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Peridynamics review

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Abstract

Peridynamics (PD) is a novel continuum mechanics theory established by Stewart Silling in 2000. The roots of PD can be traced back to the early works of Gabrio Piola according to dell'Isola et al. PD has been attractive to researchers as it is a non-local formulation in an integral form, unlike the local differential form of classical continuum mechanics. Although the method is still in its infancy, the literature on PD is fairly rich and extensive. The prolific growth in PD applications has led to a tremendous number of contributions in various disciplines. This manuscript aims to provide a concise description of the PD theory together with a review of its major applications and related studies in different fields to date. Moreover, we succinctly highlight some lines of research that are yet to be investigated.

Keywords

Peridynamics, continuum mechanics, fracture, damage, non-local elasticity

I. Introduction

The analysis of material behavior owing to various types of loading and boundary conditions may be carried out at different length scales. At the nanoscale, often molecular dynamics (MD) is used to analyze the behavior of atoms and molecules. However, simulation time, integration algorithms, and the required computational power are limiting factors to the method's capabilities. On the other hand, at the macroscale, the behavior of a body is usually analyzed using the classical continuum mechanics (CCM) formalism. In CCM, a body is assumed to be a continuum surrounded within its boundary for which the balance laws must be satisfied locally. Traction t on the surface of a material point can be

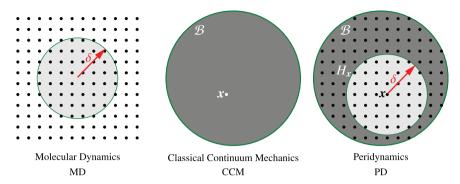


Figure 1. Comparison of MD, CCM, and PD. MD (left) analyzes the interactions between discrete entities, i.e., atoms and molecules. These local interactions are governed by the cutoff radius δ . On the other hand, CCM (center) and PD (right) are formulations defined over a continuum body \mathcal{B} . The latter is subdivided into points with a finite volume. In CCM, the state of a point is only influenced by its immediate neighbors. However, in PD, a material point \mathbf{x} interacts with other material points within a neighborhood $H_{\mathbf{x}}$ delimited by the horizon δ . PD is similar to CCM in the sense that it is still a continuum formulation and also, is similar to MD in the sense that it is non-local and borrows certain notions of MD such as the cutoff radius δ or interactions between points.

expressed as $t = \sigma \cdot n$ where σ is a stress tensor and n represents the unit normal of the surface cut the traction is acting on. Local conservation of linear and angular momentum can be expressed as $\rho(x)\ddot{u}(x,t) = \text{div}\sigma + b(x,t)$ and $\sigma = \sigma^t$, respectively, where ρ , \ddot{u} , and b correspond to the density, acceleration, and body force associated with the material point x, respectively. For the past two centuries, these balance equations have been successfully used to solve many problems in solid mechanics. Despite the fact that these equations are well established, they encounter difficulties when discontinuities such as cracks are present within the body since mathematically, the divergence term yields singular values. Various approaches such as linear elastic fracture mechanics (LEFM) [1, 2] and cohesive zone model (CZM) [3, 4] have been proposed to overcome these issues. The CZM dates back to the seminal works of Barenblatt [3, 5] and Dudgale [4] and has subsequently been extended in [6–9] among others.

Peridynamics (PD) belongs to the class of non-local continuum mechanics formulations. Etymologically the term is derived from two Greek words $\pi \varepsilon \rho i$ ("peri-" around) and $\delta \dot{\nu} \nu \alpha \mu \eta$ ("dýnami" force). In PD, a continuum is subdivided into material points occupying volume in space. The core of the PD formulation is that the behavior of each material point is governed by its interaction with other material points located within its neighborhood. In other words, the PD theory is about the interaction forces between material points within a given neighborhood. In contrast to CCM, the governing equation of PD is an integro-differential equation which makes it suitable for problems involving discontinuities in the body. Figure 1 highlights the similarities and dissimilarities among MD, CCM, and PD schematically.

There are other continuum formulations such as non-local elasticity and strain-gradient theories. Although both are non-local formulations, non-local elasticity and PD are fundamentally different. Eringen's non-local elasticity theory assumes that the stress state at a point depends on the strain state at that point as well as the strain states of all the points within the body [10]. Moreover, the balance of linear momentum is expressed in terms of the divergence of the stress tensor as in the CCM formulation. In contrast, PD precludes spatial derivatives and does not explicitly involve stress and strain. Figure 2 shows that there has been an increasing interest in PD as a novel continuum mechanics formulation.

The main purpose of this paper is to expound the PD theory to researchers of various backgrounds. The main differences between the CCM formulation and the PD theory are highlighted, an overview of the related contributions and applications of PD is presented and the challenges and new perspectives in the development of PD are discussed. Though the PD theory was formally established by Silling in 2000 [11], dell'Isola et al. [12] claimed that Gabrio Piola is the pioneer of higher-gradient and non-local continuum models, including PD. They showed that the fundamental ideas behind PD were already presented in Piola's works, who derived non-local continuum theories and higher-gradient formulations by means of the virtual work principle. dell'Isola and coworkers indicated that Piola's works have remained

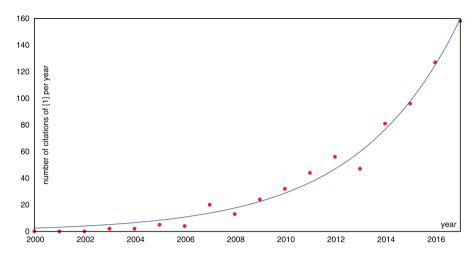


Figure 2. Number of citations of [11] per year versus year from its birth (2000) until today. The fitted curve is an exponential function and the points represent the data obtained from SCOPUS.

obscure and have been overlooked despite of their potential. On the other hand, there are strong connections yet differences between the PD theory and particle systems [13, 14]. As pointed out by Fried [13]

"The starting point of peridynamic theory is a continuum level field equation imposing linear-momentum balance with the essential difference being that the conventional term involving the divergence of the stress is replaced by a non-local term in which an integral operator is applied to the displacement field. This operator determines not only the range over which material points interact but also the nature of allowed interactions. Peridynamic theory therefore mixes kinematics, kinetics and constitutive equations from the outset. It seems likely that the conceptual basis for particle mechanics can be adapted to provide an alternative formulation of peridynamic theory in which these ingredients are treated separately." Page 1473

It is worth mentioning that various continuum models in relation to PD have been developed such as a one-dimensional elastic continuum model with long-range forces [15], modified beam and plate equations [16, 17], coupling of local and non-local continuum formulations [18, 19], and atomistic-continuum models [20]. Murdoch [21] attempted to clarify the misconceptions regarding the notions of particles and long-range forces in the PD theory in [11] from an atomistic perspective. In a related work, Drapaca and Sivaloganathan [22] introduced a new non-local continuum model based on fractional derivatives, which encompasses both CCM and non-local formulations such as PD.

