Peridynamic Theory of Solid Mechanics

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Dedicated to the memory of James K. Knowles

Contents

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1 Introduction

1.1 Purpose of the peridynamic theory

The peridynamic theory of mechanics attempts to unite the mathematical modeling of continuous media, cracks, and particles within a single framework. It does this by replacing the partial differential equations of the classical theory of solid mechanics with integral or integro-differential equations. These equations are based on a model of internal forces within a body in which material points interact with each other directly over finite distances.

The classical theory of solid mechanics is based on the assumption of a continuous distribution of mass within a body. It further assumes that all internal forces are contact forces [73] that act across zero distance. The mathematical description of a solid that follows from these assumptions relies on partial differential equations that additionally assume sufficient smoothness of the deformation for the PDEs to make sense in either their strong or weak forms. The classical theory has been demonstrated to provide a good approximation to the response of real materials down to small length scales, particularly in single crystals, provided these assumptions are met [52]. Nevertheless, technology increasingly involves the design and fabrication of devices at smaller and smaller length scales, even interatomic dimensions. Therefore, it is worthwhile to investigate whether the classical theory can be extended to permit relaxed assumptions of continuity, to include the modeling of discrete particles such as atoms, and to allow the explicit modeling of nonlocal forces that are known to strongly influence the behavior of real materials.

Similar considerations apply to cracks and other discontinuities: the PDEs of the classical theory do not apply directly on a crack or dislocation because the deformation is discontinuous on these features. Consequently, the techniques of fracture mechanics introduce relations that are extraneous to the basic field equations of the classical theory. For example, linear elastic fracture mechanics (LEFM) considers a crack to evolve according to a separate constitutive model that predicts, on the basis of nearby conditions, how fast a crack grows, in what direction, whether it should arrest, branch, and so on. Although the methods of fracture mechanics provide important and reliable tools in many applications, it is uncertain to what extent this approach can meet the future needs of fracture modeling in complex media under general conditions, particularly at small length scales. Similar considerations apply to certain methods in dislocation dynamics, in which the motion of a dislocation is determined by a supplemental relation.

Aside from requiring these supplemental constitutive equations for the growth of defects within LEFM and dislocation dynamics, the classical theory predicts some well-known nonphysical features in the vicinity of these

singularities. The unbounded stresses and energy densities predicted by the classical PDEs are conventionally treated in idealized cases by assuming that their effect is confined to a small process zone near the crack tip or within the core of a dislocation [38]. However, the reasoning behind neglecting the singularities in this way becomes more troublesome as conditions and geometries become more complex. For example, it is not clear that the energy within the core of a dislocation is unchanged when it moves near or across grain boundaries. Any such change in core energy could affect the driving force on a dislocation.

Molecular dynamics (MD) provides an approach to understanding the mechanics of materials at the smallest length scales that has met with important successes in recent years. However, even with the fastest computers, it is widely recognized that MD cannot model systems of sufficient size to make it a viable replacement for continuum modeling.

These considerations motivate the development of the peridynamic theory, which attempts to treat the evolution of discontinuities according to the same field equations as for continuous deformation. The peridynamic theory also has the goal of treating discrete particles according to the same field equations as for continuous media. The ability to treat both the nanoscale and macroscale within the same mathematical system may make the method an attractive framework in which to develop multiscale and atomistic-to-continuum methods.

1.2 Summary of the literature

The term "peridynamic" first appeared in [60] and comes from the Greek roots for *near* and *force*. The model proposed in [60] treats internal forces within a continuous solid as a network of pair interactions similar to springs. In this respect it is similar to Navier's theory of solids (see Section 6). In the peridynamic model, the springs can be nonlinear. The responses of the springs can depend on their direction in the reference configuration, leading to anisotropy, and on their length. The maximum distance across which a pair of material points can interact through a spring is called the *horizon*, because a given point cannot "see" past its horizon. The horizon is treated as a constant material property in [60]. The equation of motion proposed in the original peridynamic theory is

$$\rho(\mathbf{x})\ddot{\mathbf{u}}(\mathbf{x},t) = \int_{\mathcal{H}} \mathbf{f}\big(\mathbf{u}(\mathbf{x}',t) - \mathbf{u}(\mathbf{x},t), \mathbf{x}' - \mathbf{x}\big)\, dV_{\mathbf{x}'} + \mathbf{b}(\mathbf{x},t) \qquad (1)$$

where $\mathbf{x}$ is the position vector in the reference configuration of the body $\mathcal{B}$, ρ is density, $\mathbf{u}$ is displacement, and $\mathbf{b}$ is a prescribed body force density. $\mathcal{H}$ is a neighborhood of $\mathbf{x}$ with radius δ, where δ is the horizon for the material. Constitutive modeling, as proposed in [60], consists of prescribing the

pairwise force function $\mathbf{f}(\boldsymbol{\eta}, \boldsymbol{\xi})$ for all *bonds* $\boldsymbol{\xi} = \mathbf{x}' - \mathbf{x}$ and for all relative displacements between the bond endpoints, $\boldsymbol{\eta} = \mathbf{u}' - \mathbf{u}$. $\mathbf{f}$ can depend nonlinearly on $\boldsymbol{\eta}$, and there is no assumption that the bond forces are zero in the reference configuration. $\mathbf{f}$ has dimensions of force/volume^2. Linearization of the equation of motion results in an expression that is formally the same as in Kunin's nonlocal theory [46, 47] although constitutive modeling and other aspects are different; a comparison between the two models is discussed in Section 6.5.

A number of papers have investigated various aspects of the linear peridynamic theory. In [70], the static loading by a body force density of an infinitely long, homogeneous bar is considered. The resulting solutions, obtained using Fourier transforms, demonstrate interesting features not present in solutions of the classical equilibrium equation. Among these are oscillations that decay at points far from where the loading is applied, a result of the nonlocality in the equations. (The physical significance of these features is not yet clear.) Dispersion curves are derived from isotropic material models in [60], along with a variational formulation and some aspects of material stability. Zimmermann [83] explored many features of theory, including certain aspects of wave motion, material stability, and numerical solution techniques. Zimmermann also studied energy balance for crack growth within the theory.

Weckner and Abeyaratne [75] studied the dynamics of a one dimensional bar and obtained a Green's function representation of the solution. They also derived expressions for the evolution of discontinuities in the displacement field. Stable discontinuities (*i.e.,* discontinuities that do not grow unboundedly over time) can occur for certain choices of the initial data, even with well-behaved material properties. For other materials, discontinuities can grow unboundedly over time, leading to a type of material instability. Green's functions for three dimensional unbounded elastic isotropic media were derived in [77] for both statics and dynamics. This work also presented a comparison between the local and peridynamic theories for linear elastic solids.

Alali and Lipton [3], Du and Zhou [18, 19], and Emmrich and Weckner [20, 21] establish various existence and uniqueness results for the linear peridynamic balance of momentum. These papers also draw equivalences with the weak solution of the classical equations of linear elasticity, and show, in a precise sense, the well-posedness of the peridynamic equations in the limit as the nonlocality vanishes. In particular, the limiting solution coincides with the conventional weak solution given sufficient regularity of the boundary data and material properties. Within the context of nonlocal steady-state diffusion, Gunzburger and Lehoucq [35] introduce a nonlocal Gauss's theorem and nonlocal Green identities to establish well-posedness

of the nonlocal boundary value problem.

The peridynamic theory as outlined in [60] suffers from significant restrictions on the scope of material behavior that can be modeled, in particular the Poisson ratio is always 1/4 for isotropic materials. This motivated a rethinking of the whole peridynamic theory. The outcome was a concept which preserves the idea of bonds carrying forces between pairs of particles. However, in the new approach, the forces within each bond are not determined independently of each other. Instead, each bond force depends on the collective deformation (and possibly the rate of deformation and history) of all the bonds within the horizon of each endpoint. The resulting modified theory is called *state-based*, because the mathematical objects that convey information about the collective deformation of bonds are called *peridynamic states* (see Section 3). The technical discussion in the present article deals primarily with the state-based theory, although the earlier *bond-based* theory is shown to be a special case of this. The state-based theory is discussed in greater detail in [67], which includes a specific isotropic solid material model in which any Poisson ratio can be prescribed.

It is also shown in [67] that any elastic constitutive model from the classical theory can be adapted to the peridynamic theory using a nonlocal approximation to the deformation gradient tensor. Application of this technique to a strain-hardening plasticity model is demonstrated in [74, 27]. The stress tensor provided by the classical constitutive model is mapped onto the bond forces in a way consistent with the approximation used for the deformation gradient (see Section 4.11).

A peridynamic stress tensor (see Section 6.2) was derived in [48], although a similar concept was previously discussed in [83]. The peridynamic stress tensor has a mechanical interpretation similar to the Piola stress tensor in the classical theory. It provides the force per unit area across any imaginary internal surface. However, in the peridynamic case, the stress tensor is nonlocal: the forces involved are the nonlocal forces in bonds that cross from one side of the surface to the other. The peridynamic operator for the internal force density can be expressed exactly as the divergence of the peridynamic stress tensor field. Thus, the peridynamic equation of motion becomes formally the same as the classical equation.

The convergence of the bond-based peridynamic theory to the equations of classical elasticity theory was demonstrated by Zimmermann [83], and in the context of isotropic linear elastic solids by Emmrich and Weckner [21]. Within the state-based framework for constitutive modeling, it was shown in [68] that if a deformation is classically smooth, then the peridynamic operator for internal force density approaches the classical operator in the limit of small horizon (see Section 6.3). The limiting process produces a classical constitutive model for Piola stress as a limiting case of the peridynamic

stress for small horizon. In this sense, the peridynamic theory converges to the classical theory.

Sears and Lehoucq [58] provide a statistical mechanical foundation for the peridynamic balance of linear momentum. The nonlocality of force interaction is intrinsic and originates in molecular force interaction that is nonlocal. This analysis is similar to the landmark work of Irving and Kirkwood [39], who had the objective of deriving the classical, rather than peridynamic, field equations from statistical physics. The classical balance of linear momentum is a consequence of the more general peridynamic balance when the integral operator is expressed as the divergence of a stress tensor. In the important special case of a pair-potential, Noll [58, 49] in effect derives the peridynamic balance of linear momentum as an intermediate step in deriving the classical balance from the principles of statistical mechanics.

Gerstle *et al.* extended the peridynamic mechanics model to diffusive processes including heat conduction and migration of species due to high electrical current density [31]. They applied the combined nonlocal equations incorporating multiple physical mechanisms, including species diffusion, heat transport, mechanics, and electrical conduction, to a model problem demonstrating the failure of an electronic component due to electromigration.

Nearly all of the applications of the peridynamic model to date rely on numerical solutions. A numerical technique for approximating the peridynamic field equations was proposed in [61]. This numerical method simply replaces the volume integral in (1) with a finite sum:

$$\frac{\rho_i}{h^2}\left(\mathbf{u}_i^{n+1} - 2\mathbf{u}_i^n + \mathbf{u}_i^{n-1}\right) = \sum_{j\in\mathcal{H}} \mathbf{f}(\mathbf{u}_j^n - \mathbf{u}_i^n, \mathbf{x}_j - \mathbf{x}_i)V_i + \mathbf{b}_i^n$$

where i is the node number, n is the time step number, h is the time step size, and V_i is the volume (in the reference configuration) of node i. This numerical method is meshless in the sense that there are no geometrical connections, such as elements, between the discretized nodes. Adaptive refinement and convergence of the discretized method in one dimension are discussed in [11].

Damage is incorporated into this numerical method by causing the "bonds" between interacting nodes to break irreversibly. Although this breakage occurs independently among all the bonds, their failure tends to organize itself along two dimensional surfaces that are interpreted as cracks. Cracks progress autonomously: their advance is determined only by the field equations and constitutive model at the bond level. There is no supplemental relation that dictates crack growth. In particular, the stress intensity factor is not used. Because of the nonlocal nature of the equations, fields near a crack tip in the numerical results are bounded. A computer solution to one

of the Kalthoff-Winkler problems [40], which is regarded in the computational fracture mechanics community as an important benchmark problem, is presented in [61]. Additional examples, as well as more details about the numerical method, are discussed in [65, 76].

Autonomy of crack growth is also demonstrated by Kilic and Madenci [43], who apply the peridynamic method in a numerical model of cracking in glass plates. The cracks are driven by a temperature gradient that causes thermal stresses [82]. In the geometry considered, the crack growth is mostly stable. In some cases, the cracks curve and branch. The numerical model reproduces many aspects of the experiments.

Dayal and Bhattacharya [16] developed a peridynamic material model designed to reproduce martensitic phase transformations. Numerical studies showed that this model predicts phase boundaries with finite thickness and detailed structure. These authors further showed that the model uniquely determines a kinetic relation for the motion of phase boundaries. This result is analogous to the autonomous growth of cracks: the motion of the defect is determined by the field equations and the constitutive model.

Finite element discretization techniques for the peridynamic equations have been proposed by Zimmermann [83] and by Weckner *et al.* [77]. Macek [50] demonstrated that standard truss elements available in the Abaqus commercial finite element code can be used to represent peridynamic bonds. These peridynamic elements can be applied in part of an FE mesh with standard elements in the remainder of the mesh. The resulting FE model of the peridynamic equations was applied in [50] to penetration problems. A finite element formulation was also developed by Chen and Gunzburger [14], who consider the one dimensional equations for a finite bar. Weckner and Emmrich investigated certain discretizations of the peridynamic equation of motion, including Gauss-Hermite quadrature, and applied these to initial value problems to demonstrate convergence [78, 22].

Among applications of the peridynamic model to real systems, Bobaru [10, 9] demonstrated the application of a numerical model to small scale structures, including nanofibers and nanotubes. The nanofiber model is multiscale in the sense that it involves both short-range forces within a fiber and long-range van der Waals forces between fibers. The meshless property of the numerical method, as well as the ability to treat long-range forces, is helpful in these applications because of the need to generate models of complex, random structures. Silling and Bobaru [66] additionally applied the method to the dynamic fracture of brittle-elastic membranes. This study demonstrated the acceleration of a crack to a limiting growth velocity that is consistent with the properties of the material.

Small scale numerical applications of the peridynamic equations are also demonstrated by Agwai, Guven, and Madenci [1, 2] and by Kilic and

Madenci [44], who studied cracking and debonding in electronic integrated circuit packaging. Their model explicitly includes a temperature-dependent term in the material model for bond forces and so can be applied to damage driven by thermal stresses.

Concrete, because it is heterogeneous and brittle unless large compressive confining stress is present, is a good example of a material in which the standard assumptions of LEFM do not apply, at least on the macroscale. The process of cracking in concrete tends to occur through the accumulation of damage over a significant volume before localizing into a discontinuity, which itself usually follows a complex, three dimensional path. Damage and its progression to cracking in concrete are often cited as processes in which nonlocality is important [8, 55]. Gerstle *et al.* [34, 30, 32, 33] have applied the peridynamic method to the failure of concrete structures, including the debonding of reinforcing bar from concrete. This includes development a micropolar version of the theory, in which rotational degrees of freedom are included in the computational nodes.

Impact against brittle structures is a natural application for the peridynamic model, because cracks grow "autonomously:" fracture nucleation and evolution occur as an outcome of the material model and equation of motion, so any number of cracks can grow in any degree of complexity. Peridynamic analysis of impact is demonstrated in [64, 17].

Application to damage and fracture in composite laminates is discussed in [7, 80, 81, 6]. It is demonstrated that the strong anisotropy in a uniaxially reinforced lamina can be reproduced by making the bond response in (1) dependent on the direction of the bond in the reference configuration. The anisotropy also applies to damage: the criterion for bond breakage can also be dependent on bond direction. From this conceptually simple treatment of anisotropy, the complexity of damage and fracture in composites can be reproduced to a surprising degree by a homogenized peridynamic model. Kilic, Agwai, and Madenci [42] developed an innovative numerical model of a composite lamina that is not homogenized, but instead treats the constituents explicitly within the mesh. This model reproduces the influence of stacking sequence on damage and progressive failure in laminates.

The peridynamic method was applied by Foster to the interpretation of experiments on dynamic fracture initiation [26]. This application used a state-based peridynamic material adapted from a viscoplastic material model for metals using the technique discussed in Section 4.11. This work successfully reproduced the effect of loading rate on crack initiation in steel.

The use of the peridynamic theory as multiscale method is currently in its early stages. Preliminary work is reported in [5]. Solution of the peridynamic continuum equations within the LAMMPS molecular dynamics code is described in [56].

Multiscale analysis of a fiber-reinforced composite in the limit of small fiber diameter is treated by Alali and Lipton [3] for different types of assumed limiting behavior of the constituent materials and their interfaces. These authors also investigate the homogenized models resulting from alternative ways of coupling the peridynamic horizon to the geometrical length scales naturally present in the material during this limiting process.

1.3 Organization of this article

The purpose of this article is to present an up-to-date, consistent development of the peridynamic theory. In Section 2 we develop systematically the equations for global and local balance of linear momentum, angular momentum, and energy. This leads to a statement of the principle of virtual work, as well as the peridynamic form of the first law of thermodynamics.

Section 3 contains a discussion of the notation and properties of peridynamic states, which are the mathematical objects used in constitutive modeling. The term "states" is chosen in analogy with the traditional usage of this term in thermodynamics: these objects contain descriptions of all the relevant variables that affect the conditions at a material point in the body. In the case of the peridynamic model, these variables are the nonlocal interactions between a point and its neighbors.

The general form of constitutive models is discussed in Section 4, including the appropriate notion of elastic materials. Conditions for isotropy and objectivity are discussed. The Coleman-Noll method for obtaining restrictions on constitutive dependencies is applied, revealing a restriction on the sign of rate-dependent terms. Specific material models are described that highlight material behavior that the peridynamic model can describe but the classical theory cannot.

Linearization is treated in Section 5. The linearized peridynamic material properties are contained in the *modulus state*, which is analogous to the fourth order elasticity tensor in the classical theory. The equation of motion becomes a linear integro-differential equation in the linearized theory. The equation of equilibrium is a linear Fredholm integral equation of the second type.

In Section 6, we compare the peridynamic theory to the classical theory. The peridynamic stress tensor is defined, and it is shown that under certain conditions, the peridynamic equation of motion converges to the classical PDE. A comparison between the peridynamic model and some other nonlocal theories is also presented.

Section 7 demonstrates that a description of discrete particles can be obtained as the limiting case of peridynamic regions of finite volume as their sizes are shrunk to zero. The resulting description involves forces that are more general than pair interactions. Then, it is shown that such a collection

of "peridynamic particles" can be represented within the peridynamic continuum equations using generalized functions. In particular, any multibody potential can be represented exactly in terms of a peridynamic constitutive model. The peridynamic stress tensor and its volume average are derived for a system of discrete particles, and it is shown that these averages obey the peridynamic equation of motion.

Damage and fracture are discussed in Section 8. It is shown how irreversible damage can be included in the peridynamic expression for free energy in a constitutive model. Damage evolution is treated as part of the material model. A peridynamic version of the J-integral is derived that gives the rate of energy dissipation of a moving defect; this is related to the Griffith criterion for crack growth. An expression for the surface energy of a crack is derived in terms of the work done on bonds that initially connected material on one side of a crack to material on the other side.

2 Balance laws

We derive the peridynamic balances of linear and angular momentum in a more systematic way than has previously appeared in the literature [67]. We then postulate the global balance of energy for a subregion in a peridynamic body, which leads to the local balance of energy. The energy balance involves both heat transport and mechanical power. The global energy balance introduces the *absorbed power* and *supplied power* for a subregion. An important result is that the internal energy defined in terms of these powers is an additive quantity, leading to a meaningful definition of internal energy *density*.

The balances of linear momentum, angular momentum, and energy are shown to adhere to a canonical structure, which we call the *master balance law*. This law expresses the rate of change of any additive quantity within a subregion as the sum of interactions between points inside and outside of the subregion, plus a source term. These interactions appear within the integrand of an integral operator in the master balance law, and the antisymmetry of this integrand plays a crucial role. This antisymmetry allows the integral operator to be written as the integral of the divergence of a nonlocal flux. (An analogous master balance law also exists in the classical theory.)

2.1 Balance of linear momentum

Let $\mathcal{B}$ be the reference configuration of a closed, bounded body with reference mass density ρ. Let $\mathbf{y}(\cdot,\cdot)$ be a motion of $\mathcal{B}$, so $\mathbf{y}(\mathbf{x},t)$ is the position at time $t \geq 0$ of a material point $\mathbf{x} \in \mathcal{B}$. The deformed image of $\mathcal{B}$ under $\mathbf{y}$ is denoted $\mathcal{B}_t$ (Figure 1). Define the velocity field by

$$\mathbf{v}(\mathbf{x},t) = \dot{\mathbf{y}}(\mathbf{x},t) \qquad \forall \mathbf{x} \in \mathcal{B},\ t \geq 0.$$

Let $\mathbf{b}$ be the external body force density field. Let $\mathbf{L}(\mathbf{x},t)$ be the force per unit volume at time t on $\mathbf{x}$ due to interactions with other points in the body. The force vector on a subregion $\mathcal{P} \subset \mathcal{B}$ is given by

$$\int_{\mathcal{P}} (\mathbf{L} + \mathbf{b})\, dV,$$

in which the integration is performed in the reference configuration. Applying Newton's second law to this subregion,

$$\frac{d}{dt}\int_{\mathcal{P}} \rho\dot{\mathbf{y}}\, dV = \int_{\mathcal{P}} \rho\ddot{\mathbf{y}}\, dV = \int_{\mathcal{P}} (\mathbf{L} + \mathbf{b})\, dV, \tag{2}$$

hence, by localization, the equation of motion in terms of $\mathbf{L}$ is

$$\rho(\mathbf{x})\ddot{\mathbf{y}}(\mathbf{x},t) = \mathbf{L}(\mathbf{x},t) + \mathbf{b}(\mathbf{x},t) \qquad \forall \mathbf{x} \in \mathcal{B},\ t \geq 0. \tag{3}$$

Newton's second law applied to $\mathcal{B}$ requires that

$$\frac{d}{dt}\int_{\mathcal{B}} \rho\dot{\mathbf{y}}\; dV = \int_{\mathcal{B}} \mathbf{b}\; dV. \tag{4}$$

Setting $\mathcal{P} = \mathcal{B}$ in (2) and comparing the result with (4) shows that $\mathbf{L}$ must be self-equilibrated:

$$\int_{\mathcal{B}} \mathbf{L}(\mathbf{x}, t)\; dV_{\mathbf{x}} = \mathbf{0} \qquad \forall t \geq 0.$$

Now let $\mathbf{f}(\cdot, \cdot, \cdot)$ be a vector-valued function such that

$$\mathbf{L}(\mathbf{x}, t) = \int_{\mathcal{B}} \mathbf{f}(\mathbf{x}', \mathbf{x}, t)\; dV_{\mathbf{x}'} \qquad \forall \mathbf{x} \in \mathcal{B},\; t \geq 0, \tag{5}$$

and such that $\mathbf{f}$ is *antisymmetric*:

$$\mathbf{f}(\mathbf{x}, \mathbf{x}', t) = -\mathbf{f}(\mathbf{x}', \mathbf{x}, t) \qquad \forall\, \mathbf{x}, \mathbf{x}' \in \mathcal{B},\; t \geq 0. \tag{6}$$

For a given $\mathbf{L}$, such an $\mathbf{f}$ can always be found; an example is

$$\mathbf{f}(\mathbf{x}', \mathbf{x}, t) = \frac{1}{V}(\mathbf{L}(\mathbf{x}, t) - \mathbf{L}(\mathbf{x}', t)) \tag{7}$$

where V is the volume of $\mathcal{B}$ in the reference configuration. The function $\mathbf{f}$, which plays a fundamental role in the peridynamic theory, is called the *dual force density*. It has dimensions of force per unit volume squared. In general, the vectors $\mathbf{f}(\mathbf{x}', \mathbf{x}, t)$ and $\mathbf{f}(\mathbf{x}, \mathbf{x}', t)$ are not parallel to the vector $\mathbf{y}(\mathbf{x}', t) - \mathbf{y}(\mathbf{x}, t)$. The particular choice of $\mathbf{f}$ given in (7) is not very useful in practice; it is given only to demonstrate that for a given $\mathbf{L}$, an $\mathbf{f}$ satisfying (5) and (6) always exists. In applications, $\mathbf{f}$ is determined by the deformation through the constitutive model.

The antisymmetry of $\mathbf{f}$ stated in (6) allows the balance of linear momentum on a subregion $\mathcal{P} \subset \mathcal{B}$ to be expressed in a form in which $\mathbf{f}$ connects only points in the interior of $\mathcal{P}$ to points in its exterior. To see this, note that (6) implies

$$\int_{\mathcal{P}}\int_{\mathcal{P}} \mathbf{f}(\mathbf{x}', \mathbf{x}, t)\; dV_{\mathbf{x}'}\; dV_{\mathbf{x}} = \mathbf{0}. \tag{8}$$

Therefore, from (2), (5), and (8),

$$\frac{d}{dt}\int_{\mathcal{P}} \rho\dot{\mathbf{y}}(\mathbf{x}, t)\; dV = \int_{\mathcal{P}}\int_{\mathcal{B}\setminus\mathcal{P}} \mathbf{f}(\mathbf{x}', \mathbf{x}, t)\; dV_{\mathbf{x}'}\; dV_{\mathbf{x}} + \int_{\mathcal{P}} \mathbf{b}(\mathbf{x}, t)\; dV_{\mathbf{x}}. \tag{9}$$

The following converse is also true: if (9) holds for all subregions $\mathcal{P} \subset \mathcal{B}$, then (6) holds. To see this, choose any two subregions $\mathcal{N} \subset \mathcal{B}$ and $\mathcal{N}' \subset \mathcal{B}$ such that $\mathcal{N} \cap \mathcal{N}' = \emptyset$ (Figure 3). Also define $\mathcal{R} = \mathcal{B} \setminus (\mathcal{N} \cup \mathcal{N}')$. Since

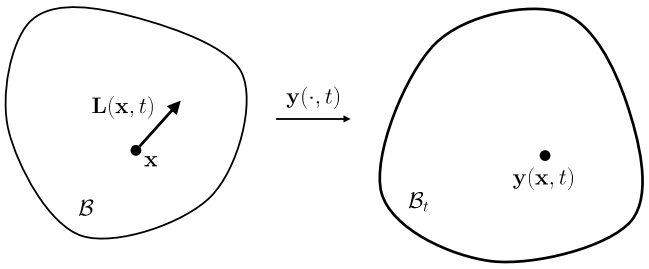

Figure 1: Peridynamic body and its motion $\mathbf{y}$.

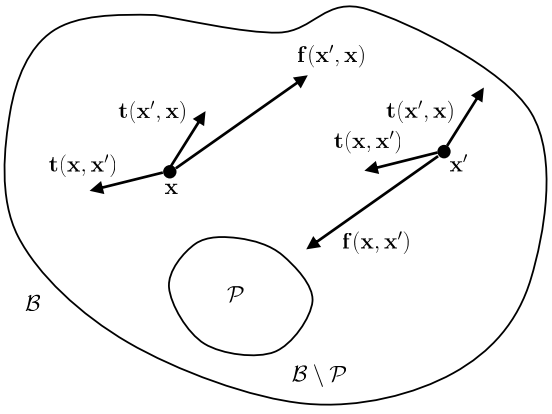

Figure 2: Dual force density $\mathbf{f}$ between two points has contributions from the bond force density $\mathbf{t}$ at both points.

