$

(27)

$\mathbf{K}$ is symmetric and real and thus positive-definite, implying that it can be inverted. The shape tensor is then used in the concept of tensor reduction, which is an operation that produces a second order tensor from two vector states:

$$\mathbf{C} = (\mathbf{A} \ast \mathbf{B}) \mathbf{K}^{-1} = \left( \int_H \omega(\xi) \mathbf{A}(\xi) \otimes \mathbf{B}(\xi) \, dV_\xi \right) \mathbf{K}^{-1}$$

(28)

### 3.2 Calculation of the deformation gradient tensor in Peridynamics

The deformation gradient tensor may be approximated as a tensor reduction of deformation vector state and reference position vector state according to eqn. (134) in [8]:

$$\mathbf{F} \approx (\mathbf{Y} \ast \mathbf{X}) \mathbf{K}^{-1}$$

(29)
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The necessary Peridynamic calculus for evaluating this quantity has been presented above. We now make the transition from the continuum representation to a discrete nodal, or particle representation, converting integrals to sums. A piecewise constant discretization of the integrals defined above yields the discrete shape tensor as

\[ K_i = \sum_{j \in H_i} V_j^0 \omega(\xi_{ij}) \xi_{ij} \otimes \xi_{ij} \]  

(30)

Here, the sum includes all particles \( j \) within the neighborhood \( H_i \) of \( i \) and \( V_j^0 \) is the volume of particle \( j \). The discrete expression for the approximate deformation gradient is obtained as:

\[ F_{PD}^i = \left( \sum_{j \in H_i} V_j^0 \omega(\xi_{ij}) x_{ij} \otimes \xi_{ij} \right) K_i^{-1} = \left( \sum_{j \in H_i} V_j^0 \omega(\xi_{ij}) u_{ij} \otimes \xi_{ij} \right) K_i^{-1} + I \]  

(31)

3.3 The Peridynamic force expression obtained from a classical stress tensor

The fundamental equation of Peridynamics is an integral equation of force densities (force per volume) which ensures local conservation of impulse, see eqn. (28). in [8]:

\[ f_{PD} = V_X \int_{H_X} \{ T[X] \langle X' - X \rangle - T[X'] \langle X - X' \rangle \} \, dV_X. \]  

(32)

Here, \( T[X] \) is a vector state, which operates on the bond \( \xi = X' - X \) in order to yield a contribution to the force density at \( X \). The antisymmetric counterpart \( T[X'] \) ensures balance of linear momentum and \( V_X \) is the volume associated with the coordinate \( X \). The vector state \( T \) is related the classical stress tensor, which can be computed using the deformation gradient and a classical material model. Specifically, this relation is stated as follows, see eqn. (142). in [8]:

\[ T[X] \langle \xi \rangle = \omega \langle \xi \rangle P_X K_X^{-1} \xi \]  

(33)

The stress tensor \( P \) above is the nominal stress tensor which applies here as the stress is expressed in the reference configuration. The dependence on \( X \) signifies that both stress and shape tensor have to be evaluated at coordinate \( X \). Converting to a discrete particle expression, one obtains:
\[ f_i^{PD} = \sum_{j \in H_i} V_i^0 V_j^0 \left\{ T_i \langle \xi_{ij} \rangle - T_j \langle \xi_{ji} \rangle \right\} \]  
\[ = \sum_{j \in H_i} V_i^0 V_j^0 \left\{ \omega \langle \xi_{ij} \rangle P_i K_j^{-1} \xi_{ij} - \omega \langle \xi_{ji} \rangle P_j K_i^{-1} \xi_{ji} \right\} \]  

4 The Correspondence between Peridynamic and SPH expressions for deformation gradient and particle forces

The discrete Peridynamic approximation of both the deformation gradient and the particle forces arising from a classical stress tensor are equal to the Total-Lagrangian SPH expressions with linear kernel gradient correction. In order to show this equivalence, we introduce some changes in nomenclature:

\[ H_i = S_i \]  
\[ \xi_{ij} = X_{ij} \]  
\[ \omega \langle \xi_{ij} \rangle = \frac{1}{X_{ij}} \frac{dW(X_{ij})}{dX_{ij}}. \]

Note that the postulated equivalence in the last line above states that the derivative of the SPH weight function has to equal the Peridynamic weight function. However, no implications arise from this requirement, as suitable weight functions can be chosen which fulfill this requirement.