This article is organized as follows. Section 2 elaborates on the fundamentals of PD in terms of its governing equation and balance laws. Section 3 discusses related contributions and various applications of PD to a plethora of problems as found in the literature to date, gathered in Figure 3. Section 4 concludes this work and provides further outlook indicating potential research trends regarding PD. Eventually, a brief guideline for the numerical implementation of PD is given in the Appendix.

2. Fundamentals of PD

The PD formulation is based on the interactions within the neighborhood H_x with the distance δ of a material point at x as shown in Figure 1. There are two main categories of PD formulation as bond-based PD and state-based PD. The latter is further divided into two types of ordinary state-based PD and non-ordinary state-based PD. Obviously, all these variants must satisfy the conservation laws. Throughout this section, the fundamentals of PD are introduced with a focus on mechanical problems. More sophisticated and coupled problems can be formulated in a similar fashion.

2.1 Bond-based PD

The PD equation can be understood as an integral expression of the linear momentum balance in CCM. The equation of motion of a material point in an elastic material can be expressed as

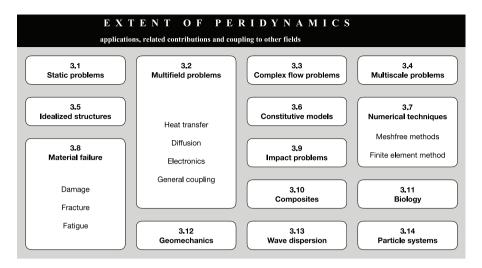


Figure 3. Extent of PD theory to date. Section 3 elaborates on each field together with a review of the topic and important contributions.

$$\rho(\mathbf{x})\ddot{\mathbf{u}}(\mathbf{x},t) = \int_{H_{\mathbf{x}}} f(\mathbf{u}' - \mathbf{u}, \mathbf{x}' - \mathbf{x}) dV' + \mathbf{b}(\mathbf{x},t), \tag{1}$$

where f(u'-u, x'-x) is a pairwise force density vector function and u is the displacement of the material point at x. The term "bond" refers to the interaction between the material points at x and x'. The bond-based PD relies on the assumption of pairwise interactions in which the force density vectors exerted by the material points on one another are equal in magnitude and parallel to the relative position vector in the deformed state. The integral equation (1) is always valid regardless of discontinuities. It can be seen that in Equation (1), the divergence of the stress tensor in the local form is replaced by the integral of the force density over the neighborhood H_x thereby f contains all the constitutive properties of the material. For instance, for a linear elastic isotropic solid f can be expressed as

$$f(u'-u, x'-x) = cs \frac{y'-y}{|y'-y|},$$
 (2)

where y = x + u is the position of the material point in the deformed configuration, c denotes the bond constant, and s is the bond stretch defined as

$$s = \frac{|y' - y| - |x' - x|}{|x' - x|}.$$
 (3)

The bond constant c is the PD material parameter and can be expressed in terms of the material constants of CCM. These relations can be established by considering a common parameter used in both approaches. For instance, for a linear isotropic material, the bond constant reads

$$c = \frac{12E}{\pi \delta^4},\tag{4}$$

where δ is the horizon and E is the elastic modulus in CCM. Note that there is only one PD parameter used in the original (bond-based PD) formulation as opposed to two independent Lamé parameters of CCM for isotropic material behavior. In other words, it is not possible to freely define a Poisson's ratio because the PD formulation automatically captures a constant Poisson's ratio of 0.33 for two-dimensional and 0.25 for three-dimensional problems, see the original work of Poisson [23] and the more recent study [24], among others. The constraints on material parameters for the bond-based PD are derived in [25].

2.2 State-based PD

The original bond-based PD formulation suffers from a limitation on material constants because it assumes that the PD forces between two material points are of equal magnitude and opposite directions. This issue has been addressed by means of a generalized formulation referred to as *state-based PD* [26]. The core of the formulation is a mathematical object called *state* which, to some extent, operates like a mapping. State is basically an array that stores information about a parameter of PD bonds associated with a particular material point. For instance, a force state stores the PD forces pertaining to a bond. State-based PD is such that the response of a material point depends on the deformation of all the material points within its horizon. Based on these new assumptions, the equation of motion of a material point can be written as

$$\rho(\mathbf{x})\ddot{\mathbf{u}}(\mathbf{x},t) = \int_{H_{\mathbf{x}}} \{ \underline{\mathbf{T}}(\mathbf{x},t) \langle \mathbf{x}' - \mathbf{x} \rangle - \underline{\mathbf{T}}(\mathbf{x}',t) \langle \mathbf{x} - \mathbf{x}' \rangle \} dV' + \mathbf{b}(\mathbf{x},t), \tag{5}$$

where $T\langle \cdot \rangle$ represents the force state.

The state-based PD can be further categorized into *ordinary* or *non-ordinary* state-based PD. Let \underline{M} denote a vector state such that $\underline{M}\langle x-x'\rangle$ is a unit vector pointing from the deformed position of x toward the deformed position of x'. If a material has a property such that for any deformation there exists a scalar state \underline{t} such that $\underline{T} = \underline{t}\underline{M}$, the material is called *ordinary* and *non-ordinary* otherwise, see Figure 4. In the ordinary state-based PD formulation, although the PD forces between two material points can have different magnitudes, their directions are assumed to be along the bond direction. For instance, for a linear elastic isotropic material, the force state is given by

$$\underline{T}(x,t)\langle x'-x\rangle = \left(\frac{2ad\delta}{|x'-x|}\theta(x,t) + bs\right)\frac{y'-y}{|y'-y|},\tag{6}$$

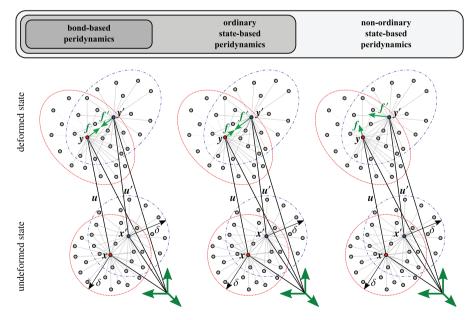


Figure 4. Illustration of the bond-based (left), ordinary state-based (center), and non-ordinary state-based PD formulations (right). The red and blue points represent two material points, each having its own horizon, represented by the red and blue circle, respectively. Each material point interacts with those in its horizon, as shown by the gray dashed lines. The difference between the three formulations lies in the magnitude and direction of the interaction forces (green arrows) between the materials points. Bondbased PD can be understood as a particular case of ordinary state-based PD. Similarly, ordinary state-based PD can be understood as a special case of non-ordinary state-based PD.

where a, b, and d are PD parameters and $\theta(x,t)$ is the PD dilatation term. This assumption can be disregarded in the non-ordinary state-based PD by allowing PD forces in arbitrary directions. By doing so, it is essential to explicitly ensure the conservation of angular momentum because it is no longer fulfilled a priori, in contrast to the bond-based and ordinary state-based formulations. Therefore, for the non-ordinary state-based PD, the following relationship must hold

$$\int_{H_{\mathbf{x}}} \{ (\mathbf{y}' - \mathbf{y}) \times \underline{\mathbf{T}}(\mathbf{x}, t) \langle \mathbf{x}' - \mathbf{x} \rangle \} dV' = 0.$$
 (7)