$\mathcal{B} \setminus \mathcal{N} = \mathcal{N}' + \mathcal{R}$ and $\mathcal{B} \setminus \mathcal{N}' = \mathcal{N} + \mathcal{R}$, it follows that for any $\mathbf{f}$, whether antisymmetric or not,

$$\left[\int_{\mathcal{N}}\int_{\mathcal{B}\setminus\mathcal{N}} + \int_{\mathcal{N}'}\int_{\mathcal{B}\setminus\mathcal{N}'} - \int_{\mathcal{N}}\int_{\mathcal{N}'} - \int_{\mathcal{N}'}\int_{\mathcal{N}} - \int_{\mathcal{N}\cup\mathcal{N}'}\int_{\mathcal{R}}\right] \mathbf{f}(\mathbf{x}', \mathbf{x})\, dV_{\mathbf{x}'}\, dV_{\mathbf{x}} = \mathbf{0}. \quad (10)$$

It follows from the linearity of the integral operator that

$$\left[\int_{\mathcal{N}} + \int_{\mathcal{N}'} - \int_{\mathcal{N}\cup\mathcal{N}'}\right] (\rho\ddot{\mathbf{y}}(\mathbf{x}, t) - \mathbf{b}(\mathbf{x}, t))\, dV_{\mathbf{x}} = \mathbf{0},$$

hence, from (9),

$$\left[\int_{\mathcal{N}}\int_{\mathcal{B}\setminus\mathcal{N}} + \int_{\mathcal{N}'}\int_{\mathcal{B}\setminus\mathcal{N}'} - \int_{\mathcal{N}\cup\mathcal{N}'}\int_{\mathcal{R}}\right] \mathbf{f}(\mathbf{x}', \mathbf{x})\, dV_{\mathbf{x}'}\, dV_{\mathbf{x}} = \mathbf{0}.$$

Subtracting this from (10) yields

$$\left[\int_{\mathcal{N}}\int_{\mathcal{N}'} + \int_{\mathcal{N}'}\int_{\mathcal{N}}\right] \mathbf{f}(\mathbf{x}', \mathbf{x})\, dV_{\mathbf{x}'}\, dV_{\mathbf{x}} = \mathbf{0}.$$

Since this equation must hold for arbitrary disjoint $\mathcal{N}$ and $\mathcal{N}'$, localization results in (6). Thus, the balance of linear momentum (9) implies that $\mathbf{f}$ possesses the antisymmetry (6).

It is convenient, but not entirely accurate, to think of $\mathbf{f}(\mathbf{x}', \mathbf{x}, t)$ as physically representing the force vector (per unit volume squared) that $\mathbf{x}'$ exerts on $\mathbf{x}$. The reason this interpretation is not accurate is that there is not necessarily a direct physical connection between $\mathbf{x}'$ and $\mathbf{x}$ that gives rise to the force. For example, if $\mathbf{L}$ is given, the particular $\mathbf{f}$ given by (7) would generate $\mathbf{L}$ regardless of whether each $\mathbf{x}'$ and $\mathbf{x}$ have any direct mechanical interaction, such as a spring connecting the two points.

For a given $\mathbf{f}$ field satisfying (5) and (6), let $\mathbf{t}(\cdot, \cdot, \cdot)$ denote a vector-valued function such that

$$\mathbf{f}(\mathbf{x}', \mathbf{x}, t) = \mathbf{t}(\mathbf{x}', \mathbf{x}, t) - \mathbf{t}(\mathbf{x}, \mathbf{x}', t) \qquad \forall\, \mathbf{x}, \mathbf{x}' \in \mathcal{B},\ t \geq 0. \quad (11)$$

Such a $\mathbf{t}$ function can always be found; an example is given by

$$\mathbf{t}(\mathbf{x}', \mathbf{x}, t) = \frac{\mathbf{f}(\mathbf{x}', \mathbf{x}, t)}{2} \qquad \forall\, \mathbf{x}, \mathbf{x}' \in \mathcal{B},\ t \geq 0.$$

The function $\mathbf{t}$ is called the *bond force density* and is the basic quantity produced by a constitutive model in the peridynamic theory (Figure 2). Like $\mathbf{f}$, the bond force density has dimensions of force per unit volume squared.

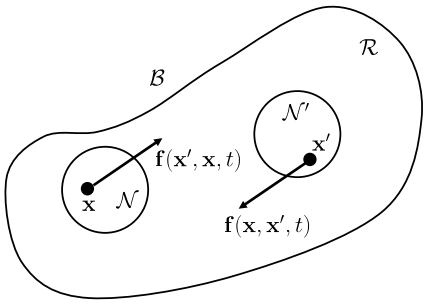

Figure 3: Antisymmetry of $\mathbf{f}$.

In order to simplify notation, set

$$\begin{aligned} \mathbf{t} &= \mathbf{t}(\mathbf{x}', \mathbf{x}, t), \quad \mathbf{t}' = \mathbf{t}(\mathbf{x}, \mathbf{x}', t), \\ \mathbf{f} &= \mathbf{f}(\mathbf{x}', \mathbf{x}, t), \quad \mathbf{f}' = \mathbf{f}(\mathbf{x}, \mathbf{x}', t) \\ \mathbf{y} &= \mathbf{y}(\mathbf{x}, t), \quad \mathbf{y}' = \mathbf{y}(\mathbf{x}', t), \\ \rho &= \rho(\mathbf{x}), \quad \mathbf{b} = \mathbf{b}(\mathbf{x}, t), \\ & \mathbf{L} = \mathbf{L}(\mathbf{x}, t), \\ dV &= dV_{\mathbf{x}}, \quad dV' = dV_{\mathbf{x}'}. \end{aligned} \tag{12}$$

From (5) and (11), the force density is given by

$$\mathbf{L} = \int_{\mathcal{B}} \left(\mathbf{t} - \mathbf{t}'\right) \, dV'. \tag{13}$$

From (9) and (11), the global balance of linear momentum for any subregion $\mathcal{P} \subset \mathcal{B}$ is

$$\frac{d}{dt} \int_{\mathcal{P}} \rho \dot{\mathbf{y}} \, dV = \int_{\mathcal{P}} \int_{\mathcal{B} \setminus \mathcal{P}} \left(\mathbf{t} - \mathbf{t}'\right) \, dV' \, dV + \int_{\mathcal{P}} \mathbf{b} \, dV. \tag{14}$$

From (3) and (5), the local balance of linear momentum is

$$\rho \ddot{\mathbf{y}} = \int_{\mathcal{B}} \mathbf{f} \, dV' + \mathbf{b} \qquad \forall \mathbf{x} \in \mathcal{B}, \; t \geq 0 \tag{15}$$

or equivalently, using (13),

$$\rho\ddot{\mathbf{y}} = \int_{\mathcal{B}} \left(\mathbf{t} - \mathbf{t}'\right)\, dV' + \mathbf{b} \qquad \forall \mathbf{x} \in \mathcal{B},\ t \geq 0. \tag{16}$$

The local balance of linear momentum is also called the *equation of motion*. By setting $\ddot{\mathbf{y}} = \mathbf{0}$ in (16), the *equilibrium equation* is found to be

$$\int_{\mathcal{B}} \left(\mathbf{t} - \mathbf{t}'\right)\, dV' + \mathbf{b} = \mathbf{0} \qquad \forall \mathbf{x} \in \mathcal{B}.$$

The double integral in (14) represents a nonlocal flux of linear momentum through the boundary of $\mathcal{P}$. This term is analogous to the contact force on a subregion in the classical, local theory. Equation (14) is an example of nonlocal balance principles whose structure is discussed in Section 2.5.

2.2 Principle of virtual work

Boundary and initial conditions can be incorporated into the balance of linear momentum (16) by formulating a variational problem [51]. Let $\mathcal{B}^* \subset \mathcal{B}$ have a nonzero volume. $\mathcal{B}^*$ consists of the points where the motion is prescribed. Let $\mathbf{w}(\cdot, \cdot)$ be a motion of $\mathcal{B}$, and use the abbreviated notation

$$\mathbf{w} = \mathbf{w}(\mathbf{x}, t), \qquad \mathbf{w}' = \mathbf{w}(\mathbf{x}', t).$$

The principle of virtual work is stated as follows:

$$\int_{\mathcal{B}} \rho\ddot{\mathbf{y}} \cdot \mathbf{w}\, dV + \int_{\mathcal{B}} \int_{\mathcal{B}} \mathbf{t} \cdot (\mathbf{w}' - \mathbf{w})\, dV'\, dV = \int_{\mathcal{B}} \mathbf{b} \cdot \mathbf{w}\, dV \tag{17}$$

for all motions $\mathbf{w}$ such that

$$\mathbf{w} = \mathbf{0} \qquad \text{on } \mathcal{B}^*. \tag{18}$$

We now demonstrate that the principle of virtual work implies the balance of linear momentum. Using the change of variables $\mathbf{x} \leftrightarrow \mathbf{x}'$ leads to the identity

$$\int_{\mathcal{B}} \int_{\mathcal{B}} \mathbf{t} \cdot (\mathbf{w}' - \mathbf{w})\, dV'\, dV = -\int_{\mathcal{B}} \int_{\mathcal{B}} (\mathbf{t} - \mathbf{t}') \cdot \mathbf{w}\, dV'\, dV. \tag{19}$$

Inserting (19) into (17) results in

$$\int_{\mathcal{B}} \left(\rho\ddot{\mathbf{y}} - \int_{\mathcal{B}} (\mathbf{t} - \mathbf{t}')\, dV' - \mathbf{b}\right) \cdot \mathbf{w}\, dV = \mathbf{0}.$$

Since this must hold for any choice of $\mathbf{w}$ satisfying (18), it follows that

$$\rho\ddot{\mathbf{y}} = \int_{\mathcal{B}} (\mathbf{t} - \mathbf{t}')\, dV' + \mathbf{b} \qquad \text{on } \mathcal{B} \setminus \mathcal{B}^*.$$

This leads to the initial boundary-value problem for the balance of linear momentum (16)

$$\begin{cases} \rho\ddot{\mathbf{y}} = \displaystyle\int_{\mathcal{B}} (\mathbf{t} - \mathbf{t}')\, dV' + \mathbf{b} & \text{on } \mathcal{B} \setminus \mathcal{B}^*, \\ \mathbf{y} = \mathbf{y}^* & \text{on } \mathcal{B}^*, \\ \dot{\mathbf{y}}(\cdot, 0) = \mathbf{v}_0(\cdot) & \text{on } \mathcal{B} \setminus \mathcal{B}^*, \end{cases} \tag{20}$$

where $\mathbf{y}^*$ and $\mathbf{v}_0$ are prescribed functions. Conversely, working backwards shows that any solution of the initial boundary-value problem (20) also satisfies the principle of virtual work (PVW) statement (17).

2.3 Balance of angular momentum

Let $\mathcal{B}$ be a closed, bounded body, and as before, let $\mathcal{P} \subset \mathcal{B}$ be a subregion. The angular momentum in $\mathcal{P}$ with respect to an arbitrary reference point $\mathbf{y}_0$ is defined by

$$\mathbf{A}(\mathcal{P}) = \int_{\mathcal{P}} (\mathbf{y} - \mathbf{y}_0) \times \rho\dot{\mathbf{y}}\, dV. \tag{21}$$

This definition asserts that there are no hidden variables or degrees of freedom other than velocity that contain angular momentum. Since $\dot{\mathbf{y}} \times \rho\dot{\mathbf{y}} = \mathbf{0}$, (21) implies

$$\dot{\mathbf{A}}(\mathcal{P}) = \int_{\mathcal{P}} (\mathbf{y} - \mathbf{y}_0) \times \rho\ddot{\mathbf{y}}\, dV.$$

From this and (3),

$$\dot{\mathbf{A}}(\mathcal{P}) = \int_{\mathcal{P}} (\mathbf{y} - \mathbf{y}_0) \times (\mathbf{L} + \mathbf{b})\, dV. \tag{22}$$

Global balance of angular momentum on $\mathcal{B}$ requires that the rate of change of total angular momentum equal the total moment due to external forces:

$$\dot{\mathbf{A}}(\mathcal{B}) = \int_{\mathcal{B}} (\mathbf{y} - \mathbf{y}_0) \times \mathbf{b}\, dV. \tag{23}$$

This equation asserts that there are no external moments other than those arising from $\mathbf{b}$. Comparing the last two equations and setting $\mathcal{P} = \mathcal{B}$ places a restriction on $\mathbf{L}$:

$$\int_{\mathcal{B}} (\mathbf{y} - \mathbf{y}_0) \times \mathbf{L}\, dV = \mathbf{0}, \tag{24}$$

which means that the moments generated by internal forces must be self-equilibrated. Conversely, (22) and (24) imply (23).

Suppose the bond force density field $\mathbf{t}$ is such that

$$\int_{\mathcal{B}} (\mathbf{y}' - \mathbf{y}) \times \mathbf{t}\, dV' = \mathbf{0} \qquad \forall \mathbf{x} \in \mathcal{B},\ t \geq 0. \tag{25}$$

A bond force density field satisfying (25) will be called *nonpolar*. This name is chosen to contrast the present situation with "micropolar" continuum theories that permit a nonzero moment to be exerted on material points: the definition (25) asserts that the net moment about $\mathbf{y}(\mathbf{x}, t)$ exerted by $\mathbf{t}(\cdot, \mathbf{x})$ vanishes. Micropolar theory has been proposed, for example, as a way of modeling granular flow [41]. A micropolar peridynamic model has been proposed [30] but is beyond the scope of the present article.

If $\mathbf{t}$ is nonpolar, then the global balance of angular momentum on $\mathcal{B}$ necessarily holds. To see this, compute the left hand side of (24) using (5), (8), and (11):

$$\begin{aligned}\int_{\mathcal{B}} (\mathbf{y} - \mathbf{y}_0) \times \mathbf{L}\, dV &= \int_{\mathcal{B}} \int_{\mathcal{B}} (\mathbf{y} - \mathbf{y}_0) \times \mathbf{f}\, dV'\, dV \\ &= \int_{\mathcal{B}} \int_{\mathcal{B}} \mathbf{y} \times \mathbf{f}\, dV'\, dV - \mathbf{y}_0 \times \int_{\mathcal{B}} \int_{\mathcal{B}} \mathbf{f}\, dV'\, dV \\ &= \int_{\mathcal{B}} \int_{\mathcal{B}} \mathbf{y} \times (\mathbf{t} - \mathbf{t}')\, dV'\, dV.\end{aligned}$$

Using the change of variables $\mathbf{x} \leftrightarrow \mathbf{x}'$ to eliminate the $\mathbf{t}'$ term and using (25) leads to

$$\int_{\mathcal{B}} (\mathbf{y} - \mathbf{y}_0) \times \mathbf{L}\, dV = \int_{\mathcal{B}} \int_{\mathcal{B}} (\mathbf{y} - \mathbf{y}') \times \mathbf{t}\, dV'\, dV = \mathbf{0},$$

so (24) holds. As discussed above, this implies that the global balance of angular momentum on $\mathcal{B}$ (23) holds.

Next, we further investigate the balance of angular momentum on subregions and use the results to derive the local balance of angular momentum. Assume that $\mathbf{t}$ is nonpolar, let $\mathcal{P} \subset \mathcal{B}$ be a subregion, and let $\mathbf{y}_0 = \mathbf{0}$. From (5), (11) and (22),

$$\dot{\mathbf{A}}(\mathcal{P}) = \int_{\mathcal{P}} \int_{\mathcal{B}} \mathbf{y} \times (\mathbf{t} - \mathbf{t}')\, dV'\, dV + \int_{\mathcal{P}} \mathbf{y} \times \mathbf{b}\, dV.$$

Add the expression

$$\mathbf{y}' \times \mathbf{t} - \mathbf{y}' \times \mathbf{t}$$

to the integrand in the double integral. Rearranging yields

$$\begin{aligned}\dot{\mathbf{A}}(\mathcal{P}) = &\int_{\mathcal{P}} \int_{\mathcal{B}} (\mathbf{y} - \mathbf{y}') \times \mathbf{t}\, dV'\, dV \\ &+ \int_{\mathcal{P}} \int_{\mathcal{B}} (\mathbf{y}' \times \mathbf{t} - \mathbf{y} \times \mathbf{t}')\, dV'\, dV + \int_{\mathcal{P}} \mathbf{y} \times \mathbf{b}\, dV. \quad (26)\end{aligned}$$

Since the bond force densities are nonpolar, by (25), the first term on the right hand side vanishes. Also, the integrand in the second term is antisymmetric in $\mathbf{x}$ and $\mathbf{x}'$, therefore

$$\int_{\mathcal{P}} \int_{\mathcal{P}} (\mathbf{y}' \times \mathbf{t} - \mathbf{y} \times \mathbf{t}') \, dV' \, dV = \mathbf{0}.$$

So, (26) implies

$$\dot{\mathbf{A}}(\mathcal{P}) = \int_{\mathcal{P}} \int_{\mathcal{B}\setminus\mathcal{P}} (\mathbf{y}' \times \mathbf{t} - \mathbf{y} \times \mathbf{t}') \, dV' \, dV + \int_{\mathcal{P}} \mathbf{y} \times \mathbf{b} \, dV,$$

or, recalling (21),

$$\frac{d}{dt} \int_{\mathcal{P}} \mathbf{y} \times \rho \dot{\mathbf{y}} \, dV = \int_{\mathcal{P}} \int_{\mathcal{B}\setminus\mathcal{P}} (\mathbf{y}' \times \mathbf{t} - \mathbf{y} \times \mathbf{t}') \, dV' \, dV + \int_{\mathcal{P}} \mathbf{y} \times \mathbf{b} \, dV, \quad (27)$$

which holds for any $\mathcal{P} \subset \mathcal{B}$. (22) and (27) are equivalent statements of the global balance of angular momentum for a subregion under the assumption of nonpolar bond force densities. The structure of (27) is similar to that of (14) in that the two terms on the right hand side represent nonlocal flux and source rate. The underlying structure of balance principles of this type is discussed further in Section 2.5.

By localizing (27), a form of the local balance of angular momentum is obtained:

$$\mathbf{y} \times \rho \ddot{\mathbf{y}} = \int_{\mathcal{B}} (\mathbf{y}' \times \mathbf{t} - \mathbf{y} \times \mathbf{t}') \, dV' + \mathbf{y} \times \mathbf{b} \qquad \forall \mathbf{x} \in \mathcal{B}, \ t \geq 0.$$

This equation is equivalent to (25).

2.4 Balance of energy

Let $q(\mathbf{x}', \mathbf{x}, t)$ denote the rate of heat transport, per unit volume squared, from $\mathbf{x}'$ to $\mathbf{x}$. It is required that q be antisymmetric:

$$q(\mathbf{x}, \mathbf{x}', t) = -q(\mathbf{x}', \mathbf{x}, t) \qquad \forall \mathbf{x}, \mathbf{x}' \in \mathcal{B}, \ t \geq 0. \quad (28)$$

Nonlocal heat transport is assumed here for consistency with the mechanical model, although the subsequent development of the energy balance could be repeated with a local heat model. Nonlocality is important in radiative heat transport. In the limit of small interaction distances, nonlocal heat conduction is physically the same as the local model.

Let $r(\mathbf{x}, t)$ denote the heat source rate at $\mathbf{x}$. The rate at which heat is supplied to a subregion $\mathcal{P} \subset \mathcal{B}$ is given by

$$\mathcal{Q}(\mathcal{P}) = \int_{\mathcal{P}} \int_{\mathcal{B}\setminus\mathcal{P}} q \, dV' \, dV + \int_{\mathcal{P}} r \, dV, \quad (29)$$

where the abbreviation $q = q(\mathbf{x}', \mathbf{x}, t)$ is used. Taking the scalar product of both sides of the balance of linear momentum (16) with the velocity $\mathbf{v}$ and integrating over $\mathcal{P}$ results in

$$\frac{d}{dt}\int_{\mathcal{P}} \frac{\rho \mathbf{v}\cdot\mathbf{v}}{2}\, dV = \int_{\mathcal{P}}\int_{\mathcal{B}} \left(\mathbf{t}-\mathbf{t}'\right)\cdot\mathbf{v}\, dV'\, dV + \int_{\mathcal{P}} \mathbf{b}\cdot\mathbf{v}\, dV. \tag{30}$$

The identity

$$\left(\mathbf{t}-\mathbf{t}'\right)\cdot\mathbf{v} = \left(\mathbf{t}\cdot\mathbf{v}' - \mathbf{t}'\cdot\mathbf{v}\right) - \mathbf{t}\cdot\left(\mathbf{v}'-\mathbf{v}\right)$$

implies that for all $\mathcal{P}\subset\mathcal{B}$,

$$\begin{aligned}
&\int_{\mathcal{P}}\int_{\mathcal{B}} \left(\mathbf{t}-\mathbf{t}'\right)\cdot\mathbf{v}\, dV'\, dV \\
&\qquad = \int_{\mathcal{P}}\int_{\mathcal{B}} \left(\mathbf{t}\cdot\mathbf{v}' - \mathbf{t}'\cdot\mathbf{v}\right) dV'\, dV - \int_{\mathcal{P}}\int_{\mathcal{B}} \mathbf{t}\cdot\left(\mathbf{v}'-\mathbf{v}\right) dV'\, dV, \\
&\qquad = \int_{\mathcal{P}}\int_{\mathcal{B}\setminus\mathcal{P}} \left(\mathbf{t}\cdot\mathbf{v}' - \mathbf{t}'\cdot\mathbf{v}\right) dV'\, dV - \int_{\mathcal{P}}\int_{\mathcal{B}} \mathbf{t}\cdot\left(\mathbf{v}'-\mathbf{v}\right) dV'\, dV,
\end{aligned} \tag{31}$$

where the antisymmetry of the *dual power density* defined by

$$p_d(\mathbf{x}', \mathbf{x}) = \mathbf{t}\cdot\mathbf{v}' - \mathbf{t}'\cdot\mathbf{v} \tag{32}$$

was used in the last step. Using (31), we may rewrite (30) as the power balance

$$\dot{\mathcal{K}}(\mathcal{P}) + \mathcal{W}_{\text{abs}}(\mathcal{P}) = \mathcal{W}_{\text{sup}}(\mathcal{P}) \tag{33}$$

where the kinetic energy in $\mathcal{P}$ is defined by

$$\mathcal{K}(\mathcal{P}) = \int_{\mathcal{P}} \frac{\rho\mathbf{v}\cdot\mathbf{v}}{2}\, dV,$$

the power *absorbed* by $\mathcal{P}$ is defined by

$$\mathcal{W}_{\text{abs}}(\mathcal{P}) = \int_{\mathcal{P}}\int_{\mathcal{B}} \mathbf{t}\cdot\left(\mathbf{v}'-\mathbf{v}\right) dV'\, dV, \tag{34}$$

and the power *supplied* to $\mathcal{P}$ is defined by

$$\mathcal{W}_{\text{sup}}(\mathcal{P}) = \int_{\mathcal{P}}\int_{\mathcal{B}\setminus\mathcal{P}} \left(\mathbf{t}\cdot\mathbf{v}' - \mathbf{t}'\cdot\mathbf{v}\right) dV'\, dV + \int_{\mathcal{P}} \mathbf{b}\cdot\mathbf{v}\, dV.$$

We postulate the following global form of the first law of thermodynamics:

$$\dot{\mathcal{E}}(\mathcal{P}) + \dot{\mathcal{K}}(\mathcal{P}) = \mathcal{W}_{\text{sup}}(\mathcal{P}) + \mathcal{Q}(\mathcal{P}) \tag{35}$$

where $\mathcal{E}(\mathcal{P})$ is the *internal energy* in $\mathcal{P}$. Subtracting (33) from (35) results in

$$\dot{\mathcal{E}}(\mathcal{P}) = \mathcal{W}_{\text{abs}}(\mathcal{P}) + \mathcal{Q}(\mathcal{P}). \tag{36}$$

This result asserts that the rate of change of internal energy is the sum of the absorbed power and the rate of heat supplied.

Using (28), it follows from the definitions (29) and (34) that both $\mathcal{W}_{\text{abs}}$ and $\mathcal{Q}$ are additive quantities, *i.e.*, for $\mathcal{P}_1, \mathcal{P}_2 \subset \mathcal{B}$ where $\mathcal{P}_1 \cap \mathcal{P}_2 = \emptyset$,

$$\mathcal{W}_{\text{abs}}(\mathcal{P}_1 \cup \mathcal{P}_2) = \mathcal{W}_{\text{abs}}(\mathcal{P}_1) + \mathcal{W}_{\text{abs}}(\mathcal{P}_2), \tag{37}$$

$$\mathcal{Q}(\mathcal{P}_1 \cup \mathcal{P}_2) = \mathcal{Q}(\mathcal{P}_1) + \mathcal{Q}(\mathcal{P}_2). \tag{38}$$

Therefore, by (36), the internal energy $\mathcal{E}$ is also additive. It follows that there exists a scalar quantity $\varepsilon(\mathbf{x}, t)$ called the *internal energy density* such that

$$\mathcal{E}(\mathcal{P}) = \int_{\mathcal{P}} \varepsilon \, dV. \tag{39}$$

From (29), (34), (36), and (39),

$$\int_{\mathcal{P}} \dot{\varepsilon} \, dV = \int_{\mathcal{P}} \int_{\mathcal{B}} \mathbf{t} \cdot \left(\mathbf{v}' - \mathbf{v}\right) dV' \, dV + \int_{\mathcal{P}} \int_{\mathcal{B}\setminus\mathcal{P}} q \, dV' \, dV + \int_{\mathcal{P}} r \, dV. \tag{40}$$

By (28),

$$\int_{\mathcal{P}} \int_{\mathcal{B}\setminus\mathcal{P}} q \, dV' \, dV = \int_{\mathcal{P}} \int_{\mathcal{B}} q \, dV' \, dV.$$

From this and (40),

$$\int_{\mathcal{P}} \left[-\dot{\varepsilon} + \int_{\mathcal{B}} \mathbf{t} \cdot \left(\mathbf{v}' - \mathbf{v}\right) dV' + \int_{\mathcal{B}} q \, dV' + r \right] dV = 0.$$

Since this must hold for any $\mathcal{P} \subset \mathcal{B}$, localization leads to the local statement of the first law of thermodynamics:

$$\dot{\varepsilon} = p_{\text{abs}} + h + r. \tag{41}$$

where the local heat transport rate at $\mathbf{x}$ is defined by

$$h = \int_{\mathcal{B}} q \, dV'$$

and the absorbed power density at $\mathbf{x}$ is defined by

$$p_{\text{abs}} = \int_{\mathcal{B}} \mathbf{t} \cdot \left(\mathbf{v}' - \mathbf{v}\right) dV'. \tag{42}$$

p_{abs} is the analogue of the stress power in the classical theory.