4.1 Equality of shape tensor and first-order correction matrix

With these changes, the Peridynamic shape tensor becomes equal to the correction matrix required for first-order consistent SPH:

\[ K_i = \sum_{j \in H_i} V_i^0 \omega \langle \xi_{ij} \rangle \xi_{ij} \otimes \xi_{ij} \]  
\[ = \sum_{j \in S_i} V_j^0 \frac{1}{X_{ij}} \frac{dW(X_{ij})}{dX_{ij}} X_{ij} \otimes X_{ij} \]  
\[ = \sum_{j \in S_i} V_j^0 \nabla W_i(X_{ij}) \otimes (X_j - X_i) \]  
\[ \vdots \]  
\[ K_i = L_i \]
4.2 Equality of the deformation gradient

In a similar manner, the Peridynamic expression of the deformation gradient can be shown to be equal to the SPH approximation:

\[ F_{PD}^i = \left( \sum_{j \in H} V_j^0 \omega (\xi_{ij}) \mathbf{u}_{ij} \otimes \xi_{ij} \right) K^{-1}_i + I \]  
\[ = \left( \sum_{j \in S} V_j^0 \frac{1}{X_{ij}} \frac{dW(X_{ij})}{dX_{ij}} \mathbf{u}_{ij} \otimes X_{ij} \right) L^{-1}_i + I \]  
\[ = \sum_{j \in S} V_j^0 \mathbf{u}_{ij} \otimes \left( L^{-1}_i \frac{1}{X_{ij}} \frac{dW(X_{ij})}{dX_{ij}} X_{ij} \right) + I \]  
\[ \therefore F_{PD}^i = F_{SPH}^i \]  

Thus, the Peridynamic concept of reduction leads to the approximation of a tensor field, which is correct to first order.

4.3 Equality of particle forces

Using the same rules for changing the Peridynamic notation into SPH notation, one obtains from the Peridynamic force expression:

\[ f_{PD}^i = \sum_{j \in H} V_i^0 V_j^0 \left\{ \omega (\xi_{ij}) P_i K^{-1}_i \xi_{ij} - \omega (\xi_{ji}) P_j K^{-1}_j \xi_{ji} \right\} \]  
\[ = \sum_{j \in S} V_i^0 V_j^0 \left\{ \frac{1}{X_{ij}} \frac{dW(X_{ij})}{dX_{ij}} P_i L^{-1}_i X_{ij} - \frac{1}{X_{ji}} \frac{dW(X_{ji})}{dX_{ji}} P_j L^{-1}_j X_{ji} \right\} \]  
\[ = \sum_{j \in S} V_i^0 V_j^0 \left\{ P_i L^{-1}_i \nabla W_i(X_{ij}) - P_j L^{-1}_j \nabla W_j(X_{ji}) \right\} \]  
\[ \therefore f_{PD}^i = f_{SPH}^i \]  

5 Discussion

We have shown that Peridynamics – when used with classical material models based on the deformation gradient tensor and nodal integration as discretization technique – is equivalent to Total Lagrangian SPH. This result allows us
to characterize this flavour of Peridynamics using the large body of studies published for SPH. SPH is a collocation method with nodal integration that suffers from two major problems: (i) the tensile instability, i.e., a numerical instability which results in particle clumping under conditions of negative pressure, and (ii) susceptibility to zero-energy modes which are caused by rank-deficiency due to nodal integration. Of these problems, the tensile instability is resolved by the Total-Lagrangian formulation [13, 16], and the rank-deficiency can be eliminated by using additional integration points [18]. Peridynamics with classical material models as presented here is a Total-Lagrangian method and therefore shows no tensile instability. However, if due to the use of nodal integration, it is still a rank-deficient method.

The rank-deficiency does usually not manifest itself until the reference configuration is updated. Such an update can be required as the Total-Lagrangian nature imposes restrictions on the magnitude of deformations that can be handled with the approximate deformation gradient. Alternatively, features of the material model, e.g. plasticity or failure, may require updates of the reference configuration. These updates result in zero-energy modes which need to be treated with dissipative mechanisms [22].

With the equivalence demonstrated in this work, Peridynamics applied to classical material models and in combination with nodal integration does not result in a new numerical method, but is instead a new derivation of an existing meshless method that is not free of problems. What are the implications of these findings for the other Peridynamic theories? The bond-based theory [7], which can be interpreted as an upscaling of the established meshless method Molecular Dynamics [23], does not require the calculation of a deformation gradient and thus does not suffer from the associated problems due to rank-deficiency. The state-based Peridynamic theory has also been formulated for some material models which are not based on the classical deformation gradient. If these unconventional material models, e.g., the linear Peridynamic solid [8], are discretized using nodal integration for computing dilatation and shear strain, rank deficiency problems are also likely to emerge.

It is worthwhile to emphasize that the mathematical foundation of Peridynamics is clear and straightforward. Correct equations of motion emerge from this theory which conserve linear and angular momentum, and approximate linear fields accurately. All of these desirable features can only introduced into the SPH approximation by ad-hoc procedures. Thus, if anything, the Peridynamic theory provides us with a better route to deriving meshless discretizations than the SPH method. If the simplest form of meshless discretization, namely nodal integration, is used, the advantages of Peridynamics over SPH vanish and the discrete expressions of both methods become equal. Future work should therefore address enhanced integration schemes for the Peridynamic theory.
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