Furthermore, in what is referred to as the *correspondence model* [26], the force density vector can be related to stress as

$$\underline{T}(x,t)\langle x'-x\rangle = \underline{w}\langle x'-x\rangle PK^{-1}(x'-x)$$
(8)

with P being the Piola¹ stress tensor K and is the shape tensor defined as

$$K = \int_{H_x} \underline{w} \langle x' - x \rangle (\underline{X} \langle x' - x \rangle \otimes \underline{X} \langle x' - x \rangle) dV', \tag{9}$$

where \underline{X} is the position state that contains the relative position of material points associated with a particular bond and the \underline{w} state contains the influence function information that defines the strength of interactions. The correspondence material model is such that the PD constitutive model is *calibrated* to yield the same results as the classical model for a given homogeneous deformation. More precisely, the two models are correspondent when the PD and classical strain energy density functions are equal under affine deformations. The deformation gradient F can be approximated in the PD framework as

$$\mathbf{F} = \frac{\int_{H_x} \underline{w} \langle \mathbf{x}' - \mathbf{x} \rangle (\underline{Y} \langle \mathbf{x}' - \mathbf{x} \rangle \otimes \underline{X} \langle \mathbf{x}' - \mathbf{x} \rangle) dV'}{\int_{H_x} \underline{w} \langle \mathbf{x}' - \mathbf{x} \rangle (\underline{X} \langle \mathbf{x}' - \mathbf{x} \rangle \otimes \underline{X} \langle \mathbf{x}' - \mathbf{x} \rangle) dV'},$$
(10)

where <u>Y</u> is the deformation state containing the relative position of material points in the deformed configuration. As the most general PD formulation, the non-ordinary state-based PD is a practical approach for a variety of problems. However, as Tupek and Radovitzky [28] demonstrated, the formulation of the non-local deformation gradient tensor allows unphysical deformation modes including material collapse, matter inter-penetration at discontinuities and zero-energy modes. The latter occur as a result of a weak coupling between a material point and its family [29]. To overcome these limitations, Tupek and Radovitzky [28] proposed an *extended constitutive correspondence formulation* by defining a non-local PD strain tensor based on alternative strain measures. To control zero-energy modes, Breitenfeld et al. [29] investigated different techniques that consist of adding another term to Equation (8). Recently, Silling [30] studied the causes of zero-energy mode instability in a meshfree discretization and established a general criterion for material stability in PD.

2.3 PD as a paradigm of continuum mechanics

Since the seminal work of Silling [11], the PD formulation has been of great interest among researchers. Notably, Silling and Lehoucq [31] and Madenci and Oterkus [25] carried out an extensive study of the balance laws, applications, and implementations of the PD formulation. Moreover, Ostoja-Starzewski et al. [32] analytically showed the restrictions imposed by the second law of thermodynamics on the pairwise forces for the bond-based PD and the force states for the state-based PD. Recently, Bobaru et al. [33] elaborated on the mathematical, numerical, and computational issues of PD, along with applications such as dynamic fracture. Aguiar and Fosdick [34] proposed a quadratic free energy function for a simple linear elastic PD material model that accounts for bond stretch and relative bond angles; the model also depends on four material constants, two of which were correlated to elastic constants from classical elasticity in the limit of small horizon. In addition, the authors indicated that their model satisfies the angular momentum balance and is a non-ordinary material model. Mitchell et al. [35] proposed an improved version of the ordinary state-based PD formulation referred to as *position-aware linear*

solid (PALS) constitutive model that employs two influence functions to address surface effects, i.e., the problems due to missing bonds in the vicinity of free surfaces thereby the influence functions are determined by means of Lagrange multipliers and calibrated at each material point, hence the name "position aware."

For computational efficiency and improved accuracy, variants of the traditional PD formulations have been developed. According to Ren et al. [36], the horizons' radii are kept constant in traditional PD to prevent the loss of accuracy in the results, owing to spurious wave reflections and ghost forces between material points. They introduced the dual-horizon concept [37] in which the discretization of the domain is analogous to that of the finite-element method (FEM) or the finite volume method (dense node distribution in critical regions and coarse distribution elsewhere), thereby reducing the computational cost. In addition to the *constant horizon* in the traditional formulation and the *dual-horizon* PD. Silling et al. [38] presented a variable horizon in a PD medium with constant bulk properties. They investigated the anomalies induced by ghost forces and concluded that these irregularities can be minimized by making the horizon a smoothly varying function. Recently, Queiruga and Moridis [39] investigated the accuracy and convergence properties of state-based PD laws including deformation gradient-based model [26] and dilation-based models [40, 41] with different influence functions for two-dimensional static problems. They observed that the convergence of the dilation state-based models is restricted to specific constant-strain problems and that the deformation gradient model exhibits a linear convergence rate but is unstable. They also noted that convergence is guaranteed with a cubic influence function. Ganzenmüller et al. [42] proposed an improvement to the prototype microbrittle model (PMB) model: a linear-elastic, bond-based PD model with brittle failure. They validated the modified model by analyzing wave propagation in a bar with non-uniform particle discretization and investigated crack propagation in a patch with initial crack. Their results were quantitatively in good agreement with the analytical

The presence of the length scale parameter δ in the PD formulation makes it suitable for analyzing material behavior at the microscale as well as the macroscale. Notably, PD has been used to analyze nano-indentation [43] and failure of graphene sheets [44], nanoscale friction and wear properties of amorphous carbon films [45]. Chowdhury et al. [46] developed a 3D state-based micropolar PD model with an additional length scale parameter. They also derived a one-dimensional homogenized micropolar PD beam model. The authors concluded that the incorporation of micropolar effects improves the prediction capabilities of the model and that dimensionally-reduced models significantly reduce computational overhead. Note, when applying a continuum model at the nanoscale, the underlying assumptions of field theories no longer hold. Nonetheless, such continuum models can be used as numerical estimates to approximate the homogenized material response. Obviously, at the nanoscale discrete models such as MD are more appropriate and physically acceptable.

Various studies have attempted to establish the connection between PD and classical elasticity. To correlate CCM with PD, Lehoucq and Silling [47] established the notion of PD stress tensor, which is not explicitly present in the PD governing equation. Silling [48] presented a coarsening method for linear elastic PD material models. In the proposed approach, the material properties are derived at different length scales. Silling indicated that, unlike the rescaling approach [49], the coarsening method accounts for material rearrangement at the small scale in response to the deformation at the large scale. An interesting study was presented by Madenci et al. [50] in which they introduced a PD differential operator that can recast local differential equations into their non-local form. The authors demonstrated the robustness and capability of the proposed operator by solving challenging differential equations. Bellido et al. [51] demonstrated that hyperelasticity is the Γ -limit of the PD macroelastic energy of deformation; the latter being a double integral of the pairwise potential function evaluated over the domain. Seleson et al. [52] analyzed the connections between nearest-neighbor discretizations of PD equilibrium equations, by means of nodal-based quadratures, and finite difference discretizations of the classical Navier-Cauchy equation of static elasticity. They concluded that the PD equations reduce to their classical discrete counterparts under appropriate choices of quadrature weights. Rahman and Foster [53] developed a statistical mechanics framework for the PD theory of solids, which incorporated MD within a PD model. Another topic of interest in the development of PD models is the investigation of non-linearities in the PD formulation, as described in [54, 55]. Liu and Hong [56] derived the

micromoduli of discretized PD models in one and three dimensions. An important consideration in the PD formulation is the handling of boundary conditions, see in particular [57–60].