It is worthwhile to contrast the peridynamic power balance developed in this section with earlier approaches that lead to *nonadditive* definitions of internal energy. The key difference lies in our usage of the peridynamic quantities *absorbed* and *supplied power*, rather than the traditional ideas of internal and external power that appear in literature on the thermodynamics of nonlocal media. To see this, define the *internal* and *external power* by

$$\mathcal{W}_{\text{int}}(\mathcal{P}) = \int_{\mathcal{P}} \int_{\mathcal{P}} \mathbf{f} \cdot \mathbf{v} \, dV' \, dV,$$
$$\mathcal{W}_{\text{ext}}(\mathcal{P}) = \int_{\mathcal{P}} \int_{\mathcal{B}\setminus\mathcal{P}} \mathbf{f} \cdot \mathbf{v} \, dV' \, dV + \int_{\mathcal{P}} \mathbf{b} \cdot \mathbf{v} \, dV.$$

$\mathcal{W}_{\text{int}}(\mathcal{P})$ consists of the rate of work done on material points in $\mathcal{P}$ by interactions with other points in $\mathcal{P}$. $\mathcal{W}_{\text{ext}}(\mathcal{P})$ represents the work done by all other interactions, including body forces. These quantities are related to $\mathcal{W}_{\text{abs}}$ and $\mathcal{W}_{\text{sup}}$ via

$$\mathcal{W}_{\text{abs}}(\mathcal{P}) = -\mathcal{W}_{\text{int}}(\mathcal{P}) + \int_{\mathcal{P}} \int_{\mathcal{B}\setminus\mathcal{P}} \mathbf{t} \cdot \big(\mathbf{v}' - \mathbf{v}\big) \, dV' \, dV$$
$$\mathcal{W}_{\text{sup}}(\mathcal{P}) = \mathcal{W}_{\text{ext}}(\mathcal{P}) + \int_{\mathcal{P}} \int_{\mathcal{B}\setminus\mathcal{P}} \mathbf{t} \cdot \big(\mathbf{v}' - \mathbf{v}\big) \, dV' \, dV.$$

Inserting the above expressions for the absorbed and supplied power replaces (33) with the following alternate statement of the power balance:

$$\dot{\mathcal{K}}(\mathcal{P}) - \mathcal{W}_{\text{int}}(\mathcal{P}) = \mathcal{W}_{\text{ext}}(\mathcal{P}).$$

However, Gurtin and Williams [36] demonstrate that $\mathcal{W}_{\text{int}}$ and $\mathcal{W}_{\text{ext}}$ are not additive quantities, in the sense of (38), leading to their conclusion that there is no additive notion of the internal energy density analogous to (36). The antisymmetretry of the dual power density p_d defined in (32) is also necessary for the additivity of the absorbed and supplied power expenditures. As the next section demonstrates, additivity and antisymmetry are intrinsic to well formulated nonlocal balance laws.

2.5 Master balance law

The global balances of linear momentum (14), angular momentum (27), and energy (35) over any subregion $\mathcal{P} \subset \mathcal{B}$ possess the following canonical structure:

$$\dot{\mathsf{E}}(\mathcal{P}) = \int_{\mathcal{P}} \int_{\mathcal{B}\setminus\mathcal{P}} \mathsf{D} \, dV' \, dV + \int_{\mathcal{P}} \mathsf{s} \, dV, \tag{43}$$

where $\mathsf{D}(\cdot,\cdot)\colon \mathcal{B} \times \mathcal{B} \to \mathbb{R}^d$ and $\mathsf{s}(\cdot)\colon \mathcal{B} \to \mathbb{R}^d$. Here, $d = 1$ if E is scalar valued or $d = 3$ if it is vector valued. It is assumed that D is antisymmetric:

$$\mathsf{D}(\mathbf{x}', \mathbf{x}) = -\mathsf{D}(\mathbf{x}, \mathbf{x}') \qquad \forall \mathbf{x}, \mathbf{x}' \in \mathcal{B}. \tag{44}$$

(In the remaining discussion, the abbreviations $\mathsf{D} = \mathsf{D}(\mathbf{x}', \mathbf{x})$ and $\mathsf{s} = \mathsf{s}(\mathbf{x})$ are used, and t does not appear explicitly.) The balance (43) states that the rate of change of the extensive quantity $\mathsf{E}(\mathcal{P})$ is composed of two terms. The first term represents interactions between $\mathcal{P}$ its exterior. The second term represents external sources. The functions D and s are called the *dual interaction density* and the *source rate* respectively. (44) implies

$$\int_{\mathcal{P}} \int_{\mathcal{B}\setminus\mathcal{P}} \mathsf{D}\, dV'\, dV = \int_{\mathcal{P}} \int_{\mathcal{B}} \mathsf{D}\, dV'\, dV,$$

hence (43) may be rewritten as

$$\dot{\mathsf{E}}(\mathcal{P}) = \int_{\mathcal{P}} \int_{\mathcal{B}} \mathsf{D}\, dV'\, dV + \int_{\mathcal{P}} \mathsf{s}\, dV. \tag{45}$$

From (45), it is immediate that

$$\dot{\mathsf{E}}(\mathcal{P}_1 \cup \mathcal{P}_2) = \dot{\mathsf{E}}(\mathcal{P}_1) + \dot{\mathsf{E}}(\mathcal{P}_2),$$

where $\mathcal{P}_1$ and $\mathcal{P}_2$ are any two disjoint subregions of $\mathcal{B}$. This establishes that E is additive. It follows that there exists a density function e on $\mathcal{B}$ such that

$$\mathsf{E}(\mathcal{P}) = \int_{\mathcal{P}} \mathsf{e}\, dV$$

for any subregion $\mathcal{P} \subset \mathcal{B}$. Inserting this expression into (45), localization leads to the local balance

$$\dot{\mathsf{e}} = \int_{\mathcal{B}} \mathsf{D}\, dV' + \mathsf{s}. \tag{46}$$

Table 1 lists the dual interaction densities and source rates for the three nonlocal balances previously introduced.

We now demonstrate that the master balance law (43) can be written in a more traditional form, *i.e.,* the first term on the right hand side of (43) corresponds to a nonlocal flux acting on the boundary of $\mathcal{P}$. This is accomplished by invoking two lemmas due to Noll [53, 49], and crucially depends upon the antisymmetry of D.

Suppose that the dual interaction density D is antisymmetric and continuously differentiable, and that

$$|\mathsf{D}(\mathbf{x}, \mathbf{x}')| \leqslant K|\mathbf{x} - \mathbf{x}'|^{-\ell} \qquad \mathbf{x} \in \mathcal{B}, \quad \mathbf{x}' \in \mathbb{R}^3 \setminus \mathcal{B},$$

for positive constants K and $\ell < 3$. Then Noll's lemma I provides a closed

Balance (Eq.)	e	D	s
Linear momentum (14)	$\rho\dot{\mathbf{y}}$	$\mathbf{t}-\mathbf{t}'$	$\mathbf{b}$
Angular momentum (27)	$\mathbf{y}\times\rho\dot{\mathbf{y}}$	$\mathbf{y}'\times\mathbf{t}-\mathbf{y}\times\mathbf{t}'$	$\mathbf{y}\times\mathbf{b}$
Energy (35)	$\varepsilon+\dfrac{\rho\dot{\mathbf{y}}\cdot\dot{\mathbf{y}}}{2}$	$q+\mathbf{t}\cdot\dot{\mathbf{y}}'-\mathbf{t}'\cdot\dot{\mathbf{y}}$	$r+\mathbf{b}\cdot\dot{\mathbf{y}}$

Table 1: Global balance principles. $\mathbf{y}$ denotes the motion of the body $\mathcal{B}$, and $\mathcal{P}\subset\mathcal{B}$.

form expression for a tensor of order one[1] or two,

$$\mathsf{T}(\mathbf{x})=-\frac{1}{2}\int_{\mathbb{R}^3}\left(\int_0^1\mathsf{D}\left(\mathbf{x}+\lambda\mathbf{z},\mathbf{x}-(1-\lambda)\mathbf{z}\right)\,d\lambda\right)\otimes\mathbf{z}\,dV, \tag{47}$$

such that

$$\nabla\cdot\mathsf{T}=\int_{\mathcal{B}}\mathsf{D}\,dV'.$$

Noll's lemma II then implies that

$$\int_{\mathcal{P}}\nabla\cdot\mathsf{T}\,dV=\int_{\mathcal{P}}\int_{\mathcal{B}}\mathsf{D}\,dV'\,dV=\int_{\mathcal{P}}\int_{\mathcal{B}\setminus\mathcal{P}}\mathsf{D}\,dV'\,dV, \tag{48}$$

where the antisymmetry of the dual density D is invoked for the second equality. Using the divergence theorem, this allows us to rewrite the master balance law (43) in the familiar form[2]

$$\dot{\mathsf{E}}(\mathcal{P})=\int_{\partial\mathcal{P}}\mathsf{T}\mathbf{n}\,dV+\int_{\mathcal{P}}\mathsf{s}\,dV.$$

Localization then gives the counterpart of (46) as

$$\dot{\mathsf{e}}=\nabla\cdot\mathsf{T}+\mathsf{s}.$$

Noll [54] calls T a *reacher*. This terminology draws a distinction with the abstract notion of a *contactor* corresponding to a surface interaction. For

[1] The integrand is understood as

$$\mathbf{z}\int_0^1\mathsf{D}\left(\mathbf{x}+\lambda\mathbf{z},\mathbf{x}-(1-\lambda)\mathbf{z}\right)\,d\lambda$$

for an order one tensor, or flux vector, T.

[2] When the tensor T is of order one, then $\mathsf{T}\mathbf{n}$ is understood to be $\mathsf{T}\cdot\mathbf{n}$.

instance, when the interaction is a force, a contactor is a contact stress associated with the classical continuum notion of contact force.

The conclusion of Noll's lemma II given by (48) implies that

$$\int_{\partial\mathcal{B}} \mathsf{T}\mathbf{n}\, dV = \mathbf{0},$$

and equivalently expresses that the sum of the internal interactions in the body is zero.

As shown in Section 2.1 for the case $\mathsf{D} = \mathbf{f}$, the second equality in (48) implies the antisymmetry of D that was assumed in (44). Lehoucq and Silling [48] provide an expression (see (120) below) for the peridynamic stress tensor in terms of the bond force density. This expression is derivable from (47) with $\mathsf{D} = \mathbf{f}$.

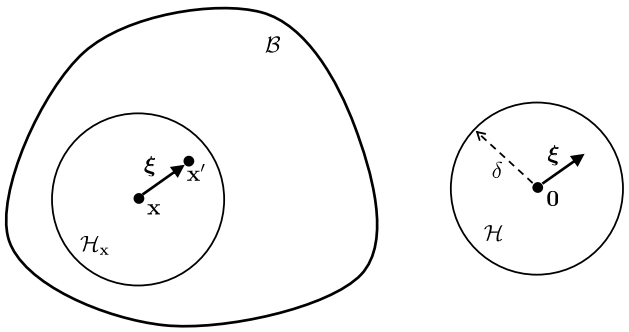

Figure 4: The family $\mathcal{H}$ contains the relative position vectors (bonds) connecting $\mathbf{x}$ to points such as $\mathbf{x}'$ within a distance δ of $\mathbf{x}$.

3 Peridynamic states: notation and properties

The remainder of this paper largely involves mappings from pairs of points $(\mathbf{x}, \mathbf{x}')$ to some quantity. As an aid to keeping track of these mappings, it is convenient to introduce objects called "peridynamic states." Consider a body $\mathcal{B}$. Let δ be a positive number, called the *horizon*. For a given $\mathbf{x} \in \mathcal{B}$, let $\mathcal{H}_\mathbf{x}$ be the neighborhood of radius δ with center $\mathbf{x}$ (Figure 4). Define the *family* of $\mathbf{x}$ by

$$\mathcal{H} = \big\{ \boldsymbol{\xi} \in (\mathbb{R}^3 \setminus \mathbf{0}) \;\big|\; (\boldsymbol{\xi} + \mathbf{x}) \in (\mathcal{H}_\mathbf{x} \cap \mathcal{B}) \big\}.$$

A vector $\boldsymbol{\xi} \in \mathcal{H}$ is called a *bond* connected to $\mathbf{x}$. $\mathcal{H}$ differs from $\mathcal{H}_\mathbf{x}$ in that the former is centered at $\mathbf{0}$ and contains bonds, while the latter is centered at $\mathbf{x}$ and contains position vectors of material points.

A peridynamic *state* $\underline{\mathsf{A}}\langle\,\cdot\,\rangle$ is a function on $\mathcal{H}$. The angle brackets $\langle\,\cdot\,\rangle$ enclose the bond vector; parentheses and square brackets will be used later to indicated dependencies of the state on other quantities. A state need not be a differentiable or continuous function of the bonds in $\mathcal{H}$.

If the value $\underline{\mathsf{A}}\langle\boldsymbol{\xi}\rangle$ is a scalar, then $\underline{\mathsf{A}}$ is a *scalar state*. The set of all scalar states is denoted $\mathcal{S}$. Two special scalar states are the *zero state* and the

unity state defined respectively by

$$\underline{0}\langle\boldsymbol{\xi}\rangle = 0, \qquad \underline{1}\langle\boldsymbol{\xi}\rangle = 1 \qquad \forall\boldsymbol{\xi} \in \mathcal{H}.$$

If the value of $\underline{\mathsf{A}}\langle\boldsymbol{\xi}\rangle$ is a vector, then $\underline{\mathsf{A}}$ is a *vector state*. The set of all vector states is denoted $\mathcal{V}$. Two special vector states are the *null vector state* and the *identity state* defined by

$$\underline{\mathbf{0}}\langle\boldsymbol{\xi}\rangle = \mathbf{0}, \qquad \underline{\mathbf{X}}\langle\boldsymbol{\xi}\rangle = \boldsymbol{\xi} \qquad \forall\boldsymbol{\xi} \in \mathcal{H} \tag{49}$$

where $\mathbf{0}$ is the null vector.

An example of a scalar state is given by

$$\underline{a}\langle\boldsymbol{\xi}\rangle = 3\mathbf{c}\cdot\boldsymbol{\xi} \qquad \forall\boldsymbol{\xi} \in \mathcal{H},$$

where $\mathbf{c}$ is a constant vector. An example of a vector state is given by

$$\underline{\mathbf{A}}\langle\boldsymbol{\xi}\rangle = \boldsymbol{\xi} + \mathbf{c} \qquad \forall\boldsymbol{\xi} \in \mathcal{H}.$$

Another useful kind of state, called a *double state*, maps pairs of bonds $\boldsymbol{\xi}, \boldsymbol{\zeta} \in \mathcal{H}$ into second order tensors, and is written $\underline{\mathbb{A}}\langle\boldsymbol{\xi}, \boldsymbol{\zeta}\rangle$. The set of all double states is denoted $\mathcal{D}$.

In the following, $\underline{a}$ and $\underline{b}$ are scalar states, $\underline{\mathbf{A}}$ and $\underline{\mathbf{B}}$ are vector states, and $\mathbf{V}$ is a vector. Some elementary operations on states are defined as follows, for any $\boldsymbol{\xi} \in \mathcal{H}$:

$$(\underline{a} + \underline{b})\langle\boldsymbol{\xi}\rangle = \underline{a}\langle\boldsymbol{\xi}\rangle + \underline{b}\langle\boldsymbol{\xi}\rangle, \qquad (\underline{\mathbf{A}} + \underline{\mathbf{B}})\langle\boldsymbol{\xi}\rangle = \underline{\mathbf{A}}\langle\boldsymbol{\xi}\rangle + \underline{\mathbf{B}}\langle\boldsymbol{\xi}\rangle$$

$$(\underline{a}\underline{b})\langle\boldsymbol{\xi}\rangle = \underline{a}\langle\boldsymbol{\xi}\rangle\underline{b}\langle\boldsymbol{\xi}\rangle, \qquad (\underline{a}\underline{\mathbf{B}})\langle\boldsymbol{\xi}\rangle = \underline{a}\langle\boldsymbol{\xi}\rangle\underline{\mathbf{B}}\langle\boldsymbol{\xi}\rangle$$

$$(\underline{\mathbf{A}}\cdot\underline{\mathbf{B}})\langle\boldsymbol{\xi}\rangle = \underline{\mathbf{A}}\langle\boldsymbol{\xi}\rangle\cdot\underline{\mathbf{B}}\langle\boldsymbol{\xi}\rangle, \qquad (\underline{\mathbf{A}}\otimes\underline{\mathbf{B}})\langle\boldsymbol{\xi}\rangle = (\underline{\mathbf{A}}\langle\boldsymbol{\xi}\rangle)\otimes(\underline{\mathbf{B}}\langle\boldsymbol{\xi}\rangle)$$

$$(\underline{\mathbf{A}}\circ\underline{\mathbf{B}})\langle\boldsymbol{\xi}\rangle = \underline{\mathbf{A}}\big\langle\underline{\mathbf{B}}\langle\boldsymbol{\xi}\rangle\big\rangle, \qquad (\underline{\mathbf{A}}\cdot\mathbf{V})\langle\boldsymbol{\xi}\rangle = (\underline{\mathbf{A}}\langle\boldsymbol{\xi}\rangle)\cdot\mathbf{V}$$

where the symbol $\cdot$ indicates the usual scalar product of two vectors in $\mathbb{R}^3$ and $\otimes$ denotes the dyadic (tensor) product of two vectors. Also define a scalar state $|\underline{\mathbf{A}}|$ by

$$|\underline{\mathbf{A}}|\langle\boldsymbol{\xi}\rangle = |\underline{\mathbf{A}}\langle\boldsymbol{\xi}\rangle| \tag{50}$$

and the *dot products*

$$\underline{a}\bullet\underline{b} = \int_{\mathcal{H}} \underline{a}\langle\boldsymbol{\xi}\rangle\underline{b}\langle\boldsymbol{\xi}\rangle\, dV_{\boldsymbol{\xi}}, \qquad \underline{\mathbf{A}}\bullet\underline{\mathbf{B}} = \int_{\mathcal{H}} \underline{\mathbf{A}}\langle\boldsymbol{\xi}\rangle\cdot\underline{\mathbf{B}}\langle\boldsymbol{\xi}\rangle\, dV_{\boldsymbol{\xi}} \tag{51}$$

where, once again, the symbol $\cdot$ denotes the scalar product of two vectors in $\mathbb{R}^3$. The *norm* of a scalar state or a vector state is defined by

$$||\underline{a}|| = \sqrt{\underline{a}\bullet\underline{a}}, \qquad ||\underline{\mathbf{A}}|| = \sqrt{\underline{\mathbf{A}}\bullet\underline{\mathbf{A}}}. \tag{52}$$

Most of the constitutive models in peridynamics involve functions of states, and it is helpful to define a notion of derivatives of such functions. If $\psi(\cdot) : \mathcal{S} \to \mathbb{R}$ is a function of a scalar state, its *Fréchet derivative* $\nabla\psi$, if it exists, is defined by

$$\psi(\underline{A} + \underline{a}) = \psi(\underline{A}) + \nabla\psi(\underline{A}) \bullet \underline{a} + o(||\underline{a}||) \tag{53}$$

for all scalar states $\underline{A}$ and $\underline{a}$. $\nabla\psi$ is a scalar state.

If $\Psi(\cdot) : \mathcal{V} \to \mathbb{R}$ is a function of a vector state, its Fréchet derivative $\nabla\Psi$, if it exists, is similarly defined by

$$\Psi(\mathbf{A} + \mathbf{a}) = \Psi(\mathbf{A}) + \nabla\Psi(\mathbf{A}) \bullet \mathbf{a} + o(||\mathbf{a}||) \tag{54}$$

for all vector states $\mathbf{A}$ and $\mathbf{a}$. $\nabla\Psi$ is a vector state.

For functions of more than one state, for example $\Psi(\underline{\mathbf{A}}, \underline{\mathbf{B}})$, the Fréchet derivatives with respect to the two arguments will be denoted $\Psi_{\underline{\mathbf{A}}}$ and $\Psi_{\underline{\mathbf{B}}}$ respectively. The notation $\partial/\partial\underline{\mathbf{A}}$ denotes the derivative of a function with respect to $\underline{\mathbf{A}}$, if the argument depends either directly or indirectly on $\underline{\mathbf{A}}$. For example, if $f(\cdot) : \mathbb{R} \to \mathbb{R}$, then

$$\frac{\partial}{\partial\underline{\mathbf{A}}} f(\psi(\underline{\mathbf{A}})) = \nabla\phi(\underline{\mathbf{A}}), \qquad \phi(\underline{\mathbf{A}}) := f(\psi(\underline{\mathbf{A}})).$$

In this case, it is easily shown from (53) that the following chain rule applies:

$$\frac{\partial}{\partial\underline{\mathbf{A}}} f(\psi(\underline{\mathbf{A}})) = f'(\psi(\underline{\mathbf{A}}))\nabla\psi(\underline{\mathbf{A}}).$$

where f' denotes the first derivative of f.

The operations on states such as the dot product defined above occur repeatedly in manipulations, but their use does not restrict the physics that can be modeled. Note that $\mathcal{S}$, $\mathcal{V}$, and $\mathcal{D}$ are infinite dimensional linear vector spaces (assuming that $\mathcal{H}$ contains an infinite number of bonds), but this does not preclude the modeling of nonlinear behavior. For example, the discussion of constitutive modeling in Section 4 below deals with nonlinear functions of states.

A *state field* is a state valued function of position in $\mathcal{B}$ and possibly time. These dependencies are written in square brackets:

$$\underline{\mathsf{A}}[\mathbf{x}, t]$$

for any $\mathbf{x} \in \mathcal{H}$ and $t \geq 0$. An example of a scalar state field is given by

$$\underline{a}[\mathbf{x}, t]\langle\boldsymbol{\xi}\rangle = |\boldsymbol{\xi} + \mathbf{x}|t \qquad \forall\boldsymbol{\xi} \in \mathcal{H},\ \mathbf{x} \in \mathcal{B},\ t \geq 0.$$

Finally, the dependence of a state valued function of other quantities is written in parentheses, for example

$$\underline{\mathsf{A}}(\underline{\mathbf{B}}).$$

An example of a state valued function of a vector state is given by

$$\underline{a}(\underline{\mathbf{B}}) = |\underline{\mathbf{B}}|^3,$$

i.e., using the definition (50),

$$\underline{a}(\underline{\mathbf{B}})\langle\boldsymbol{\xi}\rangle = |\underline{\mathbf{B}}\langle\boldsymbol{\xi}\rangle|^3 \qquad \forall\boldsymbol{\xi} \in \mathcal{H},\ \mathbf{x} \in \mathcal{B},\ t \geq 0.$$

A vector state is analogous to a second order tensor in the classical theory, because it maps vectors (bonds) into vectors. However, the mapping performed by a vector state is not necessarily a linear transformation on the bond vectors, *i.e.,* $\underline{\mathbf{A}}\langle\boldsymbol{\xi}\rangle$ is not necessarily a linear function of $\boldsymbol{\xi}$. The additional notation described above is needed because of this nonlinearity and nonlocality.

The mappings defined by states provide the fundamental objects on which constitutive models operate in the nonlocal setting of peridynamics. In the classical theory, a constitutive model for a simple material specifies a tensor (stress) as a function of another tensor (deformation gradient). In the peridynamic theory, a constitutive model instead provides a vector state (called the *force state*) as a function of another vector state (called the *deformation state*). The way this works is discussed in the next section.

4 Constitutive modeling

The discussion in Section 2 introduced the bond force density field $\mathbf{t}$ without specifying how this $\mathbf{t}$ is determined in a particular motion. This determination is provided by the *constitutive model*, also called the *material model*, which contains all information about the response of a particular material. In the peridynamic theory, the constitutive model supplies $\mathbf{t}(\mathbf{x}', \mathbf{x}, t)$ in terms of the deformation at any given time, the history of deformation, and any other physically relevant quantities. This discussion does not include damage, which is the subject of Section 8.

The state that maps bonds connected to $\mathbf{x}$ into their deformed images is called the *deformation state* and denoted $\underline{\mathbf{Y}}[\mathbf{x}, t]$. Angle brackets are used to indicate a bond that this state operates on. For a motion $\mathbf{y}$, at any $t \geq 0$,

$$\underline{\mathbf{Y}}[\mathbf{x}, t]\langle \mathbf{x}' - \mathbf{x} \rangle = \mathbf{y}(\mathbf{x}', t) - \mathbf{y}(\mathbf{x}, t) \tag{55}$$

for any $\mathbf{x} \in \mathcal{B}$ and any $\mathbf{x}' \in \mathcal{B}$ such that $\mathbf{x}' - \mathbf{x} \in \mathcal{H}$ (Figure 5). The values of any $\mathbf{t}(\mathbf{x}', \mathbf{x}, t)$ are given by the *force state* $\underline{\mathbf{T}}$:

$$\mathbf{t}(\mathbf{x}', \mathbf{x}, t) = \underline{\mathbf{T}}[\mathbf{x}, t]\langle \mathbf{x}' - \mathbf{x} \rangle. \tag{56}$$

With this definition, the absorbed power density defined in (42) takes the form

$$p_{\text{abs}} = \underline{\mathbf{T}} \bullet \dot{\underline{\mathbf{Y}}} \tag{57}$$

where the dot product is defined in the previous section. Recall that this absorbed power density is the peridynamic analogue of the stress power $\boldsymbol{\sigma} \cdot \dot{\mathbf{F}}$, where $\boldsymbol{\sigma}$ is the Piola stress tensor and $\mathbf{F} = \partial \mathbf{y} / \partial \mathbf{x}$ is the deformation gradient tensor.

In terms of the force state, the equation of motion (16) has the form

$$\rho(\mathbf{x}) \ddot{\mathbf{y}}(\mathbf{x}, t) = \int_{\mathcal{B}} \left(\underline{\mathbf{T}}[\mathbf{x}, t]\langle \mathbf{x}' - \mathbf{x} \rangle - \underline{\mathbf{T}}[\mathbf{x}', t]\langle \mathbf{x} - \mathbf{x}' \rangle \right) dV_{\mathbf{x}'} + \mathbf{b}(\mathbf{x}, t) \tag{58}$$

for all $\mathbf{x} \in \mathcal{B}$, $t \geq 0$. The equilibrium equation is then

$$\int_{\mathcal{B}} \left(\underline{\mathbf{T}}[\mathbf{x}]\langle \mathbf{x}' - \mathbf{x} \rangle - \underline{\mathbf{T}}[\mathbf{x}']\langle \mathbf{x} - \mathbf{x}' \rangle \right) dV_{\mathbf{x}'} + \mathbf{b}(\mathbf{x}) = \mathbf{0}$$

for all $\mathbf{x} \in \mathcal{B}$.

4.1 Simple materials

The constitutive model determines the force state at any $\mathbf{x}$ and t. For a *simple* material and a homogeneous body, the force state depends only on the deformation state:

$$\underline{\mathbf{T}}[\mathbf{x}, t] = \hat{\underline{\mathbf{T}}}(\underline{\mathbf{Y}}[\mathbf{x}, t])$$

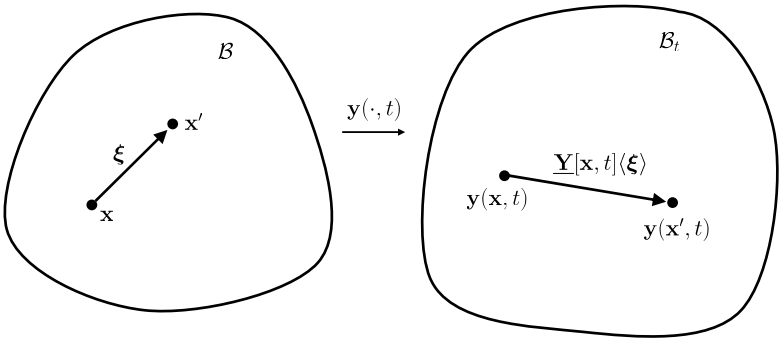

Figure 5: The deformation state $\underline{\mathbf{Y}}[\mathbf{x}, t]$ maps each bond in the family of $\mathbf{x}$ to its deformed image.

where $\underline{\hat{\mathbf{T}}}(\cdot) : \mathcal{V} \to \mathcal{V}$ is a function whose value is a force state. Suppressing from the notation the dependence on $\mathbf{x}$ and t,

$$\underline{\mathbf{T}} = \underline{\hat{\mathbf{T}}}(\underline{\mathbf{Y}}) \tag{59}$$

which is analogous to the Piola stress in a simple material in the classical theory, $\boldsymbol{\sigma} = \hat{\boldsymbol{\sigma}}(\mathbf{F})$. If the body is heterogeneous, an explicit dependence on $\mathbf{x}$ is included:

$$\underline{\mathbf{T}} = \underline{\hat{\mathbf{T}}}(\underline{\mathbf{Y}}, \mathbf{x}).$$

If the material is rate dependent, the constitutive model would additionally depend on the time derivative of the deformation state:

$$\underline{\mathbf{T}} = \underline{\hat{\mathbf{T}}}(\underline{\mathbf{Y}}, \underline{\dot{\mathbf{Y}}}, \mathbf{x}).$$

4.2 Kinematics of deformation states

The deformation state defined in (55) provides a mapping from each bond $\boldsymbol{\xi}$ in the family of $\mathbf{x}$ to its deformed image $\underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle$. It is assumed that at any $t \geq 0$, $\mathbf{y}(\cdot, t)$ is invertible:

$$\mathbf{x}_1 \neq \mathbf{x}_2 \implies \mathbf{y}(\mathbf{x}_1, t) \neq \mathbf{y}(\mathbf{x}_2, t) \qquad \forall \mathbf{x}_1, \mathbf{x}_2 \in \mathcal{B}.$$

This assumption implies

$$\underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle \neq \mathbf{0} \qquad \forall \boldsymbol{\xi} \in \mathcal{H}.$$

Otherwise, there are essentially no kinematical restrictions on $\underline{\mathbf{Y}}$. All of the following are allowed:

- Nondifferentiability (as might occur near an inclusion or a phase boundary).
- Discontinuities (such as a crack).
- Voids and other defects.

However, not all these allowable features would appear, or be capable of appearing, in a given application.

4.3 Directional decomposition of a force state

As discussed in Section 2.3, bond force densities are assumed to be non-polar, as defined in (25). This provides an admissibility condition on the constitutive model. In terms of the force state, the condition for nonpolarity is written as

$$\int_{\mathcal{H}} \underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle \times \underline{\hat{\mathbf{T}}}(\underline{\mathbf{Y}})\langle\boldsymbol{\xi}\rangle \, dV_{\boldsymbol{\xi}} = \mathbf{0} \qquad \forall \underline{\mathbf{Y}} \in \mathcal{V}. \tag{60}$$

This requirement means that the force state at $\mathbf{x}$ exerts no net moment on a small volume surrounding $\mathcal{B} \setminus \mathbf{x}$.

For any deformation state $\underline{\mathbf{Y}}$, define the *direction state* by

$$\underline{\mathbf{M}} = \frac{\underline{\mathbf{Y}}}{|\underline{\mathbf{Y}}|} \tag{61}$$

(see (50) for notation). Using the abbreviation $\underline{\mathbf{T}} = \hat{\underline{\mathbf{T}}}(\underline{\mathbf{Y}})$, define the *collinear* and *orthogonal* parts of the force state by

$$\underline{\mathbf{T}}_{\|} = (\underline{\mathbf{M}} \otimes \underline{\mathbf{M}})\underline{\mathbf{T}}, \qquad \underline{\mathbf{T}}_{\perp} = \underline{\mathbf{T}} - \underline{\mathbf{T}}_{\|}. \tag{62}$$

Thus, for any $\boldsymbol{\xi} \in \mathcal{H}$,

$$\underline{\mathbf{T}}_{\|}\langle\boldsymbol{\xi}\rangle = (\underline{\mathbf{M}}\langle\boldsymbol{\xi}\rangle \cdot \underline{\mathbf{T}}\langle\boldsymbol{\xi}\rangle)\underline{\mathbf{M}}\langle\boldsymbol{\xi}\rangle \tag{63}$$

which is parallel to the deformed bond. Similarly, $\underline{\mathbf{T}}_{\perp}\langle\boldsymbol{\xi}\rangle$ is orthogonal to the deformed bond. From (61) and (63),

$$\int_{\mathcal{H}} \underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle \times \underline{\mathbf{T}}_{\|}\langle\boldsymbol{\xi}\rangle \, dV_{\boldsymbol{\xi}} = \mathbf{0}$$

regardless of constitutive model. From this and the second of (62), the condition for nonpolarity (60) is equivalent to

$$\int_{\mathcal{H}} \underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle \times \underline{\mathbf{T}}_{\perp}\langle\boldsymbol{\xi}\rangle \, dV_{\boldsymbol{\xi}} = \mathbf{0}.$$

The constitutive model $\hat{\underline{\mathbf{T}}}$ is called *ordinary* if, for all $\underline{\mathbf{Y}} \in \mathcal{V}$,

$$\underline{\mathbf{T}}_{\|} = \underline{\mathbf{T}} \tag{64}$$

where $\underline{\mathbf{T}} = \hat{\underline{\mathbf{T}}}(\underline{\mathbf{Y}})$. Otherwise, the constitutive model is *nonordinary*. From (60) and (64), evidently all ordinary constitutive models are nonpolar. (The converse of this is not true.)

4.4 Examples

An example of a simple peridynamic material model is given by

$$\hat{\underline{\mathbf{T}}}(\underline{\mathbf{Y}}) = a\big(|\underline{\mathbf{Y}}| - |\underline{\mathbf{X}}|\big)\underline{\mathbf{M}}, \qquad \underline{\mathbf{M}} = \frac{\underline{\mathbf{Y}}}{|\underline{\mathbf{Y}}|} \qquad \forall \underline{\mathbf{Y}} \in \mathcal{V},$$

where a is a constant. Writing this out in detail,

$$\underline{\mathbf{T}}\langle\boldsymbol{\xi}\rangle = a\big(|\underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle| - |\boldsymbol{\xi}|\big)\frac{\underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle}{|\underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle|} \qquad \forall \underline{\mathbf{Y}} \in \mathcal{V},$$

for any bond $\boldsymbol{\xi} \in \mathcal{H}$. In this material, the magnitude of the bond force density vector $\mathbf{t}$ is proportional to the bond extension (change in length of the bond). The direction is parallel to the deformed bond. In this example, the bonds respond independently of each other: $\underline{\mathbf{T}}\langle\boldsymbol{\xi}\rangle$ depends only on $\underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle$. Materials with this property are called *bond-based* and are discussed in Section 4.7.

A much larger class of materials incorporates the *collective* response of bonds. This means that the force density in each bond depends not only on its own deformation, but also on the deformation of other bonds. A simple example is given by

$$\underline{\mathbf{T}}\langle\boldsymbol{\xi}\rangle = a\big(|\underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle| - |\underline{\mathbf{Y}}\langle -\boldsymbol{\xi}\rangle|\big)\underline{\mathbf{M}}\langle\boldsymbol{\xi}\rangle.$$

In this material, the bond force density for any bond $\boldsymbol{\xi}$ is proportional to the difference in deformed length between itself and the bond opposite to $\boldsymbol{\xi}$. (Note that in general $\underline{\mathbf{Y}}\langle -\boldsymbol{\xi}\rangle \neq -\underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle$, since the two bonds $\boldsymbol{\xi}$ and $-\boldsymbol{\xi}$ can deform independently of each other.) This material is an example of a *bond-pair* model, discussed in Section 4.12.

The mean elongation of all the bonds in a family is defined by

$$\bar{e} = \frac{1}{V_{\mathcal{H}}}\int_{\mathcal{H}} \left(|\underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle| - |\boldsymbol{\xi}|\right) dV_{\boldsymbol{\xi}}, \qquad V_{\mathcal{H}} = \int_{\mathcal{H}} dV.$$

A material model in which the magnitudes of forces in the bonds are identical to each other and depend only on the mean elongation is provided by

$$\underline{\mathbf{T}} = a\bar{e}\underline{\mathbf{M}}.$$

In Section 4.10, the mean elongation in the bonds (weighted by scalar state) is used to define a nonlocal volume change. This provides a way to characterize an isotropic solid using the conventional bulk modulus and shear modulus.

4.5 Thermodynamic restrictions on constitutive models

In this section it is shown that the force state can be related to a free energy function, which is subject to certain restrictions due to the second law of thermodynamics. The first law of thermodynamics asserts the equivalence of mechanical energy and heat energy. At any point $\mathbf{x} \in \mathcal{B}$, the local form of the first law (41) with the absorbed power density given by (57) takes the form

$$\dot{\varepsilon} = \underline{\mathbf{T}} \bullet \underline{\dot{\mathbf{Y}}} + h + r \tag{65}$$

where ε is the internal energy density, h is the rate of heat transfer due to interaction with other points in $\mathcal{B}$, and r is a prescribed source rate (all these quantities are per unit volume in the reference configuration).

The second law of thermodynamics is expressed by the Clausius-Duhem inequality:

$$\theta\dot{\eta} \geq r + h \tag{66}$$

where θ is the absolute temperature and η is the entropy density. Now define the free energy density by

$$\psi = \varepsilon - \theta\eta. \tag{67}$$

Following Coleman and Noll [15], certain restrictions on the constitutive response will now be derived. Taking the time derivative of (67) leads to

$$\dot{\psi} = \dot{\varepsilon} - \dot{\theta}\eta - \theta\dot{\eta}.$$

From this and (65), it follows that

$$\dot{\psi} = \underline{\mathbf{T}} \bullet \underline{\dot{\mathbf{Y}}} + h + r - \dot{\theta}\eta - \theta\dot{\eta}. \tag{68}$$

Combining this expression with (66), the variables ε, $\dot{\eta}$, and r are eliminated to yield

$$\underline{\mathbf{T}} \bullet \underline{\dot{\mathbf{Y}}} - \dot{\theta}\eta - \dot{\psi} \geq 0. \tag{69}$$

Now assume that ψ and η have the following dependencies:

$$\psi = \psi(\underline{\mathbf{Y}}, \underline{\dot{\mathbf{Y}}}, \theta), \qquad \eta = \eta(\underline{\mathbf{Y}}, \underline{\dot{\mathbf{Y}}}, \theta),$$

hence $\dot{\psi}$ involves the Fréchet derivatives of ψ with respect to $\underline{\mathbf{Y}}$ and $\underline{\dot{\mathbf{Y}}}$, which are denoted $\psi_{\underline{\mathbf{Y}}}$ and $\psi_{\underline{\dot{\mathbf{Y}}}}$ respectively:

$$\dot{\psi} = \psi_{\underline{\mathbf{Y}}} \bullet \underline{\dot{\mathbf{Y}}} + \psi_{\underline{\dot{\mathbf{Y}}}} \bullet \underline{\ddot{\mathbf{Y}}} + \psi_\theta \dot{\theta},$$

with a similar expression for $\dot{\eta}$. Combining these with (69) leads to

$$\Big(\underline{\mathbf{T}} - \psi_{\underline{\mathbf{Y}}}\Big) \bullet \underline{\dot{\mathbf{Y}}} - \psi_{\underline{\dot{\mathbf{Y}}}} \bullet \underline{\ddot{\mathbf{Y}}} - \Big(\psi_\theta + \eta\Big)\dot{\theta} \geq 0. \tag{70}$$

The method of Coleman and Noll assumes that, in the present case of peridynamics, the quantities $\underline{\dot{\mathbf{Y}}}$, $\underline{\ddot{\mathbf{Y}}}$, and $\dot{\theta}$ can, in principle, be varied independently. The inequality (70) must hold for all such choices. This results in the following conclusions:

$$\eta = -\psi_\theta, \qquad \psi_{\underline{\dot{\mathbf{Y}}}} = \mathbf{0}.$$

The first of these is a standard relation in thermodynamics. The second states that the free energy is independent of $\underline{\dot{\mathbf{Y}}}$. Next, following Fried's development [29] for the thermodynamics of discrete particles, decompose the force state into parts that are independent of and dependent on $\underline{\dot{\mathbf{Y}}}$ respectively:

$$\underline{\mathbf{T}}(\underline{\mathbf{Y}}, \underline{\dot{\mathbf{Y}}}, \theta) = \underline{\mathbf{T}}^e(\underline{\mathbf{Y}}, \theta) + \underline{\mathbf{T}}^d(\underline{\mathbf{Y}}, \underline{\dot{\mathbf{Y}}}, \theta) \tag{71}$$

where the superscript e stands for "equilibrium" and d stands for "dissipative." Then, setting $\dot{\theta} = 0$ and $\ddot{\underline{\mathbf{Y}}} = \underline{\mathbf{0}}$ in (70) and using (71),

$$\left(\underline{\mathbf{T}}^e(\underline{\mathbf{Y}}, \theta) - \psi_{\underline{\mathbf{Y}}}(\underline{\mathbf{Y}}, \theta)\right) \bullet \dot{\underline{\mathbf{Y}}} + \underline{\mathbf{T}}^d(\underline{\mathbf{Y}}, \dot{\underline{\mathbf{Y}}}, \theta) \bullet \dot{\underline{\mathbf{Y}}} \geq 0$$

where the terms that are independent of $\dot{\underline{\mathbf{Y}}}$ have been grouped together. The conclusions are therefore

$$\underline{\mathbf{T}}^e(\underline{\mathbf{Y}}, \theta) = \psi_{\underline{\mathbf{Y}}}(\underline{\mathbf{Y}}, \theta) \tag{72}$$

and

$$\underline{\mathbf{T}}^d(\underline{\mathbf{Y}}, \dot{\underline{\mathbf{Y}}}, \theta) \bullet \dot{\underline{\mathbf{Y}}} \geq 0. \tag{73}$$

Equation (73) is the dissipation inequality for rate-dependent materials in peridynamics, and it must hold for all choices of $\dot{\underline{\mathbf{Y}}}$. It states that the rate-dependent part of the constitutive model must dissipate energy at a nonnegative rate. Interestingly, (73) does *not* imply that

$$\underline{\mathbf{T}}^d\langle\boldsymbol{\xi}\rangle \cdot \dot{\underline{\mathbf{Y}}}\langle\boldsymbol{\xi}\rangle \geq 0 \qquad \forall \boldsymbol{\xi} \in \mathcal{H}.$$

In other words, there can be some bonds that "generate energy" provided there are other bonds that dissipate at least this much energy. A version of the dissipation inequality for materials undergoing damage will be discussed in Section 8.2.

4.6 Elastic materials

If the free energy density depends only on $\underline{\mathbf{Y}}$, the material is called *elastic*, and by convention the free energy density is called the *strain energy density* and denoted $W = \hat{W}(\underline{\mathbf{Y}})$. Then by (72),

$$\dot{W} = \underline{\mathbf{T}} \bullet \dot{\underline{\mathbf{Y}}} \tag{74}$$

for any $\underline{\mathbf{Y}}$ and

$$\hat{\underline{\mathbf{T}}} = \hat{W}_{\underline{\mathbf{Y}}}.$$

Since $\hat{W}$ is a function of only one variable, this can also be written as

$$\hat{\underline{\mathbf{T}}} = \nabla \hat{W}. \tag{75}$$

For a body composed of an elastic material (not necessarily homogeneous), by setting $\mathbf{w} = \dot{\mathbf{y}}$ in the principle of virtual work expression (17) and using (56) and (74), it follows that for an elastic material,

$$\frac{d}{dt}\int_{\mathcal{B}} \frac{\rho \dot{\mathbf{y}} \cdot \dot{\mathbf{y}}}{2}\, dV + \frac{d}{dt}\int_{\mathcal{B}} W\, dV = \int_{\mathcal{B}} \mathbf{b} \cdot \dot{\mathbf{y}}\, dV.$$

Thus, as in the classical theory, work performed on an elastic peridynamic body by external loads is converted into a combination of kinetic energy and recoverable strain energy.

A mechanical interpretation of the Fréchet derivative of $\hat{W}$ in an elastic material is as follows. Suppose the family is deformed, then held fixed. Choose a single bond $\boldsymbol{\xi}$, surrounded by a small volume dV. While continuing to hold all other bonds fixed, increment the position of the small volume by a small vector ϵ. If the material is elastic, then there is a vector $\mathbf{t}$, independent of ϵ, such that the resulting change in W is given by

$$dW = \mathbf{t} \cdot \epsilon \, dV.$$

The value of this vector is $\mathbf{t} = \underline{\mathbf{T}}\langle\boldsymbol{\xi}\rangle$. An elastic material model can be either ordinary or nonordinary: elasticity does not require that $\underline{\mathbf{T}}\langle\boldsymbol{\xi}\rangle \parallel \underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle$.

4.7 Bond-based materials

Suppose that each bond has its own constitutive relation, independent of the others. Then there is a function $\hat{\mathbf{t}}(\cdot,\cdot)$ on $\mathbb{R}^3 \times \mathcal{H}$ such that

$$\underline{\mathbf{T}}\langle\boldsymbol{\xi}\rangle = \hat{\mathbf{t}}(\underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle, \boldsymbol{\xi}) \tag{76}$$

for all $\underline{\mathbf{Y}} \in \mathcal{V}$ and all $\boldsymbol{\xi} \in \mathcal{H}$. Such a material model is called *bond-based*.

The requirement of nonpolarity (60) implies that any bond-based material model is ordinary. To see this, suppose that it is nonordinary. Then, by definition, there is some deformation state $\underline{\mathbf{Y}}_0$ and some bond $\boldsymbol{\xi}_0$ such that

$$\mathbf{c} := \underline{\mathbf{Y}}_0\langle\boldsymbol{\xi}_0\rangle \times \mathbf{t}_0 \neq \mathbf{0}, \qquad \mathbf{t}_0 = \hat{\mathbf{t}}(\underline{\mathbf{Y}}_0\langle\boldsymbol{\xi}_0\rangle, \boldsymbol{\xi}_0).$$

Start with this $\underline{\mathbf{Y}}_0$ and let all other bonds except $\boldsymbol{\xi}_0$ be held fixed while $\boldsymbol{\xi}_0$ is further deformed. (Strictly speaking, we are deforming the material point $\mathbf{x} + \boldsymbol{\xi}_0$, while holding all other material points fixed, where $\mathbf{x}$ is the point whose constitutive model is under consideration.) Because (60) must continue to hold during this process, any choice of $\underline{\mathbf{Y}}\langle\boldsymbol{\xi}_0\rangle$ leaves $\underline{\mathbf{Y}}\langle\boldsymbol{\xi}_0\rangle \times \hat{\mathbf{t}}(\underline{\mathbf{Y}}\langle\boldsymbol{\xi}_0\rangle, \boldsymbol{\xi}_0)$ unchanged, *i.e.*,

$$\mathbf{z} \times \hat{\mathbf{t}}(\mathbf{z}, \boldsymbol{\xi}_0) = \mathbf{c} \tag{77}$$

for any vector $\mathbf{z} = \underline{\mathbf{Y}}\langle\boldsymbol{\xi}_0\rangle$. One such choice is

$$\mathbf{z} = \alpha\mathbf{c}$$

where α is a nonzero scalar with the appropriate dimensions for this expression to make sense. Then by (77),

$$\alpha\mathbf{c} \times \hat{\mathbf{t}}(\alpha\mathbf{z}, \boldsymbol{\xi}_0) = \mathbf{c}.$$

This can only hold if $\mathbf{c} = \mathbf{0}$, proving that the material model is ordinary.[3]

In an *elastic* bond-based body, there is a scalar-valued function $\hat{w}(\mathbf{p}, \boldsymbol{\xi})$ called the *bond potential*, where $\mathbf{p}$ is a vector, such that

$$\hat{W}(\underline{\mathbf{Y}}) = \int_{\mathcal{H}} \hat{w}(\underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle, \boldsymbol{\xi})\, dV_{\boldsymbol{\xi}}, \qquad \hat{\mathbf{t}}(\underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle, \boldsymbol{\xi}) = \hat{w}_{\mathbf{p}}(\underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle, \boldsymbol{\xi}). \tag{78}$$

Note that the first argument of $\hat{w}$ in this integrand is a *vector*, not a vector state. $\hat{w}_{\mathbf{p}}$ denotes the partial derivative with respect to this argument.

Recall the result proved above that any bond-based material model is ordinary. An implication of this result for elastic bond-based materials is that $\hat{w}(\mathbf{p}, \boldsymbol{\xi})$ can depend on $\mathbf{p}$ only through $|\mathbf{p}|$, *i.e.*, through the deformed length of the bond. To confirm this, choose a deformed bond vector $\mathbf{p}$ and consider a rotation of this vector at some angular velocity $\boldsymbol{\omega}$. Then $d\mathbf{p}/dt = \boldsymbol{\omega} \times \mathbf{p}$. Therefore

$$\frac{d}{dt}\hat{w}(\mathbf{p}, \boldsymbol{\xi}) = \hat{w}_{\mathbf{p}}(\mathbf{p}, \boldsymbol{\xi}) \cdot \frac{d\mathbf{p}}{dt} = \hat{w}_{\mathbf{p}}(\mathbf{p}, \boldsymbol{\xi}) \cdot (\boldsymbol{\omega} \times \mathbf{p}).$$

Since the material is ordinary, there is some scalar β, with appropriate dimensions, such that

$$\hat{w}_{\mathbf{p}}(\mathbf{p}, \boldsymbol{\xi}) = \beta \mathbf{p}.$$

Combining the last two equations,

$$\frac{d}{dt}\hat{w}(\mathbf{p}, \boldsymbol{\xi}) = \beta \mathbf{p} \cdot (\boldsymbol{\omega} \times \mathbf{p}).$$

Since, for any vector $\boldsymbol{\omega}$, $\mathbf{p} \perp (\boldsymbol{\omega} \times \mathbf{p})$, it follows that

$$\frac{d}{dt}\hat{w}(\mathbf{p}, \boldsymbol{\xi}) = 0.$$

This proves that $\hat{w}(\mathbf{p}, \boldsymbol{\xi})$ is unchanged by a rigid rotation of $\mathbf{p}$; therefore, $\hat{w}$ depends on $\mathbf{p}$ only through $|\mathbf{p}|$. So, we can write, for an elastic bond-based material model,

$$\hat{w}(\mathbf{p}, \boldsymbol{\xi}) = w(e, \boldsymbol{\xi}), \qquad e = |\mathbf{p}| - |\boldsymbol{\xi}|$$

for some function w. Then, by the first of (78),

$$\hat{W}(\underline{\mathbf{Y}}) = \int_{\mathcal{H}} w(\underline{e}\langle\boldsymbol{\xi}\rangle, \boldsymbol{\xi})\, dV_{\boldsymbol{\xi}},$$

[3] The discussion of this result in [60] is flawed because it treats only pairs of material points in isolation from all other material points, neglecting the possibility that these other points could somehow cancel out a couple between the pair.

where $\underline{e}$ is the scalar extension state, defined by

$$\underline{e} = |\underline{\mathbf{Y}}| - |\underline{\mathbf{X}}| \qquad \text{or} \qquad \underline{e}\langle\boldsymbol{\xi}\rangle = |\underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle| - |\boldsymbol{\xi}| \quad \forall \boldsymbol{\xi} \in \mathcal{H}.$$

Let the partial derivative of $w(e, \boldsymbol{\xi})$ with respect to e be denoted $w_e(e, \boldsymbol{\xi})$. By the second of (78) and the chain rule,

$$\hat{\mathbf{t}}(\underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle, \boldsymbol{\xi}) = w_e(\underline{e}\langle\boldsymbol{\xi}\rangle, \boldsymbol{\xi})\mathbf{M}, \qquad \mathbf{M} = \frac{\underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle}{|\underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle|}. \tag{79}$$

If the body is homogeneous and composed of bond-based material, it is sometimes convenient to consider each bond as the fundamental object for purposes of constitutive modeling: set

$$W(\mathbf{x}) = \frac{1}{2}\int_{\mathcal{H}_\mathbf{x}} \breve{w}\big(e, \mathbf{x}', \mathbf{x}\big)\, dV_{\mathbf{x}'}, \qquad e = |\mathbf{y}(\mathbf{x}') - \mathbf{y}(\mathbf{x})| - |\mathbf{x}' - \mathbf{x}|$$

where $\mathcal{H}_\mathbf{x}$ is the neighborhood of $\mathbf{x}$ with radius equal to the horizon, and

$$\breve{w}(e, \mathbf{x}', \mathbf{x}) = 2w(e, \mathbf{x}' - \mathbf{x}).$$

This change allows the resulting "bond-based theory" to be developed without using the formalism of states. The bond-based theory is the subject of [60], in which $\breve{w}$ is called the *micropotential* and the material model is called *microelastic*. Because the bond-based theory was developed earlier than the state-based theory, and because its constitutive models do not require the additional complexity of Fréchet derivatives, the vast majority of applications of peridynamics have been performed within the bond-based theory. However, as noted in Section 1.2, the bond-based theory suffers from severe limitations on the material response it can reproduce, notably the restriction on the Poisson ratio $\nu = 1/4$ for isotropic microelastic solids. It is demonstrated in Section 4.10 below that this restriction is removed in the state-based theory.