3 Extent of PD

As the PD formulation can inherently account for discontinuities in the displacement field, PD has been predominantly used for the solution of fracture and damage problems. However, its extent is not restricted to fracture mechanics. This section attempts to present a concise categorization of the PD applications and related contributions in the literature gathered in Figure 3. Obviously, some categories may overlap.

3.1 Static problems

PD has been applied to various static and quasistatic problems. For instance, Dayal and Bhattacharya [61] applied the PD theory to study martensitic phase transformations. They conducted both quasistatic and dynamic analyses of phase boundaries and observed that for the quasistatic responses, the accuracy of the results is highly dependent on the choice of numerical method as well as the incremental load step. Huang et al. [62] presented an extended bond-based PD formulation to investigate the quasistatic response and crack propagation in cantilever beams. Mikata [63] made a significant contribution by investigating analytical solutions of peristatic and PD problems for a one-dimensional infinite rod. Furthermore, Zaccariotto et al. [64] applied PD for the solution of static equilibrium problems and static crack propagation problems using an implicit Newton–Raphson method. In addition, Buryachenko [65] used PD to study the properties of peristatic bars of random structure.

3.2 Multifield problems

To solve complex problems encountered in practice, coupled formulations involving PD have been developed for the analysis of thermal, chemical, diffusion, and electrical problems as well as porous flow. In particular, see the pioneering work of Gerstle et al. [66] and the more recent work of Oterkus et al. [57] among others.

- 3.2.1 Heat transfer. The classical heat transfer equations are not applicable to bodies with emerging discontinuities since they involve temperature gradients. This issue motivated Bobaru and Duangpanya [67] to present a PD formulation for one-dimensional transient heat conduction. They also analyzed the convergence to the classical solution in the limit of vanishing horizon, which was then extended to multiple dimensions [68]. In addition, Oterkus et al. [57] derived a generalized state-based PD heat transfer model based on the Lagrangian formalism and demonstrated its advantage in handling discontinuities. To account for the effects of thermal state on the deformation of a body, fully coupled PD thermomechanics were presented in [69]. An important study was carried out by Chen et al. [70] in which, by means of the one-point quadrature, they investigated the effect of the kernel choice on PD solutions for transient heat and mass diffusion. The authors underlined that the one-point quadrature converges to the classical solution in the limit of vanishing horizon.
- 3.2.2 Diffusion. Considering the major issues caused by moisture in different applications, Diyaroglu et al. [71] used a PD model based on the wetness approach to predict moisture concentration and diffusion. Oterkus et al. [57] derived a generalized state-based PD thermal diffusion model that can also be adapted to account for concentration. For various benchmark problems, the results from the model were in good agreement with the analytical solutions. Furthermore, PD provides a suitable platform to study non-local diffusion arising in several disciplines such as biology, image processing, and particle systems, see [72] among others.
- 3.2.3 Electronics. Device failure due to thermal stresses is a major concern regarding electronic packages. This failure mode stems from the mismatch of material properties at interfaces as well as the presence

of geometric discontinuities. In that context, the PD formulation has been applied to investigate crack propagation in multi-layer thin-film structures [73]. Thermomechanical modeling of microelectronic packages has been addressed in [74]. Another crucial issue regarding electronic components is their potential moisture absorption, leading to degradation whereby the PD wetness approach [71] can be utilized to predict moisture concentration in electronic packages.

3.2.4 General coupling techniques. To accurately simulate coupled processes, various formulations can be merged into a single framework. In particular, the PD formulation has been coupled with different numerical methods. For instance, PD has been implemented within a coupling framework to investigate soil dynamics applicable to geomaterials exhibiting inelastic behavior under high-pressure loads or soil fragmentation owing to high strain rates under explosion-induced shock waves. As soil is essentially a medium in which various particles such as sand and rocks are assembled, conventional FEMs are not suitable to capture the complex dynamic interactions. To address the technical difficulties in the simulation of explosion-induced fragmentation, coupled PD-smoothed particle hydrodynamics (SPH) formulations have been developed [75, 76]. PD has also been applied in the context electrothermomechanics, for instance to model dielectric breakdown in solids [77]. The works of Prakash et al. [78] illustrate the application of electromechanical PD to study composite materials. Specifically, the coupled framework was used to investigate conductivity and piezoresistivity of carbon nanotube (CNT)-reinforced polymer composites and to carry out damage sensing in nanocomposite bonded explosive materials. PD-FEM coupling is an approach aimed at taking advantage of both methods [79–82]. The interest in PD can also be understood from the coupling of PD with other formulations such as classical elasticity [83], poroelasticity [41, 84], MD [85, 86], finite point method [87] as well as damage models [88].

3.3 Complex flow problems

The governing equations of transport phenomena are typically convection—diffusion equations. However, in some natural systems such as porous media, anomalous diffusion occurs. The work of Katiyar et al. [89] presented a state-based PD formulation to simulate the convective transport of a single-phase flow of a fluid in heterogeneous porous media. Motivated by the problem of desiccation cracking owing to the soil's variable moisture content, Jabakhanji and Mohtar [90] proposed a PD model for transient moisture flow in unsaturated, heterogeneous, and anisotropic soils.

It is worth mentioning that Silling et al. [91] proposed an Eulerian PD model for compressible fluids. The bond forces are dependent only on the positions of the material points in the deformed configuration in contrast to the Lagrangian formulation in the classical PD. The proposed model was used to analyze problems involving very large deformations. The authors reported that the behavior of soft materials such as gels can be modeled via a framework combining Lagrangian and Eulerian PD models.

3.4 Multiscale problems

There exists a wide range of phenomena and processes whose characterization requires a simultaneous and consistent modeling at multiple spatial and temporal scales. Multiscale modeling is typically used for the analysis of complex materials such as biomaterials, crystalline materials, polymers, and composite materials. Various numerical techniques have been developed to perform multiscale modeling and simulation, amongst them PD is of particular interest here. Askari et al. [92] demonstrated that PD is a viable multiscale material model, suitable for length scales ranging from nanoscale to macroscale. One of the early applications of PD to multiscale modeling is found in [49], in which adaptive refinement for one dimension, later extended to two dimensions [93], was introduced. It has been shown that the PD horizon δ is essentially a *length scale*. Bobaru et al. [94] addressed the natural connections between PD and multiscale modeling. Alali and Lipton [95] developed a two-scale evolution equation based on the PD formulation to study the dynamics of heterogeneous media.