4.8 Objectivity

As in the classical theory, invariance of a strain energy density function in the peridynamic theory with respect to rigid rotation following a deformation leads to a notion of material frame indifference, or *objectivity*. Let $\mathcal{O}^+$ denote the set of all proper orthogonal tensors. For any $\mathbf{Q} \in \mathcal{O}^+$ and any $\underline{\mathbf{A}} \in \mathcal{V}$, let $\mathbf{Q}\underline{\mathbf{A}}$ be the vector state defined by

$$(\mathbf{Q}\underline{\mathbf{A}})\langle\boldsymbol{\xi}\rangle = \mathbf{Q}(\underline{\mathbf{A}}\langle\boldsymbol{\xi}\rangle) \qquad \forall \boldsymbol{\xi} \in \mathcal{H}$$

and similarly define the state $\underline{\mathbf{A}}\mathbf{Q}$ by

$$(\underline{\mathbf{A}}\mathbf{Q})\langle\boldsymbol{\xi}\rangle = \underline{\mathbf{A}}\langle\mathbf{Q}\boldsymbol{\xi}\rangle \qquad \forall \boldsymbol{\xi} \in \mathcal{H}.$$

Consider an elastic material such that

$$\hat{W}(\mathbf{Q}\underline{\mathbf{Y}}) = \hat{W}(\underline{\mathbf{Y}}) \qquad \forall \mathbf{Q} \in \mathcal{O}^+,\ \underline{\mathbf{Y}} \in \mathcal{V}. \tag{80}$$

Let $\mathbf{Q}$ be fixed. Consider any $\underline{\mathbf{Y}} \in \mathcal{V}$ and a small increment $\delta\underline{\mathbf{Y}} \in \mathcal{V}$. From (54), (75), and (80), neglecting terms of higher order than $\delta\underline{\mathbf{Y}}$,

$$\underline{\hat{\mathbf{T}}}(\mathbf{Q}\underline{\mathbf{Y}}) \bullet \delta(\mathbf{Q}\underline{\mathbf{Y}}) = \underline{\hat{\mathbf{T}}}(\underline{\mathbf{Y}}) \bullet \delta\underline{\mathbf{Y}}.$$

Since $\underline{\mathbf{T}}$ is vector valued, by the properties of the transpose of a tensor,

$$\big(\mathbf{Q}^T\underline{\hat{\mathbf{T}}}(\mathbf{Q}\underline{\mathbf{Y}})\big) \bullet \delta\underline{\mathbf{Y}} = \underline{\hat{\mathbf{T}}}(\underline{\mathbf{Y}}) \bullet \delta\underline{\mathbf{Y}}.$$

Since this must hold for every small $\delta\underline{\mathbf{Y}}$, and since $\mathbf{Q}^T = \mathbf{Q}^{-1}$, it follows that (80) implies

$$\underline{\hat{\mathbf{T}}}(\mathbf{Q}\underline{\mathbf{Y}}) = \mathbf{Q}\underline{\hat{\mathbf{T}}}(\underline{\mathbf{Y}}) \qquad \forall \mathbf{Q} \in \mathcal{O}^+,\ \underline{\mathbf{Y}} \in \mathcal{V}. \tag{81}$$

Any simple material model, whether elastic or not, that satisfies (81) is called *objective*. Objectivity can be assumed as an admissibility requirement for any material model in the absence of some externally dictated special direction in space, such as an electric field. It is easily shown [63] that an objective elastic material necessarily satisfies the condition for nonpolarity (60).

4.9 Isotropy

Consider an elastic material model with the property that

$$\hat{W}(\underline{\mathbf{Y}}\mathbf{Q}) = \hat{W}(\underline{\mathbf{Y}}) \qquad \forall \mathbf{Q} \in \mathcal{O}^+,\ \underline{\mathbf{Y}} \in \mathcal{V}. \tag{82}$$

Proceeding as in the previous section, choose any $\mathbf{Q} \in \mathcal{O}^+$ and any $\underline{\mathbf{Y}} \in \mathcal{V}$, then consider a small increment $\delta\underline{\mathbf{Y}} \in \mathcal{V}$. From (54), (75), and (82),

$$\begin{aligned}
\underline{\hat{\mathbf{T}}}(\underline{\mathbf{Y}}) \bullet \delta\underline{\mathbf{Y}} &= \underline{\hat{\mathbf{T}}}(\underline{\mathbf{Y}}\mathbf{Q}) \bullet \delta(\underline{\mathbf{Y}}\mathbf{Q}) \\
&= \int_{\mathcal{H}} \underline{\hat{\mathbf{T}}}(\underline{\mathbf{Y}}\mathbf{Q})\langle\boldsymbol{\xi}\rangle \cdot \delta\underline{\mathbf{Y}}\langle\mathbf{Q}\boldsymbol{\xi}\rangle \, dV_{\boldsymbol{\xi}} \\
&= \int_{\mathcal{H}} \underline{\hat{\mathbf{T}}}(\underline{\mathbf{Y}}\mathbf{Q})\langle\mathbf{Q}^{-1}\boldsymbol{\xi}'\rangle \cdot \delta\underline{\mathbf{Y}}\langle\boldsymbol{\xi}'\rangle \, dV_{\boldsymbol{\xi}'} \\
&= \big(\underline{\hat{\mathbf{T}}}(\underline{\mathbf{Y}}\mathbf{Q})\mathbf{Q}^{-1}\big) \bullet \delta\underline{\mathbf{Y}}
\end{aligned}$$

where the change of variable $\boldsymbol{\xi}' = \mathbf{Q}\boldsymbol{\xi}$ has been used. Since this result must hold for every $\delta\underline{\mathbf{Y}}$, it follows that (82) implies

$$\underline{\hat{\mathbf{T}}}(\underline{\mathbf{Y}}\mathbf{Q}) = \underline{\hat{\mathbf{T}}}(\underline{\mathbf{Y}})\mathbf{Q} \qquad \forall \mathbf{Q} \in \mathcal{O}^+,\ \underline{\mathbf{Y}} \in \mathcal{V}. \tag{83}$$

Any material model, whether elastic or not, satisfying (83) is called *isotropic*. If the material model is isotropic, then the force state is invariant with respect to pre-rotations applied before the stretch.

4.10 Isotropic elastic solid

A peridynamic material model for a constitutively linear isotropic elastic solid was proposed in Section 15 of [67]. A nonlocal dilatation is defined by

$$\vartheta = \frac{3}{m}(\underline{\omega}\underline{x}) \bullet \underline{e}, \qquad m = (\underline{\omega}\underline{x}) \bullet \underline{x} \tag{84}$$

where $\underline{\omega}$ is the scalar *influence state*, which serves as a weighting function, and the scalar *extension state* is defined by

$$\underline{e} = |\underline{\mathbf{Y}}| - \underline{x}, \qquad \underline{x} = |\underline{\mathbf{X}}|.$$

It can be shown [67] that for any choice of $\underline{\omega}$, if the deformation is small and homogeneous, ϑ defined in (84) equals the trace of the classical linear strain tensor. (The coefficient $3/m$ in (84) is chosen so that this is true.)

Define an elastic material in which the strain energy density contains two terms representing the contribution of the volume change and of everything else in the deformation state, respectively:

$$\hat{W}(\underline{\mathbf{Y}}) = \frac{k\vartheta^2}{2} + \frac{\alpha}{2}(\underline{\omega}\underline{e}^{\mathrm{d}}) \bullet \underline{e}^{\mathrm{d}} \tag{85}$$

where k and α are constants and

$$\underline{e}^{\mathrm{d}} := \underline{e} - \underline{e}^{\mathrm{i}}, \qquad \underline{e}^{\mathrm{i}} := \frac{\vartheta \underline{x}}{3}.$$

The scalar state $\underline{e}^{\mathrm{i}}$ is called the *isotropic part* of the extension state, and $\underline{e}^{\mathrm{d}}$ is called the *deviatoric part*. The isotropic part contains length changes of bonds due to isotropic expansion of the family. The deviatoric part contains the remainder of the length changes, which may be due to shear or to other types of deformation within the family. After evaluating the applicable Fréchet derivatives [67], the force state is given by

$$\underline{\hat{\mathbf{T}}}(\underline{\mathbf{Y}}) = \left(\frac{3k\vartheta}{m} \underline{\omega}\underline{x} + \alpha \underline{\omega}\underline{e}^{\mathrm{d}} \right) \underline{\mathbf{M}}, \qquad \underline{\mathbf{M}} = \frac{\underline{\mathbf{Y}}}{|\underline{\mathbf{Y}}|}.$$

Since the bond force densities are parallel to the deformed bonds, this is an ordinary material model. This material model is constitutively linear in the sense that the force state depends linearly on the extension state. However, it does not assume linear kinematics as will be assumed in the linearized peridynamic theory discussed below in Section 5. For small, homogeneous deformations, the strain energy density in the peridynamic material model (85) equals that of an isotropic linear elastic solid in the *classical* theory provided k is the bulk modulus for the material and $\alpha = 15\mu/m$, where μ is the shear modulus [67].

4.11 Peridynamic material derived from a classical material

Suppose a material model from the classical theory is given in the following form:

$$\boldsymbol{\sigma} = \hat{\boldsymbol{\sigma}}(\mathbf{F}), \qquad \mathbf{F} = \frac{\partial \mathbf{y}}{\partial \mathbf{x}}$$

where $\boldsymbol{\sigma}$ is the Piola stress tensor, $\hat{\boldsymbol{\sigma}}$ is a function, and $\mathbf{F}$ is the deformation gradient tensor. A peridynamic material model can be derived from this as follows [67, 74, 27]. (An alternative approach making use of the principle of virtual work can also be used [51].) A nonlocal approximation to the deformation gradient tensor is defined by

$$\bar{\mathbf{F}} = \left(\int_{\mathcal{H}} \underline{\omega}\langle \boldsymbol{\xi} \rangle \underline{\mathbf{Y}}\langle \boldsymbol{\xi} \rangle \otimes \boldsymbol{\xi} \, dV_{\boldsymbol{\xi}} \right) \mathbf{K}^{-1}$$

where $\underline{\omega}$ is the scalar influence state and $\mathbf{K}$ is the symmetric positive definite *shape tensor* defined by

$$\mathbf{K} = \int_{\mathcal{H}} \underline{\omega}\langle \boldsymbol{\xi} \rangle \boldsymbol{\xi} \otimes \boldsymbol{\xi} \, dV_{\boldsymbol{\xi}}.$$

The force state is determined by mapping the resulting $\boldsymbol{\sigma}$ back onto the bonds as follows:

$$\hat{\underline{\mathbf{T}}}(\underline{\mathbf{Y}}) = \underline{\omega} \hat{\boldsymbol{\sigma}}(\bar{\mathbf{F}}) \mathbf{K}^{-1} \underline{\mathbf{X}}.$$

The peridynamic stress tensor (see Section 6.2) corresponding to this peridynamic material model equals $\hat{\boldsymbol{\sigma}}(\underline{\mathbf{F}})$ in the special case of homogeneous deformation of a homogeneous body.

4.12 Bond-pair materials

Let w be a scalar-valued function of four vectors:

$$w(\mathbf{p}, \mathbf{q}, \mathbf{r}, \mathbf{s})$$

with partial derivatives with respect to the first two arguments denoted by

$$w_{\mathbf{p}}(\mathbf{p}, \mathbf{q}, \mathbf{r}, \mathbf{s}), \qquad w_{\mathbf{q}}(\mathbf{p}, \mathbf{q}, \mathbf{r}, \mathbf{s}).$$

Suppose an elastic material has its strain energy density function given by

$$\hat{W}(\underline{\mathbf{Y}}) = \int_{\mathcal{H}} w(\underline{\mathbf{Y}}\langle \boldsymbol{\xi} \rangle, \underline{\mathbf{Y}}\langle \boldsymbol{\chi}(\boldsymbol{\xi}) \rangle, \boldsymbol{\xi}, \boldsymbol{\chi}(\boldsymbol{\xi})) \, dV_{\boldsymbol{\xi}} \tag{86}$$

where $\boldsymbol{\chi}(\cdot) : \mathcal{H} \to \mathcal{H}$ is a continuously differentiable and invertible function. (Note that the four arguments of w in the integrand are *vectors*, not *vector*

states, because $\underline{\mathbf{Y}}$ is evaluated at the specific bonds $\boldsymbol{\xi}$ and $\boldsymbol{\chi}(\boldsymbol{\xi})$.) Let $\boldsymbol{\chi}^{-1}$ be the inverse mapping of $\boldsymbol{\chi}$:

$$\boldsymbol{\zeta} = \boldsymbol{\chi}(\boldsymbol{\xi}) \qquad \Longleftrightarrow \qquad \boldsymbol{\xi} = \boldsymbol{\chi}^{-1}(\boldsymbol{\zeta}).$$

Let the Jacobian determinants of the forward and inverse mappings be defined by

$$J(\boldsymbol{\xi}) = \Big|\det \operatorname{grad} \boldsymbol{\chi}(\boldsymbol{\xi})\Big|, \qquad J^{-1}(\boldsymbol{\zeta}) = \Big|\det \operatorname{grad} \boldsymbol{\chi}^{-1}(\boldsymbol{\zeta})\Big|.$$

Mechanically, the $\hat{W}$ defined in (86) sums up energies due to interactions between pairs of bonds $\boldsymbol{\xi}$ and $\boldsymbol{\chi}(\boldsymbol{\xi})$. Such a material is called a *bond-pair material* (Figure 6).

To determine the associated force state, the Fréchet derivative of this $\hat{W}$ is evaluated as follows. Consider an increment in the deformation state $\delta\underline{\mathbf{Y}}$. Then, from (86),

$$\delta\hat{W} = \int_{\mathcal{H}} \Big[w_{\mathbf{p}}\big(\underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle, \underline{\mathbf{Y}}\langle\boldsymbol{\chi}(\boldsymbol{\xi})\rangle, \boldsymbol{\xi}, \boldsymbol{\chi}(\boldsymbol{\xi})\big) \cdot \delta\underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle + w_{\mathbf{q}}\big(\underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle, \underline{\mathbf{Y}}\langle\boldsymbol{\chi}(\boldsymbol{\xi})\rangle, \boldsymbol{\xi}, \boldsymbol{\chi}(\boldsymbol{\xi})\big) \cdot \delta\underline{\mathbf{Y}}\langle\boldsymbol{\chi}(\boldsymbol{\xi})\rangle \Big] \, dV_{\boldsymbol{\xi}}.$$

Now use the change of variables $\boldsymbol{\zeta} = \boldsymbol{\chi}(\boldsymbol{\xi})$ in the $w_{\mathbf{q}}$ term to obtain

$$\delta\hat{W} = \int_{\mathcal{H}} w_{\mathbf{p}}\big(\underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle, \underline{\mathbf{Y}}\langle\boldsymbol{\chi}(\boldsymbol{\xi})\rangle, \boldsymbol{\xi}, \boldsymbol{\chi}(\boldsymbol{\xi})\big) \cdot \delta\underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle \, dV_{\boldsymbol{\xi}} + \int_{\mathcal{H}} w_{\mathbf{q}}\big(\underline{\mathbf{Y}}\langle\boldsymbol{\chi}^{-1}(\boldsymbol{\zeta})\rangle, \underline{\mathbf{Y}}\langle\boldsymbol{\zeta}\rangle, \boldsymbol{\chi}^{-1}(\boldsymbol{\zeta}), \boldsymbol{\zeta}\big) \cdot \delta\underline{\mathbf{Y}}\langle\boldsymbol{\zeta}\rangle \, J^{-1}(\boldsymbol{\zeta}) \, dV_{\boldsymbol{\zeta}}.$$

In the second integral, replace the dummy variable of integration $\boldsymbol{\zeta}$ by $\boldsymbol{\xi}$:

$$\delta\hat{W} = \int_{\mathcal{H}} \Big[w_{\mathbf{p}}\big(\underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle, \underline{\mathbf{Y}}\langle\boldsymbol{\chi}(\boldsymbol{\xi})\rangle, \boldsymbol{\xi}, \boldsymbol{\chi}(\boldsymbol{\xi})\big) + w_{\mathbf{q}}\big(\underline{\mathbf{Y}}\langle\boldsymbol{\chi}^{-1}(\boldsymbol{\xi})\rangle, \underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle, \boldsymbol{\chi}^{-1}(\boldsymbol{\xi}), \boldsymbol{\xi}\big) J^{-1}(\boldsymbol{\xi}) \Big] \cdot \delta\underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle \, dV_{\boldsymbol{\xi}}.$$

Comparing this result with (75), the force state can be read off:

$$\underline{\mathbf{T}}\langle\boldsymbol{\xi}\rangle = \nabla\hat{W}\langle\boldsymbol{\xi}\rangle = w_{\mathbf{p}}\big(\underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle, \underline{\mathbf{Y}}\langle\boldsymbol{\chi}(\boldsymbol{\xi})\rangle, \boldsymbol{\xi}, \boldsymbol{\chi}(\boldsymbol{\xi})\big) + w_{\mathbf{q}}\big(\underline{\mathbf{Y}}\langle\boldsymbol{\chi}^{-1}(\boldsymbol{\xi})\rangle, \underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle, \boldsymbol{\chi}^{-1}(\boldsymbol{\xi}), \boldsymbol{\xi}\big) J^{-1}(\boldsymbol{\xi}). \quad (87)$$

Bond-based materials are a special case of bond pair materials with $\boldsymbol{\chi}\langle\boldsymbol{\xi}\rangle = \boldsymbol{\xi}$ for all $\boldsymbol{\xi}$.

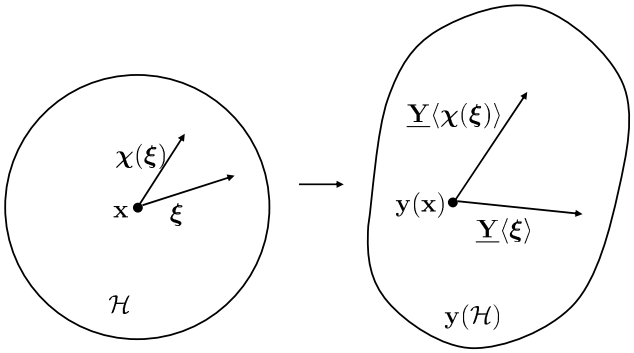

Figure 6: In a bond-pair material, the bond force density in each bond $\boldsymbol{\xi}$ is determined by its own deformation and that of another bond $\boldsymbol{\chi}(\boldsymbol{\xi})$.

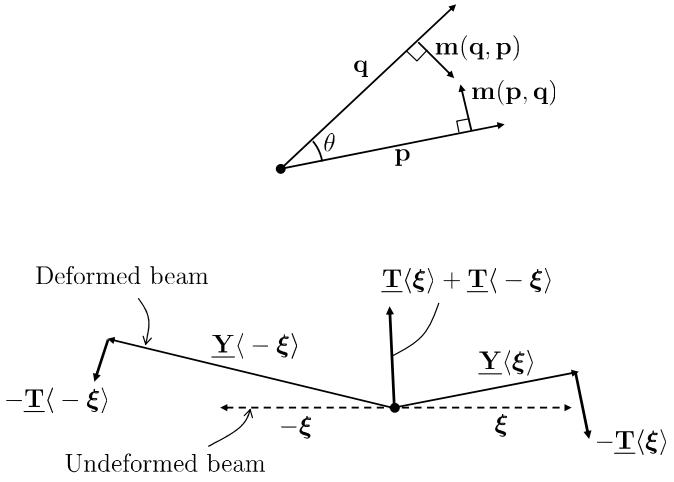

Figure 7: Top: Unit vectors $\mathbf{m}(\mathbf{p},\mathbf{q})$ and $\mathbf{m}(\mathbf{q},\mathbf{p})$. Bottom: Peridynamic beam based on a bond-pair material. The forces tend to restore the relative bond angles to their initial value, which in this case is π.

4.13 Example: a bond-pair material in bending

Consider the bond-pair material defined by (86) with

$$w(\mathbf{p},\mathbf{q},\mathbf{r},\mathbf{s}) = \frac{c}{4}(\theta-\theta_0)^2, \tag{88}$$

$$\theta = \cos^{-1}\frac{\mathbf{p}\cdot\mathbf{q}}{|\mathbf{p}||\mathbf{q}|}, \quad \theta_0 = \cos^{-1}\frac{\mathbf{r}\cdot\mathbf{s}}{|\mathbf{r}||\mathbf{s}|}$$

where c is a constant and both θ and θ_0 are in the interval $[0,\pi]$. ($\boldsymbol{\chi}$ will be defined later.) θ is the angle between the deformed bonds $\mathbf{p}$ and $\mathbf{q}$, while θ_0 is the angle between the undeformed bonds $\mathbf{r}$ and $\mathbf{s}$. Mechanically, if $c>0$, this material resists changes in the angle between the bonds $\mathbf{r}$ and $\mathbf{s}$. The elastic material model defined by (86) and (88) is objective, because it does not refer to any special direction in space. Using (88) and the chain rule to obtain $w_{\mathbf{p}}$, one finds, for $\theta \neq 0$,

$$\begin{aligned} w_{\mathbf{p}} = \frac{\partial w}{\partial\theta}\frac{\partial\theta}{\partial\mathbf{p}} &= \frac{c(\theta-\theta_0)}{2}\left(\frac{-1}{\sin\theta}\frac{\partial\cos\theta}{\partial\mathbf{p}}\right) \\ &= \frac{c(\theta_0-\theta)}{2\sin\theta}\frac{1}{|\mathbf{p}||\mathbf{q}|}\left(\mathbf{q}-\frac{|\mathbf{q}|\cos\theta}{|\mathbf{p}|}\mathbf{p}\right). \end{aligned}$$

A more suggestive form of this expression is

$$w_{\mathbf{p}} = \frac{c(\theta_0-\theta)}{2|\mathbf{p}|}\,\mathbf{m}(\mathbf{p},\mathbf{q}) \tag{89}$$

where

$$\mathbf{m}(\mathbf{p},\mathbf{q}) = \begin{cases} \mathbf{0} & \text{if } \theta = 0, \\ \dfrac{1}{\sin\theta}\left(\dfrac{\mathbf{q}}{|\mathbf{q}|}-\cos\theta\dfrac{\mathbf{p}}{|\mathbf{p}|}\right), & \text{if } \theta \neq 0. \end{cases}$$

Geometrically, $\mathbf{m}(\mathbf{p},\mathbf{q})$ is the unit vector normal to $\mathbf{p}$ that is coplanar with $\mathbf{p}$ and $\mathbf{q}$ such that $\mathbf{q}\cdot\mathbf{m}(\mathbf{p},\mathbf{q}) \geq 0$ (Figure 7). Similarly,

$$w_{\mathbf{q}} = \frac{c(\theta_0-\theta)}{2|\mathbf{q}|}\,\mathbf{m}(\mathbf{q},\mathbf{p}). \tag{90}$$

To define the pairing of bonds, take

$$\boldsymbol{\chi}(\boldsymbol{\xi}) = -\boldsymbol{\xi} \qquad \forall\boldsymbol{\xi}\in\mathcal{H}, \tag{91}$$

hence $J = J^{-1} = 1$. Then, by (87), (89), and (90),

$$\begin{aligned} \underline{\mathbf{T}}\langle\boldsymbol{\xi}\rangle &= w_{\mathbf{p}}\big(\underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle,\underline{\mathbf{Y}}\langle-\boldsymbol{\xi}\rangle,\boldsymbol{\xi},-\boldsymbol{\xi}\big) + w_{\mathbf{q}}\big(\underline{\mathbf{Y}}\langle-\boldsymbol{\xi}\rangle,\underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle,-\boldsymbol{\xi},\boldsymbol{\xi}\big) \\ &= \frac{c(\pi-\theta)}{|\underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle|}\,\mathbf{m}(\underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle,\underline{\mathbf{Y}}\langle-\boldsymbol{\xi}\rangle) \end{aligned}$$

where

$$\theta = \cos^{-1} \frac{\underline{\mathbf{Y}}\langle \boldsymbol{\xi} \rangle \cdot \underline{\mathbf{Y}}\langle -\boldsymbol{\xi} \rangle}{|\underline{\mathbf{Y}}\langle \boldsymbol{\xi} \rangle||\underline{\mathbf{Y}}\langle -\boldsymbol{\xi} \rangle|}, \qquad 0 \leq \theta \leq \pi.$$

Note that $\underline{\mathbf{T}}\langle \boldsymbol{\xi} \rangle \perp \underline{\mathbf{Y}}\langle \boldsymbol{\xi} \rangle$ (see Figure 7).

This material does not offer resistance to any homogeneous deformation. The strain energy density W changes only in response to nonhomogeneous deformations. This response is an aspect of nonlocality, because the finiteness of the bond lengths is what gives rise to the angle changes that result in changes in strain energy density.

An application of this material model is the bending of a beam. The strain energy increases according to deformations of the beam involving curvature. This can be thought of as a nonlocal version of an Euler beam. However, in the traditional treatment of an Euler beam, a new PDE is introduced, reflecting the resistance to curvature. This fourth order PDE is virtually unrelated to the second order PDEs of the classical theory of elasticity. In contrast, in the peridynamic beam model proposed here, the fundamental equation of motion is unchanged from the basic three dimensional peridynamic equation of motion. The peridynamic beam model simply uses a particular choice of material model, which is the bond-pair model with the choice of $\boldsymbol{\chi}$ given in (91).

5 Linear theory

Like the linear classical theory, the linear peridynamic theory concerns small deformations. However, the applicable notion of smallness is different in the peridynamic theory, because it does not restrict the deformation gradient, and even allows discontinuities. Under this assumption of smallness, the peridynamic equation of equilibrium reduces to a linear integral equation.

Linearization of the bond-based peridynamic theory is discussed in [60, 83]. The discussion below pertains to the more general state-based theory and largely follows [63]. See Section 1.2 for a summary of work to date making use of the linear theory.

5.1 Small displacements

Let $\mathcal{B}$ be a body with horizon δ. Consider a time-independent deformation $\mathbf{y}^0$, which may be large. (The role of $\mathbf{y}^0$ in the linearization will become clear in Section 5.3 below.) Let $\mathbf{u}$ be a displacement field superposed on $\mathbf{y}^0$, and define a vector state field by

$$\underline{\mathbf{U}}[\mathbf{x},t]\langle\mathbf{q}-\mathbf{x}\rangle = \mathbf{u}(\mathbf{q},t) - \mathbf{u}(\mathbf{x},t), \qquad \forall \mathbf{x} \in \mathcal{B},\ (\mathbf{q}-\mathbf{x}) \in \mathcal{H}. \tag{92}$$

The displacement field is said to be *small* if

$$\ell \ll \delta \tag{93}$$

where

$$\ell = \sup_{|\mathbf{q}-\mathbf{x}|\le\delta} |\mathbf{u}(\mathbf{q},t) - \mathbf{u}(\mathbf{x},t)|. \tag{94}$$

(Strictly speaking, (93) is actually a condition on the *relative* displacements, rather than the displacements themselves.) This idea of a small displacement field is a nonlocal analogue of the concept in classical linear theory that $|\text{grad } \mathbf{u}| \ll 1$. The peridynamic definition of a small displacement field (93) does not restrict rigid translations of a body, but it does restrict rigid body rotations to small angles. More importantly, it allows for possible small discontinuities in $\mathbf{u}$, a key difference from the classical linear theory.

Recalling the definition of the norm of a vector state (52), for a small displacement field, (93) and (94) imply that

$$||\underline{\mathbf{U}}|| = O(\ell).$$

5.2 Double states

In the linear peridynamic theory, the analogue of the classical fourth order elasticity tensor is a double state (see definition following (49)). Before developing the linear theory further, it is helpful to introduce some properties of double states.