The determination of material properties across different length scales is often carried out by means of an atomistic-to-continuum coupling approach. As indicated in [86], the transition from the microscale to the macroscale is challenging because the coupling must be consistent. In that regard, multiscale

computational models were developed based on an MD–PD coupling [85, 86, 96]. Talebi et al. [97] introduced an open-source, multiscale modeling software for failure simulation in solids named PERMIX that has an interface to LAMMPS [98]. In addition, Du et al. [99] implemented the two-scale convergence model to study the homogenization of the non-local convection-diffusion equation and the state-based PD for heterogeneous media. Xu et al. [100] developed a two-dimensional multiscale implementation of finite-element discretization of non-local models, see also [101]. It is noted that PD has been used for mesoscale fracture analysis in aggregate materials, specifically in multiphase cementitious composites [102]. Shelke et al. [103] addressed the multiscale estimation of damage in composite materials by means of a non-local elastic kernel. For more details on the application of PD in the context of multiscale modeling, see [104] among others.

3.5 Idealized structures

The behavior of engineering structures under different loadings and constraints can be sufficiently described by imposing suitable conditions on partial differential equations (PDEs) of CCM resulting in simple models such as the Euler–Bernoulli beam equation, Timoshenko beam equation, and the thin plate equation. In general, the numerical simulation and design of complex engineering structures involve a combination of *idealized* structural elements such as beams, bars, shells, plates, and membranes. The advancement of the PD theory has brought a new perspective in continuum mechanics as it recovers the reformulation of established PDEs governing the behavior of idealized structural elements. The pioneering work by Silling and Bobaru [105] presented the PD equations for membranes and fibers used to investigate membrane failure and large deformations in fibers. Later, Diyaroglu et al. [106] derived the PD equations for a Timoshenko beam and Mindlin plate that could account for transverse shear deformations. A PD equation of motion for antiplane shear and torsional deformations in structural elements is presented in [58]. See [107, 108] for PD models for beams, [109] for thin plates, [110–113] for fiber networks, and [114] for shells, among others.

It is a very challenging task to determine material properties at the microscale and nanoscale, essentially due to the scale effect. In that context, Celik et al. [115] carried out the mechanical characterization of nickel nanowires via experimental procedures and numerical simulations using FEM and PD, to determine their elastic modulus and yield stress. In addition, Reddy et al. [16] presented modified beam and plate theories based on gradient elasticity theories, which account for size effects and geometric non-linearity. Moreover, they proposed a discrete PD formulation as an alternative to the classical PD whereby the advantages of the discrete PD approach were highlighted. An interesting study by Li et al. [116] presented a PD model for the non-linear static analysis of truss and tensegrity structures. To understand the relationship between microstructure and mechanical behavior, Le et al. [117] used a state-based PD to analyze the stress distribution in round wires under uniaxial tensile load and investigated the effects of defects on the properties of the wires.

3.6 Constitutive models

Different materials can be categorized based on their constitutive behavior such as elasticity, plasticity, and viscoelasticity. For the examples of elasticity in PD see the bond-based model proposed by Silling [11], the ordinary state-based model proposed by Silling et al. [26], the non-ordinary state-based model proposed by Aguiar and Fosdick [34], and the higher gradient expansion for linear isotropic PD materials proposed by Silhavy [118], among others. Foster et al. [119] incorporated a viscoplasticity model within the state-based PD framework. The first PD crystal plasticity model was implemented by Sun and Sundararaghavan [120]. In addition, Madenci and Oterkus [59] developed ordinary state-based PD constitutive relations for plastic deformation based on von-Mises yield criteria with isotropic hardening. Viscoelastic material models have been incorporated within the PD framework to simulate the response of viscoelastic materials under point loads [121] as well as mechanical and thermal loads [122].

3.7 Numerical techniques

The governing equations of physical phenomena are often solved numerically, essentially due to the complexities of the formulations such as strong coupling, non-linearity, and complex geometries. With

proper refinement, numerical methods usually yield approximate solutions with sufficiently high accuracy. For engineering analyses, the FEM and meshfree methods are among the most common approaches. This section briefly reviews the relationship of such numerical techniques with PD.

3.7.1 Meshfree methods. Even though mesh-based approximation techniques such as FEM are widely used in many applications, there are cases in which they may not be well suited. These include complex three-dimensional geometries, domains with discontinuities, and transient fluid flow through porous media [41]. It is known that a highly distorted mesh results in large errors and constant remeshing is impractical. The meshfree methods preclude the use of predefined mesh for the domain discretization but instead, a set of nodes are scattered over the domain and its boundaries, see [123, 124] among others. The PD approach bears certain similarities to the meshfree method in the sense that the domain must be discretized into a set of points and not elements.

Silling and Askari [125] elaborated on the numerical implementation of the PD governing equation namely the meshfree discretization, the integration procedures and the boundary conditions. The discretized formulation was then applied to case studies involving dynamic crack growth. Bessa et al. [126] made a significant contribution by establishing a connection between the original state-based PD formulation with other meshfree methods. Furthermore, the authors introduced the reproducing kernel particle method so as to overcome certain limitations of the original formulation. Regarding the comparison of PD and other meshfree methods, Ganzenmüller et al. [127] investigated the similarities between the meshfree discretizations of PD and SPH. Yaghoobi and Chopeza [128] presented a meshfree method based on the non-ordinary state-based PD to analyze fiber-reinforced concrete structures. An interesting study by O'Grady and Foster [129] presented a meshfree implementation of a state-based PD model to analyze the bending and failure of shells, thereby rotational springs are introduced between pairs of PD bonds. Seleson and Littlewood [130] investigated the accuracy and convergence of meshfree static PD simulations.

3.7.2 Finite element methods. The finite element method is one of the most important numerical methods in computational mechanics. To optimize computational efficiency and accuracy, the concurrent implementation of FEM and PD has been investigated. A significant contribution by Macek and Silling [131] described the implementation of PD within a FE code, in which the PD bonds were represented by truss elements. Chen and Gunzburger [132] developed continuous and discontinuous Galerkin FEM for the PD model, by means of a variational formulation. In order to reduce the computational cost in PD computations, Wang and Tian [133] proposed a fast Galerkin method with efficient matrix assembly and storage for a PD model. Later, their proposed model was extended by Liu et al. [134] to higher-order discretizations and hp adaptivity. Interesting studies were presented by Du et al. [135, 136] in which an adaptive FEM was developed for non-local diffusion equations and PD models by establishing a posteriori error analysis. Tian and Du [137] introduced a non-conforming discontinuous Galerkin finite-element scheme for non-local, volumetrically constrained problems associated with some linear non-local diffusion and non-local PD operators.

A potentially useful and practical technique is the integration of PD within an established finite-element framework, such as commercial softwares. In that context, Beckmann et al. [138] investigated the damage of a two-dimensional bi-material strip owing to thermal loading by means of an implicit finite-element implementation of PD in Abaqus®. It is worth mentioning the work of Schweitzer and Wu [139], who studied the discretization of the particle unity method, a generalized FEM, with embedded PD enrichment.

Owing to its relative simplicity, attempts have been made to reformulate FEM to tackle challenging problems such as fatigue and damage. Reddy and Srinivasa [140] presented displacement-based finite-element models for hyperelastic materials. It was demonstrated that the magnitude of the discretized nodal forces can be expressed in terms of the axial strains along the element edges. The nodal force expressions were then compared with the bond force in PD. Based on this work, Khodabakhshi et al. [141] introduced a non-local framework known as graph-based finite elements to study fracture in brittle materials. It was shown that fracture problems can be solved using FEM if the classical formulation is reformulated into truss-like models, thereby preserving the simplicity of the FEM. Recently, Ren et al.

[142] investigated the dynamic fracture process in a 3D elastic solid, based on a discontinuous Galerkin method of the bond-based PD. Aiming to design a numerical framework for the failure analysis of new corrosion-resistant materials, De Meo and Oterkus [143] presented FE implementation of a PD pitting corrosion damage model. Gerstle et al. [144, 145] presented a finite element PD model to analyze the structural behavior of concrete structures. Very recently, PD modeling of diffusion using FE analysis was discussed in detail by [146] whereby the accuracy and capability of this approach is demonstrated through several benchmark problems. See [147–156] for further contributions dealing with PD and finite element techniques.

3.8 Material failure

In order to prevent safety risks and casualties, significant effort is put into the investigation and prediction of failure. From the perspective of computational simulation, the eXtended Finite Element Method (XFEM) [157, 158] has been introduced as an extension of the conventional FEM to capture discontinuities. On the other hand, PD inherently provides a suitable framework to predict material failure. Comparisons of PD, XFEM and CZM are presented in [159].

In the context of PD, failure can be categorized depending on the material characteristics and the type of PD formulation used. For instance, for brittle materials such as glass or PMMA and if the bond-based PD formulation is utilized, the failure can depend on a critical stretch parameter. For each step of a PD analysis, the stretches of all bonds are monitored and if any of these bonds exceeds the critical stretch value, then these bonds get broken and their forces reduce to zero such that the associated material points will no longer interact with each other. The critical stretch parameter has a direct connection to Griffith's failure criterion [1] based on the critical energy release rate. According to the PD theory, a crack emerges when the bonds within a certain region are broken. The local damage state of a material point is quantified as the ratio of the number of broken interactions to the original number interactions associated with it. A novel energy-based failure criterion was proposed by Foster et al. [160] for a rate-dependent plastic material model within PD. Material failure is often categorized into damage, fracture and fatigue discussed in the remainder of this section. Obviously, the three categories are not mutually exclusive. For instance, low-cycle fatigue can be related to crack propagation and fracture.

3.8.1 Damage. Considering that experimental tests for damage investigation may not be cost effective, numerical techniques have been developed to provide qualitative as well as quantitative prediction of structural damage. A crucial process used to assess the damage state of a structure during its service life is Structural Health Monitoring (SHM). Ibrahim [162] assessed the recent advances of Structural Life Assessment (SLA) and explained the differences between SLA and SHM in PD. To accurately simulate the material degradation involving discontinuities, Han et al. [88] introduced an adaptive coupling of local continuum damage mechanics and PD. PD has been used for damage prediction in different classes of materials including composite materials [163, 164] and layered heterogeneous materials [165]. Emmrich and Puhst [166] applied PD to investigate the conditions for the existence and uniqueness of solutions in the case of damage. Considerable effort has been dedicated to the study of damage due to pitting corrosion; a form of localized corrosion generally in the form of cavities. De Meo et al. [167] presented for the first time a numerical multiphysics PD framework for the modeling of adsorbed-hydrogen stress-corrosion cracking, based on the adsorption-induced decohesion mechanism. More recently, De Meo and Oterkus [143] implemented a PD-based pitting corrosion damage model in a commercial FE software, see also [168, 169]. Recently, Jiang et al. [170] applied the PD theory to analyze micro breakage in cemented carbide cutting tool.

¹For the sake of completeness and in contrast to "material failure", one shall not neglect "structural failure" due to geometrical instabilities such as buckling phenomena. In this regard, Kilic and Madenci [161] investigated the elastic stability of structures by means of PD, in order to determine buckling characteristics of columns under compression and plates under thermal loads.

3.8.2 Fracture. Peridynamics has proven to be powerful strategy to capture various types of fracture in materials due to its integro-differential nature with no spatial derivatives. Taking advantage of the PD formulation, Kilic and Madenci [171] predicted crack growth patterns in quenched glass plates. Ha et al. [172] used a bond-based PD to characterize dynamic brittle fracture. In a related work, Shi [173] simulated crack propagation in brittle glasses by means of a modified Lennard–Jones potential. Liu and Hong [174] used discretized PD and parallel computing to study brittle and ductile solids. The first study on dynamic fracture using PD has been presented by Silling [175], for further developments see [138, 176–183] among others. In that context, Shojaei et al. [87] coupled finite point method to PD in order to study dynamic fracture. Recently, Madenci et al. [184] predicted crack propagation in isotropic materials under complex loading conditions. Dynamic fracture has also been studied with PD for various types of structures such as polymers [185], fiber networks [186], concrete structures [187], anisotropic materials [188–190], functionally graded materials [191], polycrystalline materials [192] as well as geomaterials [62, 193–196]. It is worth mentioning that Evangelatos and Spanos [197] presented the application of PD to stochastic fracture modeling, with a novel spatial discretization of the PD equation.

3.8.3 Fatigue. Hu and Madenci [198] presented a fatigue damage model to predict damage in laminates under cyclic loading. The performed numerical simulations were found to be consistent with the experimental fatigue data. Crack nucleation and growth was also investigated in [199] using a PD fatigue model. Zhang et al. [190] developed a PD-based fatigue crack model to analyze fatigue cracking in two-phase composite materials. Their numerical results were consistent with the experimental data.

3.9 Impact problems

Silling and Askari [200] pioneered the study on impact by means of PD. The numerical code EMU was used to implement the bond-based PD and solve a set of case studies. Then, using EMU, Demmie and Silling [201] considered the problem of extreme loadings of structures. Their work was extended by Oterkus et al. [202] by presenting an impact damage assessment of building components. The PD theory has been used to study impact damage in composite materials [203], layered glass systems [204, 205], and ceramic materials [206]. Recently, Liu et al. [207] studied impact damage in a beam with an offset notch. Lee et al. [208] presented a modeling framework for the interaction of PD domain and conventional finite elements, to effectively analyze impact problem and damage thereof. In a related work, Kosteski et al. [209] introduced the lattice discrete element method to model the impact test of poly (methyl methacrylate) (PMMA) specimens. It is noted that Demmie and Ostoja-Starzewski [210] elaborated on a computational stochastic PD model that was used to study impact loading in geological materials. See also [211–214] for further contributions on impact and damage using PD.