If $\underline{\mathbb{D}}$ is a double state, then for every pair of bonds $\boldsymbol{\xi}$ and $\boldsymbol{\zeta}$ in $\mathcal{H}$, the value of $\underline{\mathbb{D}}\langle\boldsymbol{\xi},\boldsymbol{\zeta}\rangle$ is a second-order tensor. The set of all double states is denoted $\mathcal{D}$. In the following, $\underline{\mathbb{D}}$ and $\underline{\mathbb{E}}$ are double states, while $\underline{\mathbf{A}}$ and $\underline{\mathbf{B}}$ are vector states. Define the vector state $\underline{\mathbb{D}} \bullet \underline{\mathbf{A}}$ by

$$(\underline{\mathbb{D}} \bullet \underline{\mathbf{A}})\langle\boldsymbol{\xi}\rangle = \int_{\mathcal{H}} \underline{\mathbb{D}}\langle\boldsymbol{\xi},\boldsymbol{\zeta}\rangle\ \underline{\mathbf{A}}\langle\boldsymbol{\zeta}\rangle\ dV_{\boldsymbol{\zeta}} \qquad \forall\boldsymbol{\xi}\in\mathcal{H}$$

where the integrand is the product of a second order tensor with a vector; the component form is $\underline{D}_{ij}\underline{A}_j$. The *adjoint* of $\underline{\mathbb{D}}$ is a double state defined by

$$\underline{\mathbb{D}}^\dagger\langle\boldsymbol{\xi},\boldsymbol{\zeta}\rangle = \underline{\mathbb{D}}^T\langle\boldsymbol{\zeta},\boldsymbol{\xi}\rangle \qquad \forall\boldsymbol{\xi},\boldsymbol{\zeta}\in\mathcal{H}.$$

where the superscript T indicates the tensor transpose. Note that the order of the bonds is switched when taking the adjoint in addition to taking the tensor transpose. $\underline{\mathbb{D}}$ is *self-adjoint* if

$$\underline{\mathbb{D}}^\dagger = \underline{\mathbb{D}}.$$

Also define the vector state $\mathbf{A} \bullet \underline{\mathbb{D}}$ by

$$\underline{\mathbf{A}} \bullet \underline{\mathbb{D}} = \underline{\mathbb{D}}^\dagger \bullet \underline{\mathbf{A}}.$$

For any vector states $\underline{\mathbf{A}}$ and $\underline{\mathbf{B}}$, the following identity holds:

$$\underline{\mathbf{B}} \bullet \underline{\mathbb{D}}^\dagger \bullet \underline{\mathbf{A}} = \underline{\mathbf{A}} \bullet \underline{\mathbb{D}} \bullet \underline{\mathbf{B}}.$$

If $\underline{\mathbf{S}}(\cdot) : \mathcal{V} \to \mathcal{V}$ is Fréchet differentiable, then

$$\underline{\mathbf{S}}(\underline{\mathbf{A}} + \underline{\mathbf{a}}) = \underline{\mathbf{S}}(\underline{\mathbf{A}}) + \nabla\underline{\mathbf{S}}(\underline{\mathbf{A}}) \bullet \underline{\mathbf{a}} + o(||\underline{\mathbf{a}}||) \qquad \forall\underline{\mathbf{A}},\underline{\mathbf{a}}\in\mathcal{V} \tag{95}$$

where $\nabla\underline{\mathbf{S}}(\underline{\mathbf{A}})$ is a double state. As before, in the case of a function of two states, such as $\underline{\mathbf{S}}(\underline{\mathbf{A}},\underline{\mathbf{B}})$, the Fréchet derivative with respect to each is denoted $\underline{\mathbf{S}}_{\underline{\mathbf{A}}}$ or $\underline{\mathbf{S}}_{\underline{\mathbf{B}}}$.

If $\Psi(\cdot) : \mathcal{V} \to \mathbb{R}$, then the second Fréchet derivative of Ψ, if it exists, is a double state defined by

$$\nabla\nabla\Psi = \nabla(\nabla\Psi) \qquad \text{on } \mathcal{V}.$$

The following list summarizes, omitting some details, three important results that are proved in [63]:

(i) If $\Psi(\cdot,\cdot) : \mathcal{V}\times\mathcal{V} \to \mathbb{R}$ and Ψ is twice continuously Fréchet differentiable, then the order of differentiation in the mixed second Fréchet derivatives of Ψ is interchangeable, *i.e.*,

$$(\Psi_{\underline{\mathbf{A}}})_{\underline{\mathbf{B}}}(\underline{\mathbf{A}},\underline{\mathbf{B}}) = (\Psi_{\underline{\mathbf{B}}})_{\underline{\mathbf{A}}}(\underline{\mathbf{A}},\underline{\mathbf{B}}) \qquad \forall\underline{\mathbf{A}},\underline{\mathbf{B}}\in\mathcal{V}.$$

(*ii*) If $\Psi(\cdot) : \mathcal{V} \to \mathbb{R}$ and Ψ is twice continuously Fréchet differentiable, then

$$(\nabla\nabla\Psi)^\dagger = \nabla\nabla\Psi \qquad \text{on } \mathcal{V}.$$

(*iii*) If $\underline{\mathbf{S}}(\cdot) : \mathcal{V} \to \mathcal{V}$ and $\underline{\mathbf{S}}$ is continuously Fréchet differentiable, then

$$(\nabla\underline{\mathbf{S}})^\dagger = \nabla\underline{\mathbf{S}} \qquad \text{on } \mathcal{V} \tag{96}$$

if and only if there exists a twice continuously Fréchet differentiable function $\Psi(\cdot) : \mathcal{V} \to \mathbb{R}$ such that

$$\underline{\mathbf{S}} = \nabla\Psi \qquad \text{on } \mathcal{V}.$$

(This result is analogous to Poincaré's theorem in vector calculus.)

5.3 Linearization of an elastic constitutive model

Let the force state for a body $\mathcal{B}$ be given by $\underline{\hat{\mathbf{T}}}(\underline{\mathbf{Y}})$, where $\underline{\hat{\mathbf{T}}}$ is the constitutive model. Suppose that $\underline{\hat{\mathbf{T}}}$ is Fréchet differentiable, and denote its Fréchet derivative by $\underline{\hat{\mathbf{T}}}_{\underline{\mathbf{Y}}}$. Consider an equilibrated deformation $\mathbf{y}^0$ corresponding to a time-independent external body force density field $\mathbf{b}^0$, and define

$$\underline{\mathbf{Y}}^0[\mathbf{x}]\langle\mathbf{q}-\mathbf{x}\rangle = \mathbf{y}^0(\mathbf{q}) - \mathbf{y}^0(\mathbf{x}) \qquad \forall \mathbf{x}, \mathbf{q} \in \mathcal{B}$$

and

$$\underline{\mathbf{T}}^0[\mathbf{x}] = \underline{\hat{\mathbf{T}}}(\underline{\mathbf{Y}}^0[\mathbf{x}], \mathbf{x}) \qquad \forall \mathbf{x} \in \mathcal{B}.$$

Define a double state field called the *modulus state* field by

$$\underline{\underline{\mathbb{K}}}[\mathbf{x}] = \underline{\hat{\mathbf{T}}}_{\underline{\mathbf{Y}}}(\underline{\mathbf{Y}}^0[\mathbf{x}], \mathbf{x}) \qquad \forall \mathbf{x} \in \mathcal{B}. \tag{97}$$

Let $\mathbf{u}$ be a small displacement field superposed on $\mathbf{y}^0$, and define the displacement state field by (92). Define the *linearized constitutive model* by

$$\underline{\mathbf{T}}[\mathbf{x}, t] = \underline{\mathbf{T}}^0[\mathbf{x}] + \underline{\underline{\mathbb{K}}}[\mathbf{x}] \bullet \underline{\mathbf{U}}[\mathbf{x}, t] \qquad \forall \mathbf{x} \in \mathcal{B},\ t \geq 0. \tag{98}$$

By (95), the linearized model differs from the full model by a term of order $o(||\underline{\mathbf{U}}||)$. If the material is elastic, then by definition

$$\underline{\hat{\mathbf{T}}}(\underline{\mathbf{Y}}, \mathbf{x}) = \hat{W}_{\underline{\mathbf{Y}}}(\underline{\mathbf{Y}}, \mathbf{x}) \qquad \forall \underline{\mathbf{Y}} \in \mathcal{V},\ \mathbf{x} \in \mathcal{B}$$

where $\hat{W}$ is the strain energy density function. Therefore, by (97),

$$\underline{\underline{\mathbb{K}}}[\mathbf{x}] = \hat{W}_{\underline{\mathbf{Y}}\underline{\mathbf{Y}}}(\underline{\mathbf{Y}}^0[\mathbf{x}], \mathbf{x}) \qquad \forall \mathbf{x} \in \mathcal{B}, \tag{99}$$

and by (96),

$$\underline{\underline{\mathbb{K}}}^\dagger = \underline{\underline{\mathbb{K}}} \quad \text{on } \mathcal{B}. \tag{100}$$

Furthermore, by result (*iii*) of Section 5.2, (100) implies that the material is elastic.

The fact that the modulus state $\underline{\underline{\mathbb{K}}}[\mathbf{x}]$ depends on $\underline{\mathbf{Y}}^0$ in (99) represents a key advantage of the peridynamic approach over other nonlocal models, because it encompasses the coupling between the large deformation state $\underline{\mathbf{Y}}^0$ and subsequent small motions of the body. This includes the coupling between a large bond force density $\underline{\mathbf{T}}^0\langle\boldsymbol{\xi}\rangle$ and small rotation of the bond. A striking example of the importance of these rotations is given in Example 4 of [63], in which large compressive forces in bonds couple to subsequent rotations to result in material instability.

For an elastic material, the force state in the linearized model (98) can be obtained from the Fréchet derivative of the following strain energy density function:

$$\underline{\mathbf{T}} = \hat{W}^{\rm lin}_{\underline{\mathbf{U}}}(\underline{\mathbf{U}}, \mathbf{x}), \qquad \hat{W}^{\rm lin}(\underline{\mathbf{U}}, \mathbf{x}) = \underline{\mathbf{T}}^0[\mathbf{x}] \bullet \underline{\mathbf{U}} + \frac{1}{2}\underline{\mathbf{U}} \bullet \underline{\underline{\mathbb{K}}}[\mathbf{x}] \bullet \underline{\mathbf{U}}.$$

5.4 Equations of motion and equilibrium

Continuing under the assumptions of the previous section, the peridynamic equation of motion (58) under a body force density field $\hat{\mathbf{b}}$ is

$$\rho(\mathbf{x})\ddot{\mathbf{y}}(\mathbf{x},t) = \int_{\mathcal{B}} \Big(\underline{\mathbf{T}}[\mathbf{x},t]\langle\mathbf{p}-\mathbf{x}\rangle - \underline{\mathbf{T}}[\mathbf{p},t]\langle\mathbf{x}-\mathbf{p}\rangle\Big)\, dV_{\mathbf{p}} + \hat{\mathbf{b}}(\mathbf{x},t)$$

for all $\mathbf{x} \in \mathcal{B}$, $t \geq 0$. Since, by assumption, $\underline{\mathbf{Y}}^0$ is equilibrated under $\mathbf{b}^0$,

$$\int_{\mathcal{B}} \Big(\underline{\mathbf{T}}^0[\mathbf{x}]\langle\mathbf{p}-\mathbf{x}\rangle - \underline{\mathbf{T}}^0[\mathbf{p}]\langle\mathbf{x}-\mathbf{p}\rangle\Big)\, dV_{\mathbf{p}} + \mathbf{b}^0(\mathbf{x}) = \mathbf{0} \qquad \forall \mathbf{x} \in \mathcal{B}.$$

Subtracting the last two equations and using (98) leads to

$$\rho(\mathbf{x})\ddot{\mathbf{u}}(\mathbf{x},t) = \int_{\mathcal{B}} \Big((\underline{\underline{\mathbb{K}}}[\mathbf{x}] \bullet \underline{\mathbf{U}}[\mathbf{x},t])\langle\mathbf{p}-\mathbf{x}\rangle - (\underline{\underline{\mathbb{K}}}[\mathbf{p}] \bullet \underline{\mathbf{U}}[\mathbf{p},t])\langle\mathbf{x}-\mathbf{p}\rangle\Big)\, dV_{\mathbf{p}} + \mathbf{b}(\mathbf{x},t) \quad (101)$$

where

$$\mathbf{b}(\mathbf{x},t) = \hat{\mathbf{b}}(\mathbf{x},t) - \mathbf{b}^0(\mathbf{x}) = \mathbf{0} \qquad \forall \mathbf{x} \in \mathcal{B},\ t \geq 0.$$

Using (92) in (101) and simplifying results in

$$\rho(\mathbf{x})\ddot{\mathbf{u}}(\mathbf{x},t) = \int_{\mathcal{B}} \mathbf{C}_0(\mathbf{x},\mathbf{q})\big(\mathbf{u}(\mathbf{q},t) - \mathbf{u}(\mathbf{x},t)\big)\, dV_{\mathbf{q}} + \mathbf{b}(\mathbf{x},t) \quad (102)$$

for all $\mathbf{x} \in \mathcal{B}$, $t \geq 0$, where $\mathbf{C}_0$ is the tensor valued function defined by

$$\mathbf{C}_0(\mathbf{x},\mathbf{q}) = \int_{\mathcal{B}} \Big(\underline{\underline{\mathbb{K}}}[\mathbf{x}]\langle\mathbf{p}-\mathbf{x},\mathbf{q}-\mathbf{x}\rangle - \underline{\underline{\mathbb{K}}}[\mathbf{p}]\langle\mathbf{x}-\mathbf{p},\mathbf{q}-\mathbf{p}\rangle + \underline{\underline{\mathbb{K}}}[\mathbf{q}]\langle\mathbf{x}-\mathbf{q},\mathbf{p}-\mathbf{q}\rangle\Big)\, dV_{\mathbf{p}} \quad (103)$$

for all $\mathbf{x}, \mathbf{q} \in \mathcal{B}$. (Recall from (51) that the dot products in (101) contain volume integrals.) If the material is elastic, then by (100) and (103),

$$\mathbf{C}_0^T(\mathbf{q}, \mathbf{x}) = \mathbf{C}_0(\mathbf{x}, \mathbf{q}) \qquad \forall \mathbf{x}, \mathbf{q} \in \mathcal{B}. \tag{104}$$

Setting the acceleration term to zero in (102) yields the linearized equation of equilibrium:

$$\int_{\mathcal{B}} \mathbf{C}_0(\mathbf{x}, \mathbf{q})\big(\mathbf{u}(\mathbf{q}) - \mathbf{u}(\mathbf{x})\big)\, dV_{\mathbf{q}} + \mathbf{b}(\mathbf{x}) = \mathbf{0} \tag{105}$$

for all $\mathbf{x} \in \mathcal{B}$. This is a Fredholm linear integral equation of the second kind. $\mathbf{C}_0$ is called the *micromodulus tensor field*.

5.5 Linear bond-based materials

If the material is bond-based as well as elastic, recall from (76) and (79) that there is a bond potential function $w(e, \boldsymbol{\xi}, \mathbf{x})$ such that

$$\underline{\hat{\mathbf{T}}}(\underline{\mathbf{Y}}, \mathbf{x})\langle\boldsymbol{\xi}\rangle = w_e(\underline{e}\langle\boldsymbol{\xi}\rangle, \boldsymbol{\xi}, \mathbf{x})\underline{\mathbf{M}}\langle\boldsymbol{\xi}\rangle \qquad \forall \boldsymbol{\xi} \in \mathcal{H} \tag{106}$$

where

$$\underline{e}\langle\boldsymbol{\xi}\rangle = |\underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle| - |\boldsymbol{\xi}|, \qquad \underline{\mathbf{M}}\langle\boldsymbol{\xi}\rangle = \frac{\underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle}{|\underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle|}. \tag{107}$$

($\mathbf{x}$ is included among the arguments in $w(e, \boldsymbol{\xi}, \mathbf{x})$ to account for heterogeneity.) To evaluate the modulus state field $\underline{\mathbb{K}}$ using (97), the Fréchet derivative of $\underline{\hat{\mathbf{T}}}$ is found as follows. For a small increment $\delta\underline{\mathbf{Y}}$ in the deformation state, according to (106) and the chain rule,

$$\delta\underline{\hat{\mathbf{T}}} = w_{ee}\underline{\mathbf{M}}\delta\underline{e} + w_e\delta\underline{\mathbf{M}}.$$

From (107),

$$\delta\underline{e} = \underline{\mathbf{M}} \cdot \delta\underline{\mathbf{Y}}, \qquad \delta\underline{\mathbf{M}} = \big(\mathbf{1} - \underline{\mathbf{M}} \otimes \underline{\mathbf{M}}\big)\frac{\delta\underline{\mathbf{Y}}}{|\underline{\mathbf{Y}}|},$$

hence

$$\delta\underline{\hat{\mathbf{T}}} = w_{ee}(\underline{\mathbf{M}} \otimes \underline{\mathbf{M}}) \cdot \delta\underline{\mathbf{Y}} + w_e\big(\mathbf{1} - \underline{\mathbf{M}} \otimes \underline{\mathbf{M}}\big)\frac{\delta\underline{\mathbf{Y}}}{|\underline{\mathbf{Y}}|}.$$

From this, (95), and (97),

$$\underline{\mathbb{K}}[\mathbf{x}]\langle\boldsymbol{\xi}, \boldsymbol{\zeta}\rangle = \Big[w_{ee}(\underline{e}^0\langle\boldsymbol{\xi}\rangle, \boldsymbol{\xi}, \mathbf{x})\underline{\mathbf{M}}^0 \otimes \underline{\mathbf{M}}^0 + w_e(\underline{e}^0\langle\boldsymbol{\xi}\rangle, \boldsymbol{\xi}, \mathbf{x})\frac{\mathbf{1} - \underline{\mathbf{M}}^0 \otimes \underline{\mathbf{M}}^0}{|\underline{\mathbf{Y}}^0\langle\boldsymbol{\xi}\rangle|}\Big]\Delta(\boldsymbol{\zeta} - \boldsymbol{\xi}). \tag{108}$$

where

$$\underline{e}^0\langle\boldsymbol{\xi}\rangle = |\underline{\mathbf{Y}}^0\langle\boldsymbol{\xi}\rangle| - |\boldsymbol{\xi}|, \qquad \underline{\mathbf{M}}^0 = \frac{\underline{\mathbf{Y}}^0\langle\boldsymbol{\xi}\rangle}{|\underline{\mathbf{Y}}^0\langle\boldsymbol{\xi}\rangle|}$$

and Δ is the three dimensional Dirac delta function. The $\underline{\mathbb{K}}$ given by (108) is clearly self-adjoint. Because of (106), the second term on the right hand side of (108) is non-null only if $\underline{\mathbf{T}}^0$ is non-null. This second term represents the change in direction of $\underline{\mathbf{T}}^0$ in response to an incremental change $d\underline{\mathbf{Y}}$. The first term on the right hand side of (106) represents the change in the magnitude of the bond force density.

In the special case of linearization near the reference configuration and of zero bond force densities in this configuration, (108) specializes to

$$\underline{\mathbb{K}}[\mathbf{x}]\langle\boldsymbol{\xi},\boldsymbol{\zeta}\rangle = w_{ee}(0,\boldsymbol{\xi},\mathbf{x})\Delta(\boldsymbol{\zeta}-\boldsymbol{\xi})\frac{\boldsymbol{\xi}\otimes\boldsymbol{\xi}}{|\boldsymbol{\xi}|^2}. \tag{109}$$

In this case, (103) and (109) imply, after evaluating the integral,

$$\begin{aligned}\mathbf{C}_0(\mathbf{x},\mathbf{q}) = {}& \big[w_{ee}(0,\mathbf{q}-\mathbf{x},\mathbf{x}) + w_{ee}(0,\mathbf{x}-\mathbf{q},\mathbf{q})\big]\frac{(\mathbf{q}-\mathbf{x})\otimes(\mathbf{q}-\mathbf{x})}{|\mathbf{q}-\mathbf{x}|^2} \\ & - \Delta(\mathbf{q}-\mathbf{x})\int_{\mathcal{B}} w_{ee}(0,\mathbf{x}-\mathbf{p},\mathbf{p})\frac{(\mathbf{x}-\mathbf{p})\otimes(\mathbf{x}-\mathbf{p})}{|\mathbf{x}-\mathbf{p}|^2}\,dV_{\mathbf{p}}.\end{aligned} \tag{110}$$

From (110), it follows that in addition to the symmetry (104) that always holds for linearized elastic material models, the following symmetries also hold if the material is bond-based:

$$\mathbf{C}_0^T(\mathbf{x},\mathbf{q}) = \mathbf{C}_0(\mathbf{x},\mathbf{q}), \qquad \mathbf{C}_0(\mathbf{q},\mathbf{x}) = \mathbf{C}_0(\mathbf{x},\mathbf{q}) \qquad \forall \mathbf{x},\mathbf{q}\in\mathcal{B}.$$

When (110) is substituted into the linearized equation of motion (102), the term involving $\Delta(\mathbf{q}-\mathbf{x})$ integrates to $\mathbf{0}$, and the resulting equation of motion for this body is

$$\rho(\mathbf{x})\ddot{\mathbf{u}}(\mathbf{x},t) = \int_{\mathcal{B}} \mathbf{C}(\mathbf{x},\mathbf{q})\big(\mathbf{u}(\mathbf{q},t)-\mathbf{u}(\mathbf{x},t)\big)\,dV_{\mathbf{q}} + \mathbf{b}(\mathbf{x},t) \tag{111}$$

for all $\mathbf{x}\in\mathcal{B}$, $t\geq 0$, where

$$\mathbf{C}(\mathbf{x},\mathbf{q}) = \big[w_{ee}(0,\mathbf{q}-\mathbf{x},\mathbf{x}) + w_{ee}(0,\mathbf{x}-\mathbf{q},\mathbf{q})\big]\frac{(\mathbf{q}-\mathbf{x})\otimes(\mathbf{q}-\mathbf{x})}{|\mathbf{q}-\mathbf{x}|^2}.$$

If the horizon δ is constant throughout $\mathcal{B}$, then the region of integration in (111) can be replaced by the neighborhood of radius δ centered at $\mathbf{x}$. This smaller region of integration can be used because $w_{ee}(0,\boldsymbol{\xi},\mathbf{x}) = 0$ whenever $|\boldsymbol{\xi}| > \delta$. The smaller region cannot be used in the more general expression (102).

5.6 Equilibrium in a one dimensional model

This section describes application of the linear theory to an infinitely long bar under static loading by a body force density field b. It is shown that the problem can be analyzed using the Fourier transform, and a Green's function solution is derived. Consider a homogeneous bar with constant cross-sectional area A, infinitely long in both directions, oriented along the x-axis. The material model is bond-based and linear elastic with horizon δ. The transverse dimensions of the bar are much smaller than δ. Define a coordinate system in which x_1 is the axial direction. Let

$$x = x_1, \quad u = u_1, \quad b = b_1,$$

$$C(q - x) = AC_{11}(x, q) \qquad \forall x, q \in \mathbb{R}^3.$$

The equilibrium equation (105) simplifies to

$$\int_{-\infty}^{\infty} C(q - x)\big(u(q) - u(x)\big)\, dq + b(x) = 0, \quad x \in \mathbb{R}. \tag{112}$$

By (104),

$$C(-\xi) = C(\xi) \qquad \forall \xi \in \mathbb{R}^3.$$

As shown in [75], this C is related to the Young's modulus E that would be measured in the static extension of a long bar by

$$E = \int_0^{\infty} \xi^2 C(\xi)\, d\xi.$$

Let v^* denote the Fourier transform of any function $v(x)$:

$$v^*(\kappa) = \int_{-\infty}^{\infty} e^{-i\kappa x} v(x)\, dx,$$

with inverse transform given by

$$v(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\kappa x} v^*(\kappa)\, d\kappa.$$

The Fourier variable κ physically represents the wave number, $\kappa = 2\pi/\lambda$, where λ is the wavelength. Taking the Fourier transform of (112) leads to

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-i\kappa x} \Big[C(q - x)\big(u(q) - u(x)\big) \Big]\, dq\, dx + b^*(x) = 0.$$

By the convolution theorem, this implies

$$C^*(\kappa) u^*(\kappa) - P u^*(\kappa) + b^*(\kappa) = 0$$

where

$$P = \int_{-\infty}^{\infty} C(\xi)\, d\xi = C^*(0).$$

The transformed displacement can therefore be written formally as

$$u^*(\kappa) = \frac{b^*(\kappa)}{M(\kappa)}, \tag{113}$$

where

$$M(\kappa) = P - C^*(\kappa). \tag{114}$$

After inversion of the transform, the displacement is given by

$$\begin{aligned} u(x) &= \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{i\kappa x} u^*(\kappa)\, d\kappa = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{i\kappa x}\frac{b^*(\kappa)}{M(\kappa)}\, d\kappa \\ &= \frac{1}{2\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{i\kappa(x-z)}\frac{b(z)}{M(\kappa)}\, dz\, d\kappa \\ &= \int_{-\infty}^{\infty} g(x,z) b(z)\, dz \end{aligned} \tag{115}$$

where g is a Green's function given by

$$g(x,z) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{e^{i\kappa(x-z)}}{M(\kappa)}\, d\kappa.$$

Some particular cases of static solutions to this one dimensional problem are discussed in [70] and [75], the latter of which also derives a dynamic Green's function. An example taken from [70] is shown in Figure 8. In this example, two opposite point loads of magnitude b_0 are applied at the points $x = \pm a$, thus

$$b(x) = b_0(\Delta(x-a) - \Delta(x+a))$$

where Δ is the one dimensional Dirac delta function. The peridynamic material model has a micromodulus function given by

$$C(\xi) = \begin{cases} 3E/\delta^2, & |\xi| \le \delta \\ 0, & \text{otherwise} \end{cases}$$

where E is the Young's modulus. The length scale in the material model (the horizon) and the length scale in the loading are related, in this example, by the arbitrary choice

$$a = \delta/4.$$

The peridynamic solution contains delta functions, indicated by the vertical arrows in the figure, located at $\pm a$. The jumps in displacement shown in the figure at $\pm 3a$ and $\pm 5a$ are a result of the discontinuities in $C(\xi)$ at $\xi = \pm\delta$;

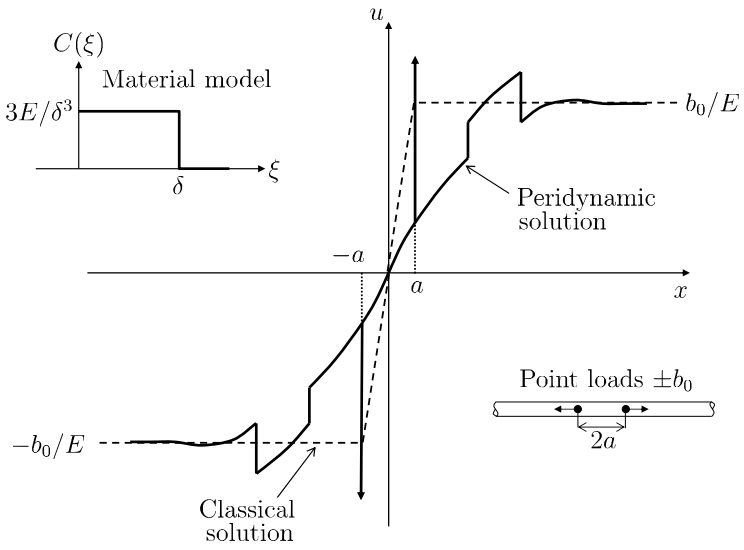

Figure 8: Peridynamic and classical displacement fields for two opposite point loads applied at $x = \pm a$, where $a = \delta/4$.

they would not appear if a continuous C were used. The solution also includes oscillations that decay with distance from the points of application of the loads. As shown in [70] analytically, each successive oscillation contains a discontinuity in a higher derivative of u than the one before it. The peridynamic result approaches the classical displacement field asymptotically at large distances.

If the length scale in the material model, *i.e.,* the horizon, is reduced so that $\delta \ll a$ while holding E constant, then the peridynamic displacement field approaches the classical field at all points except $x = \pm a$. At these two points, the delta functions persist regardless of δ (see [70] for details). The convergence in the limit of small horizon is consistent with the results of Section 6.3. The analysis in that section does not apply at the points $x = \pm a$ because the deformation is not smooth there; thus the peridynamic operator is not expected to converge to the classical operator.

For a given body force density field b, if a solution u to the equilibrium equation (112) exists, then the function u' defined by

$$u' = u + u_h$$

is also a solution to (112), where u_h is any solution to the following homo-

geneous equilibrium equation:

$$Lu_h := \int_{-\infty}^{\infty} C(q-x)\big(u_h(q) - u_h(x)\big)\, dq = 0, \quad x \in \mathbb{R},\ t \geq 0. \tag{116}$$

where L is a linear operator. For any C, one such u_h is provided by $u_h \equiv c$, where c is any constant. (A similar statement is true of the classical theory: any rigid translation of an equilibrium solution is also an equilibrium solution.)

Other homogeneous solutions may also exist for certain choices of C. The set of all these u_h functions is the null space of L. If $M(\kappa)$ has a nonzero root κ_0, then it is easily confirmed that the function

$$u_h(x) = e^{i\kappa_0 x}$$

is a solution to the homogeneous equation (116). For such a material, the transformed displacement u^* given by (113) does not exist if $b^*(\kappa_0) \neq 0$. In other words, there is no deformation of the bar that can equilibrate an applied body force density that has a nonzero Fourier component at κ_0. In this case, (115) may not apply.

Materials having a micromodulus C such that M has a nonzero root are not typical well-behaved materials. For example, if C is nonnegative and continuous on $\mathbb{R}$, it follows from (114) that M has only the root $\kappa = 0$. (It is too restrictive to assume that C is strictly positive, since this excludes some materials that have physically reasonable behavior.)

An example of a material for which M does have nonzero roots has its micromodulus given by

$$C(\xi) = \Delta(\xi - \alpha) + \Delta(\xi + \alpha)$$

where α is a positive constant that is similar to the interatomic spacing in a discrete lattice model. For this material, by (114),

$$M(\kappa) = 2(1 - \cos \alpha\kappa),$$

which has an infinite number of roots $\kappa_0 = 2\pi n/\alpha$, where n is any integer. If the loading has nonzero Fourier components at these roots, *i.e.,* if

$$b^*\left(\frac{2\pi n}{\alpha}\right) \neq 0$$

for some integer n, then a solution to the equilibrium equation (112) fails to exist. However, if b contains no Fourier components κ outside the set $(-2\pi/\alpha, 0) \cup (0, 2\pi/\alpha)$, then the solution exists and is given by (115). This means that as $\alpha \to 0$, there is a larger and larger interval on the κ axis

for which the peridynamic model behaves, for purposes of existence and uniqueness, like the classical theory. This observation is consistent with the general rule that in the limit of small material length scale, the peridynamic theory behaves similarly to the classical theory, provided certain smoothness conditions are met. (In the classical theory, only the Fourier component $\kappa = 0$ is excluded from b, because it represents loading that is not self-equilibrated.)

In summary, the existence of solutions to the equilibrium problem (112) depends on both the material properties and the loading. A solution u for well-behaved materials (no nonzero roots of M) is given by (115), provided $b^*(0) = 0$. For any such solution u, $u + c$ is also a solution for any constant c. If M has nonzero roots, the existence of solutions depends on the Fourier spectrum of the loading.

5.7 Plane waves and dispersion in one dimension

The equation of motion corresponding to (112) for the infinite, homogeneous bar is given by

$$\rho\ddot{u}(x,t) = \int_{-\infty}^{\infty} C(q-x)\big(u(q,t)-u(x,t)\big)\,dq + b(x,t), \quad x \in \mathbb{R},\ t \geq 0. \tag{117}$$

To investigate plane waves in the bar with wave number κ and angular frequency ω, assume a motion of the form

$$u(x,t) = e^{i(\kappa x - \omega t)}$$

with $b \equiv 0$. Substituting this expession into (117) results in

$$-\rho\omega^2 e^{i(\kappa x-\omega t)} = e^{-i\omega t}\int_{-\infty}^{\infty} C(q-x)\big(e^{i\kappa q} - e^{i\kappa x}\big)\,dq$$

which implies the condition

$$\rho\omega^2 = M(\kappa)$$

where M is given by (114). This provides the following dispersion relation:

$$\omega(\kappa) = \pm\sqrt{\frac{M(\kappa)}{\rho}}.$$

The corresponding phase velocity is given by

$$c(\kappa) = \frac{\omega(\kappa)}{\kappa} = \pm\frac{1}{\kappa}\sqrt{\frac{M(\kappa)}{\rho}}.$$

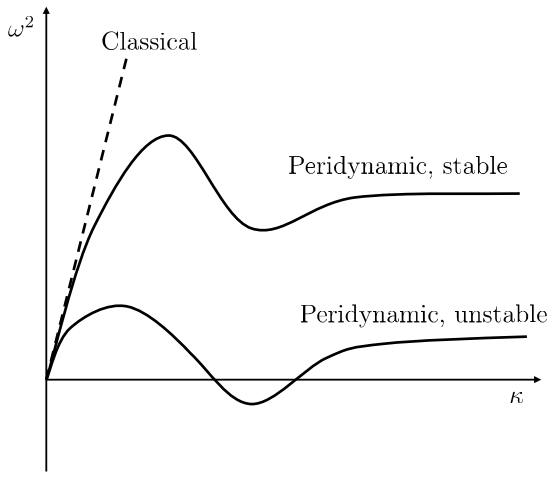

Figure 9: Dispersion curves for stable and unstable peridynamic materials.

Evidently, stable waves exist for a given κ only if $M(\kappa) > 0$. Figure 9 illustrates possible dispersion curves for a peridynamic material exhibiting stable waves at all wave numbers, and also a material that is unstable for some wave numbers due to "imaginary wave speeds." The peridynamic dispersion curves have the same slope at the origin as the classical dispersion line if their Young's moduli are the same.

6 Relation to other theories

In this section we identify quantities and principles that allow comparison between the peridynamic and the classical theories, as well as some non-local theories. This comparison would not be complete without discussing Navier's theory of solids (see [71, 72]). Navier conceived of a continuum as a smoothed out distribution of masses that interact with each other through a central potential. This model treated the relative motion of each such pair according to a first order approximation based on the displacement gradient components. In this sense, Navier's model was a local theory, even though conceptually it involved long-range forces. Because of the assumption of central potentials, isotropic materials were restricted to a Poisson ratio of 1/4 in Navier's theory. The local theory of Cauchy that was introduced after Navier's does not suffer from this restriction, and this is the classical continuum theory that continues to enjoy wide usage and acceptance today. In the next section, we compare the kinematics of this classical theory with those in the peridynamic theory.

6.1 Deformation gradient and the deformation state

Recall the definition of the deformation state (55) at a point $\mathbf{x} \in \mathcal{B}$, where $\mathcal{B}$ is a body with horizon δ:

$$\underline{\mathbf{Y}}[\mathbf{x}]\langle\boldsymbol{\xi}\rangle = \mathbf{y}(\mathbf{x}+\boldsymbol{\xi}) - \mathbf{y}(\mathbf{x}) \qquad \forall \boldsymbol{\xi} \in \mathcal{H}. \tag{118}$$

(In this discussion, the time variable will not be included explicitly.) If the deformation is continuously differentiable on $\mathcal{B}$, then the first two terms of a Taylor expansion yield

$$\mathbf{y}(\mathbf{x}+\boldsymbol{\xi}) = \mathbf{y}(\mathbf{x}) + \mathbf{F}(\mathbf{x})\boldsymbol{\xi} + O(|\boldsymbol{\xi}|^2) \qquad \forall \boldsymbol{\xi} \in \mathcal{H}$$

where the deformation gradient tensor field $\mathbf{F}$ is defined by

$$\mathbf{F}(\mathbf{x}) = \frac{\partial \mathbf{y}}{\partial \mathbf{x}}(\mathbf{x}) \qquad \forall \mathbf{x} \in \mathcal{B}.$$

Comparing the last two equations,

$$\underline{\mathbf{Y}}[\mathbf{x}]\langle\boldsymbol{\xi}\rangle = \mathbf{F}(\mathbf{x})\boldsymbol{\xi} + O(|\boldsymbol{\xi}|^2) \qquad \forall \boldsymbol{\xi} \in \mathcal{H},\ \mathbf{x} \in \mathcal{B}. \tag{119}$$

For a given continuously differentiable deformation, since $|\boldsymbol{\xi}| \leq \delta$, it follows that

$$\underline{\mathbf{Y}}[\mathbf{x}] = \mathbf{F}(\mathbf{x})\underline{\mathbf{X}} + O(\delta^2) \qquad \forall \mathbf{x} \in \mathcal{B}$$

where $\underline{\mathbf{X}}$ is the identity state defined in (49). In this sense, conceptually, the deformation gradient approximates the deformation state. The key distinctions are as follows:

- The deformation state is nonlocal in that it explicitly relates the deformation of material points separated by finite distances, while the deformation gradient is local.
- The deformation state can be evaluated even if the deformation is not differentable or continuous.
- The deformation gradient tensor maps small spheres into ellipsoids. (This is implied by the polar decomposition theorem.) The deformation state can describe more complex kinematics.

6.2 Peridynamic stress tensor

Recall from Section 2.5 that, as a consequence of Noll's lemma I [53, 49], the flux of linear momentum through a surface, *i.e.*, the force per unit area, can be expressed as the divergence of a tensor field. This tensor field is called the *peridynamic stress tensor* field, denoted $\boldsymbol{\nu}$. This can be expressed in terms of the primitive quantity $\mathbf{t}$ as

$$\boldsymbol{\nu}(\mathbf{x}) = \int_{\mathcal{U}} \int_0^\infty \int_0^\infty (y+z)^2 \mathbf{t}(\mathbf{x}+y\mathbf{m}, \mathbf{x}-z\mathbf{m}) \otimes \mathbf{m} \, dz \, dy \, d\Omega_{\mathbf{m}} \qquad (120)$$

where $\mathcal{U}$ is the unit sphere and $d\Omega_{\mathbf{m}}$ is a differential element of solid angle in the direction of the unit vector $\mathbf{m}$. The integrand can be alternatively expressed in terms of the force state by substituting

$$\mathbf{t}(\mathbf{x}+y\mathbf{m}, \mathbf{x}-z\mathbf{m}) = \underline{\mathbf{T}}[\mathbf{x}-z\mathbf{m}]\langle (y+z)\mathbf{m}\rangle. \qquad (121)$$

The peridynamic equation of motion in terms of the peridynamic stress tensor is formally identical to the classical equation of motion:

$$\rho\ddot{\mathbf{y}} = \operatorname{div} \boldsymbol{\nu} + \mathbf{b} \qquad \text{on } \mathcal{B},\ t \geq 0, \qquad (122)$$

in other words

$$\int_{\mathcal{B}} (\mathbf{t} - \mathbf{t}') \, dV' = \operatorname{div} \boldsymbol{\nu} \qquad \text{on } \mathcal{B},\ t \geq 0. \qquad (123)$$

The peridynamic stress tensor is similar to the Piola stress in the classical theory in that it provides the net force per unit area through a closed surface $\partial\mathcal{P}$ with unit normal $\mathbf{n}$:

$$\mathbf{F}_{\mathcal{P}} = \int_{\partial\mathcal{P}} \boldsymbol{\nu}\mathbf{n} \, dA.$$

However, the forces described by $\boldsymbol{\nu}$ are nonlocal; they represent direct interaction between points such as $\mathbf{x}+y\mathbf{m}$ in the exterior of $\partial\mathcal{P}$ with points such as $\mathbf{x}-z\mathbf{m}$ in the interior.

6.3 Convergence in the limit of small horizon

Under the assumption of a continuously differentiable deformation, the approximation (119) becomes more accurate as the horizon δ is reduced, because $|\boldsymbol{\xi}| \leq \delta$. It is also reasonable to expect that, since $\mathbf{t}$ in (121) is non-null only when $y + z \leq \delta$, the (nonlocal) peridynamic stress tensor should approach the (local) Piola stress tensor as δ is reduced.

To further investigate the convergence of the peridynamic equations to the classical equations, it is necessary to specify what it means for a peridynamic constitutive model to change horizon. Restricting attention to elastic materials, one way to do this is to require that for a homogeneous deformation of a homogeneous body, the strain energy density should be invariant as the horizon changes. To make this precise, suppose a material model $\hat{W}_1$ is given with horizon δ_1. For any horizon $\delta > 0$, define $s = \delta/\delta_1$. Let $\mathcal{H}_s$ be the family with horizon δ, and let $\mathcal{V}_s$ be the set of vector states on $\mathcal{H}_s$. Define an elastic material model by

$$\hat{W}_s(\underline{\mathbf{Y}}_s) = \hat{W}_1\big(\underline{\mathbf{E}}_s(\underline{\mathbf{Y}}_s)\big) \qquad \forall\, \underline{\mathbf{Y}}_s \in \mathcal{V}_s \tag{124}$$

where $\underline{\mathbf{E}}_s(\cdot) : \mathcal{V}_s \to \mathcal{V}_1$ is defined by

$$\underline{\mathbf{E}}_s(\underline{\mathbf{Y}}_s)\langle\boldsymbol{\xi}\rangle = \frac{\underline{\mathbf{Y}}_s\langle s\boldsymbol{\xi}\rangle}{s}, \qquad \forall\, \boldsymbol{\xi} \in \mathcal{H}_1. \tag{125}$$

Geometrically, $\underline{\mathbf{E}}_s$ rescales the length of bonds $\boldsymbol{\xi} \in \mathcal{H}_s$ to the original family $\mathcal{H}_1$. To confirm that the new material model defined in (124) possesses the required invariance under rescaling, let a homogeneous deformation of a large body $\mathcal{B}$ be defined by

$$\mathbf{y}(\mathbf{x}) = \mathbf{F}_0\mathbf{x} + \mathbf{c} \qquad \forall\, \mathbf{x} \in \mathcal{B}$$

where $\mathbf{F}_0$ is a constant tensor, $\det \mathbf{F}_0 > 0$, and $\mathbf{c}$ is a constant vector. If $\mathbf{x} \in \mathcal{B}$ is sufficiently far from the boundary of the body that its family does not include any points on this boundary, then from (118),

$$\underline{\mathbf{Y}}_s\langle\boldsymbol{\xi}\rangle = \mathbf{F}_0\boldsymbol{\xi} \qquad \forall\, \boldsymbol{\xi} \in \mathcal{H}_s. \tag{126}$$

Then for any $\boldsymbol{\xi} \in \mathcal{V}_1$, from (125) and (126),

$$\underline{\mathbf{E}}_s(\underline{\mathbf{Y}}_s)\langle\boldsymbol{\xi}\rangle = \frac{\underline{\mathbf{Y}}_s\langle s\boldsymbol{\xi}\rangle}{s} = \frac{\mathbf{F}_0 s\boldsymbol{\xi}}{s} = \mathbf{F}_0\boldsymbol{\xi}.$$

So, if the deformation is homogeneous, $\underline{\mathbf{E}}_s(\underline{\mathbf{Y}}_s)$ is independent of s. Therefore, under this assumption, $\hat{W}_s(\underline{\mathbf{Y}}_s)$ defined through (124) is also independent of s. This proves that this rescaled material model is invariant under changes in δ if the deformation is homogeneous.

Now let $\hat{\underline{\mathbf{T}}}_s$ denote the constitutive model for the force state derived from $\hat{W}_s$:

$$\hat{\underline{\mathbf{T}}}_s(\underline{\mathbf{Y}}_s) = \nabla \hat{W}_s(\underline{\mathbf{Y}}_s) \qquad \forall \underline{\mathbf{Y}}_s \in \mathcal{V}_s.$$

It is easily shown [68] that this force state scales with s as follows:

$$\hat{\underline{\mathbf{T}}}_s(\underline{\mathbf{Y}}_s)\langle \boldsymbol{\xi} \rangle = s^{-4} \hat{\underline{\mathbf{T}}}_1\big(\underline{\mathbf{E}}_s(\underline{\mathbf{Y}}_s)\big)\langle \boldsymbol{\xi}/s \rangle \qquad \forall \boldsymbol{\xi} \in \mathcal{H}_s. \tag{127}$$

Let $\boldsymbol{\nu}_s$ denote the peridynamic stress tensor obtained from its definition (120) for this $\hat{\underline{\mathbf{T}}}_s$ using (121):

$$\boldsymbol{\nu}_s(\mathbf{x}) = \int_{\mathcal{U}} \int_0^\infty \int_0^\infty (y+z)^2 \hat{\underline{\mathbf{T}}}_s(\underline{\mathbf{Y}}_s)[\mathbf{x} - z\mathbf{m}]\langle (y+z)\mathbf{m} \rangle \otimes \mathbf{m} \, dz \, dy \, d\Omega_{\mathbf{m}}.$$

Returning to the case of a given continuously differentiable deformation with deformation gradient tensor field $\mathbf{F}$, it can be shown [68] that $\boldsymbol{\nu}_s$ approaches a limit given by

$$\boldsymbol{\nu}_s(\mathbf{x}) \to \boldsymbol{\sigma}(\mathbf{F}(\mathbf{x})) \quad \text{as } s \to 0 \quad \forall\, \mathbf{x} \in \mathcal{B}$$

where $\boldsymbol{\sigma}$ is the function defined by

$$\boldsymbol{\sigma}(\mathbf{F}) = \int_{\mathcal{H}_1} \hat{\underline{\mathbf{T}}}_1(\mathbf{F}\underline{\mathbf{X}})\langle \boldsymbol{\xi} \rangle \otimes \boldsymbol{\xi} \, dV_{\boldsymbol{\xi}} \quad \forall\, \mathbf{F} \in \mathcal{L}^+ \tag{128}$$

where $\mathcal{L}^+$ is the set of all second order tensors with positive determinant. $\boldsymbol{\sigma}$ is called the *collapsed stress tensor* because it represents the limit, under the present assumptions, of the peridynamic stress tensor for the horizon collapsing to zero. It can further be shown [68] that

$$\text{div } \boldsymbol{\nu}_s(\mathbf{x}) \to \text{div } \boldsymbol{\sigma}(\mathbf{F}(\mathbf{x})) \quad \text{as } s \to 0, \quad \forall \mathbf{x} \in \mathcal{B}, \tag{129}$$

and that

$$\boldsymbol{\sigma}(\mathbf{F}) = \frac{\partial \Omega}{\partial \mathbf{F}}(\mathbf{F}) \qquad \forall \mathbf{F} \in \mathcal{L}^+$$

where Ω is defined by

$$\Omega(\mathbf{F}) = \hat{W}_1(\mathbf{F}\underline{\mathbf{X}}) \qquad \forall \mathbf{F} \in \mathcal{L}^+.$$

Furthermore, $\boldsymbol{\sigma}$ and Ω inherit properties from the peridynamic material with horizon δ_1 characteristic of a Piola stress tensor:

- Objectivity: Let $\mathcal{O}^+$ be the set of all proper orthogonal tensors. Then

$$\begin{aligned} &\hat{W}_1(\mathbf{Q}\underline{\mathbf{Y}}) = \hat{W}_1(\underline{\mathbf{Y}}) \quad \forall \underline{\mathbf{Y}} \in \mathcal{V}_1,\ \mathbf{Q} \in \mathcal{O}^+ \\ &\quad \Longrightarrow \quad \Omega(\mathbf{Q}\mathbf{F}) = \Omega(\mathbf{F}) \quad \forall \mathbf{F} \in \mathcal{L}^+,\ \mathbf{Q} \in \mathcal{O}^+. \end{aligned}$$

- Isotropy:

$$\hat{W}_1(\underline{\mathbf{Y}}\mathbf{Q}) = \hat{W}_1(\underline{\mathbf{Y}}) \quad \forall \underline{\mathbf{Y}} \in \mathcal{V}_1,\ \mathbf{Q} \in \mathcal{O}^+$$
$$\Longrightarrow \quad \Omega(\mathbf{F}\mathbf{Q}) = \Omega(\mathbf{F}) \quad \forall \mathbf{F} \in \mathcal{L}^+,\ \mathbf{Q} \in \mathcal{O}^+.$$

- Balance of angular momentum:

$$\int_{\mathcal{H}_1} \underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle \times \hat{\underline{\mathbf{T}}}_1(\underline{\mathbf{Y}})\langle\boldsymbol{\xi}\rangle \, dV_{\boldsymbol{\xi}} = \mathbf{0} \qquad \forall \underline{\mathbf{Y}} \in \mathcal{V}_1$$
$$\Longrightarrow \quad \boldsymbol{\sigma}(\mathbf{F})\mathbf{F}^T = \mathbf{F}\boldsymbol{\sigma}^T(\mathbf{F}) \qquad \forall \mathbf{F} \in \mathcal{L}^+.$$

(129) means that if a given deformation is twice continuously differentiable, we can compare the acceleration fields $\ddot{\mathbf{y}}_s$ computed by the peridynamic theory, for a material with horizon $s\delta_1$, to those of the classical theory $\ddot{\mathbf{y}}_0$:

$$\ddot{\mathbf{y}}_s \to \ddot{\mathbf{y}}_0 \qquad \text{as } s \to 0$$

where

$$\ddot{\mathbf{y}}_s = \int_{\mathcal{H}} \left[\underline{\mathbf{T}}_s[\mathbf{x}]\langle \mathbf{x}' - \mathbf{x} \rangle - \underline{\mathbf{T}}_s[\mathbf{x}']\langle \mathbf{x} - \mathbf{x}' \rangle \right] dV_{\mathbf{x}'} + \mathbf{b}$$

and

$$\ddot{\mathbf{y}}_0 = \operatorname{div} \boldsymbol{\sigma} + \mathbf{b}.$$

In these equations, $\underline{\mathbf{T}}_s$ and $\boldsymbol{\sigma}$ are derived from the same peridynamic material model with horizon δ_1 through (127) and (128) respectively.

In this sense, the peridynamic theory converges to the classical theory in the limit of small horizon. Stated differently, the PDEs of the classical theory are obtainable from the peridynamic equations as a limiting case.

6.4 Elasticity tensor derived from a peridynamic material

Recall from Section 6.3 that a classical material model can be derived from a peridynamic model by requiring that the two produce the same stress tensor for all homogeneous deformations. The classical material model is given by (128), which provides a Piola stress tensor $\boldsymbol{\sigma}(\mathbf{F})$, where $\mathbf{F}$ is the deformation gradient tensor.

By specializing this approach to linear peridynamic material models, a fourth order elasticity tensor can be derived. To do this, substitute the linear constitutive model (98) into (128) and assume $\underline{\mathbf{T}}^0 = \underline{\mathbf{0}}$. Consider a displacement gradient tensor $\mathbf{H}$, not necessarily symmetric, where $|\mathbf{H}| \ll 1$. By setting $\mathbf{F} = \mathbf{1} + \mathbf{H}$, the following expression for the components of stress is obtained [63]:

$$\sigma_{ij} = \left[\int_{\mathcal{H}} \int_{\mathcal{H}} \underline{K}_{ik}\langle \boldsymbol{\xi}, \boldsymbol{\zeta} \rangle \xi_j \zeta_l \, dV_{\boldsymbol{\zeta}} \, dV_{\boldsymbol{\xi}} \right] H_{kl}.$$

The classical constitutive model for linear elasticity is

$$\sigma_{ij} = \mathsf{C}_{ijkl} H_{kl}$$

where C_{ijkl} is the fourth order elasticity tensor. Since $\mathbf{H}$ is arbitrary, comparing the last two equations leads to the conclusion that

$$\mathsf{C}_{ijkl} = \int_{\mathcal{H}} \int_{\mathcal{H}} \underline{K}_{ik}\langle \boldsymbol{\xi}, \boldsymbol{\zeta} \rangle \xi_j \zeta_l \, dV_{\boldsymbol{\zeta}} \, dV_{\boldsymbol{\xi}}.$$

Thus, a classical linear elastic material model has been obtained from a peridynamic linear elastic model. The two models give the same stress tensor for homogeneous deformations of a homogeneous body. They are expected to disagree for nonhomogeneous deformations, and the classical model is not applicable at all if a discontinuity in the deformation is present.

6.5 Nonlocal theories

In this section, the peridynamic model is compared with other *strongly nonlocal* theories, *i.e.,* theories in which points separated from each other by a finite distance interact directly. Also included is a comparison with higher order gradient models, which are *weakly nonlocal* because they contain a length scale in the constitutive model but do not explicitly include interactions across finite distances. The literature on such nonlocal models is large, and only a few representative models are discussed here to illustrate the main similarities and differences.

Strongly nonlocal theories have been proposed as a way to gain insight into the role of the finiteness of the interaction distance between atoms, particularly microstructure in crystals. A pioneering example of such a nonlocal theory is Kröner's [45] , which added nonlocal terms, in the form of an integral operator, to the local equation of motion for a body $\mathcal{B}$:

$$\rho(\mathbf{x})\ddot{u}_i(\mathbf{x},t) = C_{ijkl} u_{k,lj} + \int_{\mathcal{B}} \Phi_{ik}(\mathbf{x}' - \mathbf{x}) u_k(\mathbf{x}') \, dV_{\mathbf{x}'} + b_i(\mathbf{x},t)$$

where C_{ijkl} is the fourth order elasticity tensor, and Φ_{ik} is a function representing the effect of long-range interactions. Kröner's nonlocal model is linear because the integral is a linear operator. Because Kröner's equation of motion, like the classical equation of motion, involves the second partial derivatives of displacement, it does not lend itself to the study of phenomena involving discontinuities.