3.10 Composites

Composite materials are used in several applications owing to their high strength-to-weight ratio, fatigue resistance, and damage tolerance among other properties. To save time and costs associated with experimental procedure, a huge effort is dedicated towards the development of effective computational models for prediction of composites behavior. Regarding the application of PD in composites, Silling [215] demonstrated that non-locality arises in a homogenized microscale model for layered composites when a smoothed displacement field is chosen. Furthermore, he derived a PD model in which the length scale is dependent on both the geometry and constituent properties. Buryachenko [216] presented a generalization of the general integral equations of micromechanics using a thermoperistatic formulation to obtain the effective properties of composite materials. To study the response of composite laminates over a wide range of impacting velocities, Sun and Huang [203] presented a PD rate-dependent constitutive model combining the prototype microelastic brittle (PMB) model and the viscoelastic Kelvin-Voigt model. They also introduced a new interlayer bond to describe interlayer interactions. Their simulations compared the impact resistance of composite laminates with that of isotropic plates. Kilic et al. [217] showed that PD is applicable to damage prediction in laminated composites and claimed that homogenization would compromise the failure prediction. In a related work, Hu et al. [218] proposed a homogenizationbased PD model for fiber-reinforced composite laminates. Their results were in agreement with the

analytical data for their benchmark problem. The effectiveness of PD in terms of damage prediction in composite laminates has also been demonstrated in [164, 188, 198, 219, 220].

Askari et al. [163] made a noteworthy contribution by proposing a hybrid continuum/PD model to analyze the degradation of laminated composites termed as *morphing coupling approach*. They indicated that the coupling occurs at the level of the constitutive model in attempts to mitigate the computational cost owing to the non-local nature of PD. Owing to their inhomogeneous nature, composite materials exhibit various failure modes such as matrix cracking, delamination, and fiber kinking. Hu et al. [221] proposed a PD model to investigate delamination growth in composite laminates. Diyaroglu et al. [222] predicted the damage behavior of composites subjected to shock loading. Sadowski and Pankowski [223] developed PD models to investigate nanoindentation of ceramic composites. The failure analysis of concrete structures and cementitious composites using PD can be found in [102, 224, 225].

Given the current trends towards nanomaterials, nanocomposites are an innovative class of materials with various industrial applications. Recently, studies have been conducted to estimate their macroscopic properties using the PD theory. For instance, Duzzi et al. [226] used the bond-based PD formulation to estimate the effective Young's modulus as a function of the filling fraction and observed good agreement of their model with experimental data. Han et al. [227] proposed a classical continuum model as well as a hybrid local/non-local PD-based model to determine the effective properties of CNT polymer composites using homogenization and concluded that the hybrid model is more effective in capturing local inhomogeneities. In addition, Decklever and Spanos [228] proposed a stochastic non-local model based on Monte Carlo simulation and the bond-based PD formulation to evaluate the properties of single-walled CNT polymer composites. They reported that their model is computationally efficient in predicting the mechanical properties and providing a realistic simulation of quasistatic fracture.

3.11 Biology

The PD theory has been successfully applied to study various problems related to living tissues. Deng et al. [229] investigated microcrack propagation and healing processes in cortical bone by means of a non-local multiscale field theory with a generalized form of PD. Taylor et al. [230] used PD to model rupture in biomembranes and investigated the transition between two types of floral and fractal spontaneous rupture. The work of Perré et al. [231] addressed the prediction of wood properties based on its cellular structure, by means of meshfree methods and image-based representation.

An interesting approach was implemented by Lejeune and Linder [232] where the dual-horizon PD framework was extended to capture biological growth by changing the interaction distance and force law between particles. With this framework, the authors note that PD is a particularly convenient approach for modeling biological systems on the cellular scale where each node represents a biological cell. The authors focused on using the framework to capture multiscale emergent behavior driven by mechanical interactions. Recently, Lejeune and Linder used PD to investigate the effect of cell division angle on population morphology [233], the buildup of residual stresses in growing monolayers and spheroids [234], and also the influence of cell shrinkage during cell death on population morphology [235]. Beyond this body of initial studies, which focuses on small populations of growing, proliferating, and dying cells, PD is a promising tool for modeling biological materials on the subcellular, cellular, and histological scales because PD readily captures non-local forces inherent to many biological systems. Furthermore, complex biological phenomena such as buckling and folding of tissues [236, 237] owing to growth are yet to be investigated by PD.

3.12 Geomechanics

Geomaterials are susceptible to cracking owing to fluid pressure. A type of fracture occurring in oil and gas extraction is *hydraulic fracturing*, also known as *fracking*, where fracture is induced in the rock formation to release natural gas and oil. Various numerical methods have been developed to study these phenomena, among which of particular interest here is PD. For instance, Hattori et al. [238] examined various numerical methods, among which PD, to analyze hydraulic fracking in shale rocks. For further details on hydraulic fracturing in the context of PD, see [41, 239–242] among others.

Lai et al. [243] derived the *U-p* PD formulations for fluid-saturated geomaterials and simulated their fragmentation under impulse loads. The *U-p* formulations are equations that describe the behavior of saturated geomaterials, expressed in terms of the displacement *U* and pore fluid pressure *p*. In the context of renewable energy exploitation, Feng et al. [244] reviewed enhanced geothermal systems (EGSs) and mentioned PD as a means of accurately modeling the multi-physics phenomena involved, namely thermal stresses and hydraulic fracture. As pointed out by Fan and Li [76], several engineering applications require an understanding of the soil response to blast loads. The problem of soil fragmentation under explosive loads was simulated using a PD/SPH coupling approach in [75, 76]. Moreover, the PD theory has been implemented to investigate crack behavior in rock materials [193, 194, 245].

3.13 Wave dispersion

The PD formulation has the interesting property that elastic wave dispersion occurs if long-range forces are present and that the PD horizon δ influences the amount of dispersion. The wave dispersion characteristic of PD was reported by Zingales [246] combining the concepts of lattice dynamics, PD and the Kröner–Eringen non-local model to investigate wave propagation in one-dimensional elastic solids, see also [247]. A mathematical study of non-linear PD wave equations was presented in [248]. Various numerical techniques [249–251] have been developed to analyze wave propagation in PD. Silling [252] analyzed the propagation of solitary, *non-dispersive* waves in a non-linear PD solid. In a related study, Vogler et al. [253] investigated the effect of the microstructure on the planar wave propagation in layered, particulate composite, and granular materials. To reduce the wave dispersion in PD, Wildman and Gazonas [254] presented a hybrid method. In addition, wave propagation in the context of PD has been studied in other classes of materials such as graphene [255], CNT [256], and brittle materials [206].

3.14 Particle systems

The nature of the PD equation (1) is particularly interesting in the sense that its discretized form is, to some extent, similar to MD. In that regard, Parks et al. [257] incorporated PD within the MD simulator LAMMPS. The authors pointed out that this approach enhanced the capabilities of the MD code towards performing simulations at larger time and length scales. Rahman and Foster [53] incorporated Langevin dynamics in the PD formulation through the fluctuation—dissipation principle. The authors stated that this approach resolved the ambiguity regarding the role of temperature in a PD system. Within the context of statistical mechanics, they showed that a homogenized PD model satisfies the conservation laws of continuum mechanics (mass, momentum, and energy). Dai et al. [258] elaborated on the similarity between the state-based PD and the reproducing kernel particle method and applied these techniques to solve dynamic problems in a multiresolution continuum. For further details on discrete systems and their potential connection to PD see [13, 14, 259], among others.

4. Concluding remarks

The primary objective of this manuscript was to provide a basic understanding of the PD theory and its main applications to date. Since its formal establishment, the PD theory has found its way to several disciplines collected in Figure 3. Despite its infancy, the method has been successfully applied to various challenging problems. Given its advantage in handling discontinuities, in contrast to CCM, the PD theory has been of great interest in the scientific community. As the inherent non-locality in PD induces high computational cost, further development of the method is required to boost its capabilities. Even though PD has been of particular interest to capture fracture, it has motivated other formulations such as dealing with large eddy simulations [260]. As discussed previously, PD has been applied to simulate flows in porous media and is yet to be extended to turbulent flow analysis. Recently, Motsch and Tadmor [261] presented a mathematical analysis of self-organized dynamics, an instance of which is PD elasticity. Fried [13] and Fosdick [14] have elegantly formulated the mechanics of particle systems that could lead to an alternative PD formulation. Beyond the initial studies in the context of biological applications, which focus on small populations of growing, proliferating, and dying cells, PD is a promising

tool for modeling biological materials on the subcellular, cellular, and histological scales because it readily captures non-local forces inherent to many biological systems.

In summary, this manuscript provides a brief explanation of the PD theory and an extensive account of the literature on the subject. Owing to its integro-differential form, the PD theory proves to be a promising alternative to CCM when dealing with discontinuities and non-localities. This generic framework is broadly applicable to improve our understanding of the material behavior with a large variety of applications.

Note, the main objective of this manuscript was to provide a brief overview of the literature on PD to date and to categorize them. This should not imply that the authors want to necessarily promote PD nor we believe that PD is an ultimate theory to understand and explain every possible phenomena. On the contrary, we regard PD as a continuum theory suffering from and taking advantage of most underlying assumptions of continuum mechanics. One may even claim that possibly PD, as the whole continuum mechanics, could become obsolete, as discrete Lagrangian models could prove more appropriate and predictive of material behavior. In our opinion, both discrete and continuum approaches have certain advantages and disadvantages and perhaps their utility must be separately assessed only based on the problem of interest.

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Note

1. The term Piola stress is adopted instead of the more commonly used first Piola–Kirchhoff stress. Nonetheless, it seems that the term *Piola stress* is more appropriate for this stress measure. Recall, *P* is essentially the *Piola transform* of the Cauchy stress and ties perfectly to the *Piola identity*. In addition, historically, Kirchhoff (1824–1877) employed this stress measure after Piola (1794–1850), see also the discussion in [27].

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Appendix A. Numerical implementation

A typical solution procedure for PD is described by Madenci and Oterkus [25], among others. The PD equation is generally solved numerically by means of a meshfree approach. A generic approach for the numerical implementation of PD is given in Figure 5.

The solution domain is discretized into a finite number of volumes, each represented by a point located at its center. The PD equation of motion in integral form for elasticity can then be expressed in terms of a finite summation of the form

$$\rho(\mathbf{x}_k)\ddot{\mathbf{u}}(\mathbf{x}_k,t) = \sum_{j=1}^N f(\mathbf{u}_j - \mathbf{u}_k, \mathbf{x}_j - \mathbf{x}_k)V_j + \mathbf{b}(\mathbf{x}_k,t),$$
(11)

where N is the number of points inside the horizon of material point k. Correction procedures such as volume and surface corrections can be applied to address the problems of intersecting regions and surface effects respectively [25].

As pointed out by Ganzenmüller et al. [42], "Within the context of mesh-free methods, Peridynamics can be classified as a Total-Lagrangian collocation method with nodal integration." Usually, the domain is discretized into a uniform grid of material points, see also [161]. The idea of adaptive grid refinement was first introduced by Bobaru et al. [49] to analyze the response of a one-dimensional PD bar. Henke and Shanbhag [262] investigated irregular meshes, specifically centroidal Voronoi tessellation, for PD discretization. They observed that careful placement of quadrature points seems to eliminate mesh sensitivity without significant increase in computational cost. Freimanis and Paeglitis [263] studied δ convergence (material point spacing h is constant but horizon size varies) and observed that the maximum accuracy is reached when $\delta = 3h$ and higher horizon sizes compromise the solution accuracy.

PD implementation in commercial finite-element software still uses meshfree discretization although it employs mass point elements to represent the material points and truss or spring elements for PD interactions [131]. This type of implementation also allows utilization of efficient solvers of commercial finite-element software that can significantly reduce the computational time. Computational codes to deal with PD have been developed at Sandia National Laboratories. In particular, Peridigm [264] and the parallel MD code LAMMPS [98] shall be mentioned. It is noted that PD equations are intrinsically compatible for parallel programming applications. The numerical implementation of PD is described in [25] wherein samples codes for numerous benchmark problems are given as well.

The discretization of the governing equations yields a matrix system. Brothers et al. [265] investigated different methods for an efficient construction of the tangent stiffness matrix within Peridigm: forward difference, central difference, and automatic differentiation. The tangent stiffness matrix is mainly required for implicit time integration [39] in dynamic problems. Although explicit integration scheme is

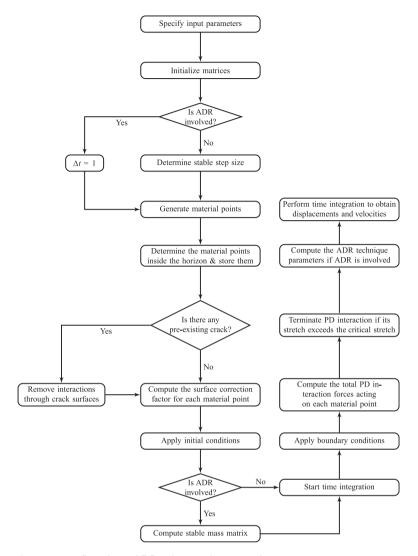


Figure 5. General PD implementation flowchart. ADR, adaptive dynamic relaxation.

more straightforward to implement and requires less storage, it is only conditionally stable, hence mainly suitable for short-duration analysis. For static problems, adaptive dynamic relaxation is a common technique that artificially drives the system to reach the steady-state condition by introducing an artificial damping [25, 266]. Kilic and Madenci [161] used a volume integration scheme over hexagonal subdomains into which Gaussian integration points were placed. Yu et al. [267] proposed a new adaptive integration method with systematic domain categorization for various geometries. To address the problem of intersecting regions (cell neighborhood and neighbor cells) in the standard meshfree approach, Seleson [268] proposed one-point quadrature algorithms to improve the accuracy of integration of two-dimensional PD models. Gu et al. [269] used the Galerkin finite element to discretize a microelastic PD material model within a finite bar. To accelerate the convergence of the iterative solver, they utilized fast circulant preconditioners.

The application of boundary conditions requires a special treatment in PD. Silling [11] showed that the variational formulation of the PD equations does not lead to natural boundary conditions, which are traction boundary conditions in the classical theory. Therefore, body forces are prescribed through a layer of finite thickness at the material boundary. On the other hand, displacement and velocity boundary conditions are enforced via a fictitious boundary layer of depth at least equal to the horizon [25, 131].