Perhaps the most widely known nonlocal elasticity theory is that of Eringen [24]. In its simplest form [23], its basic equations for an isotropic solid can be expressed as

$$\rho(\mathbf{x})\ddot{u}_i(\mathbf{x},t) = t_{ij,j}(\mathbf{x},t) + b_i(\mathbf{x},t)$$

$$t_{ij}(\mathbf{x},t) = \int_{\mathcal{B}} \alpha(|\mathbf{x}'-\mathbf{x}|)\sigma_{ij}(\mathbf{x}',t)\, dV_{\mathbf{x}'}$$
$$\sigma_{ij}(\mathbf{x},t) = \lambda\delta_{ij}u_{kk}(\mathbf{x},t) + 2\mu u_{i,j}(\mathbf{x},t)$$

where λ and μ are the usual Lamé moduli and α is a weighting function. Thus, in this version of Eringen's model, a nonlocal stress tensor t_{ij} is evaluated from the weighted volume average of the local stress tensor σ_{ij}. Like Kröner's model (and the classical local model), the form of Eringen's equations prevents it from achieving the goal of peridynamics, which is to apply the same field equations on or off of discontinuities. (However, Eringen, Speziale, and Kim [25] successfully treat the problem of a crack in a nonlocal elastic medium by, essentially, representing the crack as a zero-traction boundary condition. The solution to this problem demonstrates the absence of unbounded stress fields near the tip of a crack represented in this way within a nonlocal continuum.)

Kunin [46, 47] developed a nonlocal model in which internal forces are expressed directly in terms of the displacement:

$$\rho(\mathbf{x})\ddot{u}_i(\mathbf{x},t) = \int_{\mathcal{B}} \Phi_{ik}(\mathbf{x}'-\mathbf{x})u_k(\mathbf{x}')\, dV_{\mathbf{x}'} + b_i(\mathbf{x},t).$$

Formally, this expression is the same as the linearized equation of motion in the peridynamic model, (102). However, in the peridynamic equation, the kernel is derived by linearization of a material model in the nonlinear theory, and therefore allows the micromodulus function $\mathbf{C}_0$ in (102) to be obtained in an unambiguous way. For example, linearization of a peridynamic model of an isotropic fluid uniquely determines the appropriate $\mathbf{C}_0$ function [63].

Deriving the linearized material model as described in Section 5.3 also preserves the coupling between the forces within a large deformation state $\underline{\mathbf{Y}}^0$ and a superposed small displacement field. These potentially large forces have a major effect on the properties of plane waves, and therefore on material stability [63]. For example, in a typical crystal, there are large forces between the atoms regardless of the deformation. If the crystal has zero stress at a point, then the net force across any plane through that point is zero. But this does not change the fact that the forces are present; they merely cancel each other out. The coupling between these forces and superposed displacements cannot be neglected in a theory aimed at providing insight into the mechanics of microstructures.

A higher order approximation to the deformation state may be obtained by adding an additional term to the Taylor expansion in (119):

$$\underline{\mathbf{Y}}[\mathbf{x}]\langle\boldsymbol{\xi}\rangle = \mathbf{F}(\mathbf{x})\boldsymbol{\xi} + (\text{grad}\,\mathbf{F}(\mathbf{x}))(\boldsymbol{\xi}\otimes\boldsymbol{\xi}) + O(|\boldsymbol{\xi}|^3). \tag{130}$$

where (grad $\mathbf{F}(\mathbf{x})$) is a third order tensor representing a "strain gradient" term. If a constitutive model explicitly involves this new term, for example

if the free energy has the form

$$\psi(\mathbf{F}, \text{grad } \mathbf{F}),$$

the resulting mathematical description of the system is a *higher order gradient* theory. Theories of this type implicitly involve a length scale because the dimensions of the two arguments of ψ differ by length. If the deformation has continuous third derivatives in space, then (130) asymptotically represents a better approximation to $\underline{\mathbf{Y}}$ then (119). However, if there is a discontinuity in the deformation such as a crack, then a higher order gradient model is no more applicable than the classical local model.

Nevertheless, Seleson *et al.* [59] have shown that a higher order gradient approximation can be used as an intermediate step in upscaling a molecular dynamics model to peridynamics. To do this, these authors construct separate higher order gradient models from both an assumed peridynamic constitutive model and from the discrete system using an inner expansion technique [4]. The parameters in the peridynamic model are determined by matching the coefficients between these two higher order gradient expressions. In effect, this provides a peridynamic model for the discrete system that is demonstrated to accurately reproduce key features of the molecular dynamics model, including wave dispersion.

7 Discrete particles as peridynamic bodies

In this section it is shown that the ODEs describing the motion of discrete particles can be obtained as the limiting case of the motion of mutually interacting peridynamic bodies of finite volume, as their volume is reduced to zero. This limiting process could not be carried out within the classical theory of continuum mechanics, because nonlocality is a fundamental aspect of the system. The resulting interactions between the discrete particles have the same basic structure as the peridynamic continuum equations. It is further shown that these particles can be represented within the continuum equations with a mass density field and constitutive model that use generalized functions. This allows any multibody potential to be represented as a peridynamic material model.

Averaging the mass density and the interactions between particles results in a conventional (smooth) continuum. The averaged peridynamic stress tensor over a collection of particles provides, in effect, a Piola stress tensor field that appears in the classical (PDE) equation of motion. This result achieves the goal of deriving a classical stress tensor field from a set of particles interacting through an arbitrary multibody potential.

7.1 Self-equilibrated subregions

Let a body $\mathcal{B}$ be defined by

$$\mathcal{B} = \bigcup_{i=1}^{N} \mathcal{P}_i,$$

where the $\mathcal{P}_i$ are N disjoint bounded subregions. Assume that the nonpolarity condition (25) holds on $\mathcal{B}$. For each subregion, define its mass and center of mass by

$$M_i = \int_{\mathcal{P}_i} \rho(\mathbf{x})\, dV_{\mathbf{x}}, \qquad \mathbf{y}_i(t) = \frac{1}{M_i} \int_{\mathcal{P}_i} \rho(\mathbf{x})\mathbf{y}(\mathbf{x},t)\, dV_{\mathbf{x}}. \tag{131}$$

Recall the abbreviated notation defined in (12). Define the net force and that $\mathcal{P}_j$ exerts on $\mathcal{P}_i$ by

$$\mathbf{F}_{ij} = \int_{\mathcal{P}_i} \int_{\mathcal{P}_j} \mathbf{f}\, dV'\, dV \tag{132}$$

and the net external body force on $\mathcal{P}_i$ by

$$\mathbf{F}_i^{\text{ext}} = \int_{\mathcal{P}_i} \mathbf{b}\, dV. \tag{133}$$

Within each $\mathcal{P}_i$, let $\mathbf{r}_i$ denoted the deformed position vector relative to the deformed center of mass:

$$\mathbf{r}_i(\mathbf{x},t) = \mathbf{y}(\mathbf{x},t) - \mathbf{y}_i(t), \qquad \forall \mathbf{x} \in \mathcal{P}_i. \tag{134}$$

The net moment about $\mathbf{y}_i$ that $\mathcal{P}_j$ exerts on $\mathcal{P}_i$ is found from

$$\boldsymbol{\tau}_{ij} = \int_{\mathcal{P}_i}\int_{\mathcal{P}_j} \mathbf{r}_i \times \mathbf{f}\, dV'\, dV. \tag{135}$$

where $\mathbf{r}_i = \mathbf{r}_i(\mathbf{x},t)$. The net external moment on $\mathcal{P}_i$ about $\mathbf{y}_i$ is given by

$$\boldsymbol{\tau}_i^{\text{ext}} = \int_{\mathcal{P}_i} \mathbf{r}_i \times \mathbf{b}\, dV. \tag{136}$$

The condition

$$\mathbf{F}_{ii} = \mathbf{0}, \qquad i = 1,\dots,N \tag{137}$$

is always satisfied because of (6) and (132). If the subregions are separated by empty space and are small in size relative to the distances between them, it is reasonable to require on physical grounds that

$$\boldsymbol{\tau}_{ii} = \mathbf{0}, \qquad i = 1,\dots,N. \tag{138}$$

A system in which (138) holds will be called *self-equilibrated*. This condition does not follow from the antisymmetry of $\mathbf{f}$, except in the special case of an ordinary material (see Section 4.3).

An alternate form of the condition (138) may be derived as follows. By (11), (132), (134), (135), and (137),

$$\begin{aligned}
\boldsymbol{\tau}_{ii} &= \int_{\mathcal{P}_i}\int_{\mathcal{P}_i} \mathbf{r}_i \times \mathbf{f}\, dV'\, dV = \mathbf{y}_i \times \mathbf{F}_{ii} + \int_{\mathcal{P}_i}\int_{\mathcal{P}_i} \mathbf{r}_i \times \mathbf{f}\, dV'\, dV \\
&= \int_{\mathcal{P}_i}\int_{\mathcal{P}_i} (\mathbf{y}_i + \mathbf{r}_i) \times (\mathbf{t} - \mathbf{t}')\, dV'\, dV \\
&= \int_{\mathcal{P}_i}\int_{\mathcal{P}_i} \mathbf{y} \times (\mathbf{t} - \mathbf{t}')\, dV'\, dV \\
&= \int_{\mathcal{P}_i}\int_{\mathcal{P}_i} (\mathbf{y}' - \mathbf{y}) \times \mathbf{t}\, dV'\, dV.
\end{aligned}$$

where the change of dummy variable of integration $\mathbf{x} \leftrightarrow \mathbf{x}'$ has been used in the last step. Since the material is assumed to be nonpolar, (25) holds. So, the last expression implies

$$\boldsymbol{\tau}_{ii} = \int_{\mathcal{P}_i}\int_{\mathcal{B}\setminus\mathcal{P}_i} (\mathbf{y}' - \mathbf{y}) \times \mathbf{t}\, dV'\, dV.$$

Therefore, an alternate form of the condition for self-equilibration (138) is

$$\int_{\mathcal{P}_i} \int_{\mathcal{B}\setminus\mathcal{P}_i} (\mathbf{y}' - \mathbf{y}) \times \mathbf{t}\, dV'\, dV = \mathbf{0}, \qquad i = 1, \ldots, N. \tag{139}$$

We emphasize that self-equilibration does not hold in general; it reflects the special physical situation of small bodies separated by large empty distances.

7.2 Linear and angular momentum in self-equilibrated subregions

From the local balance of linear momentum (15) integrated over $\mathcal{P}_i$,

$$\int_{\mathcal{P}_i} \rho \ddot{\mathbf{y}}\, dV = \int_{\mathcal{P}_i} \int_{\mathcal{B}} \mathbf{f}\, dV'\, dV + \int_{\mathcal{P}_i} \mathbf{b}\, dV.$$

In view of (131), (132), (133), and (137), this is equivalent to

$$M_i \ddot{\mathbf{y}}_i = \sum_{j \neq i} \mathbf{F}_{ij} + \mathbf{F}_i^{\text{ext}}, \qquad i = 1, \ldots, N. \tag{140}$$

Equation (140) is the balance of linear momentum for the subregions expressed in terms of the centers of mass, the net force between the subregions, and the net external forces. It holds regardless of whether the subregions are self-equilibrated.

Now consider the balance of angular momentum about the origin in subregion $\mathcal{P}_i$:

$$\frac{d}{dt} \int_{\mathcal{P}_i} \rho \mathbf{y} \times \dot{\mathbf{y}}\, dV = \int_{\mathcal{P}_i} \rho \mathbf{y} \times \ddot{\mathbf{y}}\, dV = \int_{\mathcal{P}_i} \int_{\mathcal{B}} \mathbf{y} \times \mathbf{f}\, dV'\, dV + \int_{\mathcal{P}_i} \mathbf{y} \times \mathbf{b}\, dV.$$

Using (134),

$$\begin{aligned} &\int_{\mathcal{P}_i} \rho(\mathbf{y}_i + \mathbf{r}_i) \times (\ddot{\mathbf{y}}_i + \ddot{\mathbf{r}}_i)\, dV \\ &\qquad = \int_{\mathcal{P}_i} \int_{\mathcal{B}} (\mathbf{y}_i + \mathbf{r}_i) \times \mathbf{f}\, dV'\, dV + \int_{\mathcal{P}_i} (\mathbf{y}_i + \mathbf{r}_i) \times \mathbf{b}\, dV. \end{aligned} \tag{141}$$

But from (131) and (134),

$$\int_{\mathcal{P}_i} \rho \mathbf{r}_i\, dV = \int_{\mathcal{P}_i} \rho \ddot{\mathbf{r}}_i\, dV = \mathbf{0}.$$

From this, the terms on the left hand side of (141) involving $\mathbf{r}_i \times \ddot{\mathbf{y}}_i$ and $\mathbf{y}_i \times \ddot{\mathbf{r}}_i$ drop out. Grouping the remaining terms involving $\mathbf{y}_i$ together and using (132) and (133) results in

$$\mathbf{y}_i \times \Big(M_i \ddot{\mathbf{y}}_i - \sum_{j \neq i} \mathbf{F}_{ij} - \mathbf{F}_i^{\text{ext}} \Big) + \int_{\mathcal{P}_i} \rho \mathbf{r}_i \times \ddot{\mathbf{r}}_i\, dV = \int_{\mathcal{P}_i} \int_{\mathcal{B}} \mathbf{r}_i \times \mathbf{f}\, dV'\, dV + \int_{\mathcal{P}_i} \mathbf{r}_i \times \mathbf{b}\, dV.$$

By the balance of linear momentum (140), the term in parentheses vanishes, so that

$$\int_{\mathcal{P}_i} \rho \mathbf{r}_i \times \ddot{\mathbf{r}}_i \, dV = \int_{\mathcal{P}_i} \int_{\mathcal{B}} \mathbf{r}_i \times \mathbf{f} \, dV' \, dV + \int_{\mathcal{P}_i} \mathbf{r}_i \times \mathbf{b} \, dV.$$

If the subregions are self-equilibrated, (138) allows this to be rewritten in the form

$$\dot{\mathbf{a}}_i = \sum_{j \neq i} \boldsymbol{\tau}_{ij} + \boldsymbol{\tau}_i^{\text{ext}}, \qquad i = 1, \ldots, N \tag{142}$$

where

$$\mathbf{a}_i = \int_{\mathcal{P}_i} \rho \mathbf{r}_i \times \dot{\mathbf{r}}_i \, dV$$

and $\boldsymbol{\tau}_{ij}$ and $\boldsymbol{\tau}_i^{\text{ext}}$ are defined in (135) and (136) respectively. Since $\mathbf{a}_i$ is the angular momentum of $\mathcal{P}_i$ about its own deformed center of mass, $\mathbf{a}_i$ can be thought of as the angular momentum due to the the "spin" of the subregion. (142) asserts that if the subregions are self-equilibrated, changes in this spin are independent of net force on the subregion.

7.3 Peridynamic particles

The next step is to investigate the balance of angular momentum in the limit of self-equilibrated subregions with zero size. This limiting case represents *peridynamic particles*. To derive the properties of these particles, we adopt an *ansatz* concerning the nature of the forces during this limiting process such that the net forces remain fixed. Suppose that each subregion $\mathcal{P}_i$ is bounded by a sphere centered at the center of mass in the reference configuration $\mathbf{x}_i$. It is assumed that there exists a number $\epsilon > 0$ such that $|\mathbf{r}_i| \leq \epsilon$ for all i and all $t \geq 0$, where $\mathbf{r}_i$ is defined in (134). The sizes of the $\mathcal{P}_i$ in the reference configuration are variable and are parameterized by ϵ.

For any $\epsilon > 0$ and any $\mathcal{P}_i$, assume that the bond force densities obey the following *ansatz*:

$$\mathbf{t} = \mathbf{T}_{ij} \varphi_{ij}(\mathbf{x}', \mathbf{x}, \epsilon) \tag{143}$$

where the $\mathbf{T}_{ij}$ are vectors independent of ϵ. φ_{ij} is a non-negative function on $\mathcal{P}_i \times \mathcal{P}_j \times \mathbb{R}^+$ such that for any $\epsilon > 0$, $\int_{\mathcal{P}_i} \int_{\mathcal{P}_j} \varphi_{ij} = 1$. From (143), it is immediate that

$$\mathbf{T}_{ij} = \int_{\mathcal{P}_i} \int_{\mathcal{P}_j} \mathbf{t} \, dV' \, dV. \tag{144}$$

From (11), (135), and (143), since $|\mathbf{r}| \leq \epsilon$, it follows that

$$\begin{aligned}
|\boldsymbol{\tau}_{ij}| &= \left| \int_{\mathcal{P}_i} \int_{\mathcal{P}_j} \mathbf{r}_i \times (\mathbf{t} - \mathbf{t}') \, dV' \, dV \right| \\
&\leq \int_{\mathcal{P}_i} \int_{\mathcal{P}_j} |\mathbf{r}_i| \, |\mathbf{T}_{ij}\varphi_{ij} - \mathbf{T}_{ji}\varphi_{ji}| \, dV' \, dV \\
&\leq \epsilon |\mathbf{T}_{ij}| \int_{\mathcal{P}_i} \int_{\mathcal{P}_j} \varphi_{ij} + \epsilon |\mathbf{T}_{ji}| \int_{\mathcal{P}_i} \int_{\mathcal{P}_j} \varphi_{ji} \, dV' \, dV \\
&\leq \epsilon \big(|\mathbf{T}_{ij}| + |\mathbf{T}_{ji}| \big),
\end{aligned}$$

hence

$$\boldsymbol{\tau}_{ij} = O(\epsilon) \quad \text{as} \quad \epsilon \to 0.$$

Adopting an *ansatz* for $\mathbf{b}$ similar to (143) leads to

$$\boldsymbol{\tau}_i^{\text{ext}} = O(\epsilon) \quad \text{as} \quad \epsilon \to 0.$$

From these results and (142), the conclusion is that

$$\dot{\mathbf{a}}_i \to \mathbf{0} \quad \text{as} \quad \epsilon \to 0. \tag{145}$$

This proves that in the limit $\epsilon \to 0$, the angular momentum of a peridynamic particle about its own deformed center of mass is independent of time.

Next we derive a condition for nonpolarity of the interparticle forces $\mathbf{T}_{ij}$. Continuing under the *ansatz* (143), since the $\mathcal{P}_i$ are self-equilibrated, (139) implies

$$\begin{aligned}
\mathbf{0} &= \int_{\mathcal{P}_i} \int_{\mathcal{B}\setminus\mathcal{P}_i} (\mathbf{y}' - \mathbf{y}) \times \mathbf{t} \, dV' \, dV \\
&= \int_{\mathcal{P}_i} \sum_{j \neq i} \int_{\mathcal{P}_j} (\mathbf{y}' - \mathbf{y}) \times \mathbf{t} \, dV' \, dV \\
&= \int_{\mathcal{P}_i} \sum_{j \neq i} \int_{\mathcal{P}_j} \big((\mathbf{y}_j + \mathbf{r}_j') - (\mathbf{y}_i + \mathbf{r}_i) \big) \times \mathbf{t} \, dV' \, dV \\
&= \sum_{j \neq i} (\mathbf{y}_j - \mathbf{y}_i) \times \mathbf{T}_{ij} + \int_{\mathcal{P}_i} \sum_{j \neq i} \int_{\mathcal{P}_j} (\mathbf{r}_j' - \mathbf{r}_i) \times \mathbf{t} \, dV' \, dV \\
&= \sum_{j \neq i} (\mathbf{y}_j - \mathbf{y}_i) \times \mathbf{T}_{ij} + O(\epsilon) \quad \text{as} \quad \epsilon \to 0
\end{aligned}$$

where $\mathbf{r}_j' = \mathbf{r}_j(\mathbf{x}', t)$. So, in the limit $\epsilon \to 0$, the requirement of nonpolarity (25) reduces to

$$\sum_{j \neq i} (\mathbf{y}_j - \mathbf{y}_i) \times \mathbf{T}_{ij} = \mathbf{0} \tag{146}$$

for all i, which states that the net moment about $\mathbf{y}_i$ exerted by the $\mathbf{T}_{ij}$ on the other particles is zero.

Using (11), (132), and (144), it follows that

$$\mathbf{F}_{ij} = \mathbf{T}_{ij} - \mathbf{T}_{ji}$$

for all i and j. Then by (140), the balance of linear momentum for peridynamic particles may be written as

$$M_i \ddot{\mathbf{y}}_i = \sum_{j \neq i} (\mathbf{T}_{ij} - \mathbf{T}_{ji}) + \mathbf{F}_i^{\text{ext}} \tag{147}$$

for all i.

We have already investigated the dependence of angular momentum of peridynamic particles about their own deformed center of mass, with the result (145). Now we consider the balance of angular momentum of particles about the origin. To do this, once again take the limit as $\epsilon \to 0$ in the global balance of angular momentum (27), leading to

$$M_i \mathbf{y}_i \times \ddot{\mathbf{y}}_i = \sum_{j \neq i} \big(\mathbf{y}_j \times \mathbf{T}_{ij} - \mathbf{y}_i \times \mathbf{T}_{ji} \big) + \mathbf{y}_i \times \mathbf{F}_i^{\text{ext}}. \tag{148}$$

It is easy to show that this relation holds if the forces are nonpolar. To see this, note that (147) implies

$$M_i \mathbf{y}_i \times \ddot{\mathbf{y}}_i = \mathbf{y}_i \times \Big(\sum_{j \neq i} (\mathbf{T}_{ij} - \mathbf{T}_{ji}) + \mathbf{F}_i^{\text{ext}} \Big).$$

Add (146) to this result to obtain (148). Thus, if nonpolarity holds, then the global balance of angular momentum follows from the balance of linear momentum.

It is a standard result in textbooks that for pairwise interactions between particles, in which the force vector $\mathbf{F}_{ij}$ is parallel to the relative deformed position vector $\mathbf{y}_j - \mathbf{y}_i$, the balance of angular momentum follows from the balance of linear momentum. In the present case of more complex interactions, the additional nonpolarity relation (146) is required. Of course, this additional relation is trivially satisfied in the special case of pairwise interactions.

By (56), (59), and (144), it follows that the $\mathbf{T}_{ij}$ can be expressed in the form

$$\mathbf{T}_{ij} = \hat{\mathbf{T}}_{ij}(\mathbf{y}_1, \ldots, \mathbf{y}_N),$$

where the $\hat{\mathbf{T}}_{ij}$ are suitably defined functions. These functions provide a constitutive model for the forces between peridynamic particles. The functions $\hat{\mathbf{T}}_{ij}$ must satisfy the nonpolarity requirement (146).

7.4 Particles as a special case of a continuum

In this section we demonstrate that a collection of discrete peridynamic particles, together with the forces between them, can be represented within the framework of the continuum theory using generalized functions. To do this, let $\mathbf{x}_i$ denote the reference positions of the particles. Define a peridynamic body and its bond force densities by

$$\rho(\mathbf{x}) = \sum_i M_i \Delta(\mathbf{x} - \mathbf{x}_i), \qquad \mathbf{b}(\mathbf{x}, t) = \sum_i \mathbf{F}_i^{\text{ext}}(t) \Delta(\mathbf{x} - \mathbf{x}_i), \tag{149}$$

$$\mathbf{t}(\mathbf{x}', \mathbf{x}, t) = \sum_i \sum_{j \neq i} \mathbf{T}_{ij}(t) \Delta(\mathbf{x} - \mathbf{x}_i) \Delta(\mathbf{x}' - \mathbf{x}_j) \tag{150}$$

where Δ is the three dimensional Dirac delta function (which has units of volume^{-1}). To confirm that this body reproduces the accelerations for peridynamic particles given by (147), substitute these expressions into the equation of motion (16):

$$\rho(\mathbf{x}) \ddot{\mathbf{y}}(\mathbf{x}, t) = \int_{\mathcal{B}} \big(\mathbf{t}(\mathbf{x}', \mathbf{x}, t) - \mathbf{t}(\mathbf{x}, \mathbf{x}', t) \big) \, dV' + \mathbf{b}(\mathbf{x}, t)$$

to obtain

$$\sum_i M_i \Delta(\mathbf{x} - \mathbf{x}_i) \ddot{\mathbf{y}}(\mathbf{x}, t) = \sum_i \mathbf{F}_i^{\text{ext}}(t) \Delta(\mathbf{x} - \mathbf{x}_i)$$
$$+ \int_{\mathcal{B}} \sum_i \sum_{j \neq i} \mathbf{T}_{ij}(t) \big(\Delta(\mathbf{x} - \mathbf{x}_i) \Delta(\mathbf{x}' - \mathbf{x}_j) - \Delta(\mathbf{x}' - \mathbf{x}_i) \Delta(\mathbf{x} - \mathbf{x}_j) \big) \, dV_{\mathbf{x}'}.$$

Taking $\mathbf{x}$ to be any of the particle reference positions, and carrying out the integration using the properties of the delta function, leads to (147).

Expressing the constitutive model (150) at $\mathbf{x}_i$ in terms of a force state, set

$$\underline{\mathbf{T}}[\mathbf{x}, t] \langle \boldsymbol{\xi} \rangle = \mathbf{t}(\mathbf{x} + \boldsymbol{\xi}, \mathbf{x}, t)$$

to obtain

$$\underline{\mathbf{T}}[\mathbf{x}, t] \langle \boldsymbol{\xi} \rangle = \sum_i \sum_{j \neq i} \mathbf{T}_{ij}(t) \Delta(\mathbf{x} - \mathbf{x}_i) \Delta(\boldsymbol{\xi} - (\mathbf{x}_j - \mathbf{x}_i)). \tag{151}$$

With this constitutive model and (149), the equations for peridynamic particles are seen to be a special case of the continuum theory.

7.5 Multibody potentials

Consider a set of N particles with masses $M_1, \ldots, M_N$ and current positions $\mathbf{y}_1, \ldots, \mathbf{y}_N$. Let the potential energy of this set of particles be given by $U(\mathbf{y}_1, \ldots, \mathbf{y}_n)$, where U is an N-body potential. Assume that U has the property of translational invariance:

$$U(\mathbf{y}_1 + \mathbf{c}, \ldots, \mathbf{y}_N + \mathbf{c}) = U(\mathbf{y}_1, \ldots, \mathbf{y}_N) \tag{152}$$

for any constant vector $\mathbf{c}$. Also assume that U satisfies the balance of linear momentum,

$$\sum_{i=1}^{N} \frac{\partial U}{\partial \mathbf{y}_i}(\mathbf{y}_1, \ldots, \mathbf{y}_N) = \mathbf{0}, \tag{153}$$

and the balance of angular momentum,

$$\sum_{i=1}^{N} \mathbf{y}_i \times \frac{\partial U}{\partial \mathbf{y}_i}(\mathbf{y}_1, \ldots, \mathbf{y}_N) = \mathbf{0}. \tag{154}$$

These two assumptions are equivalent to requiring that each N-tuple of particles have constant total linear and angular momentum in the absence of any other interactions. Define arbitrary reference positions of the particles $\mathbf{x}_1, \ldots, \mathbf{x}_N$ independent of time, and let the particle locations be described by the motion $\mathbf{y}(\mathbf{x}, t)$, so that

$$\mathbf{y}_i = \mathbf{y}(\mathbf{x}_i, t), \qquad i = 1, \ldots, N. \tag{155}$$

Let $\mathbf{x}_0$ be an arbitrary fixed point called the *reference point* for this N-tuple of particles. This reference point may or may not coincide with the reference positions of any of the particles. Define an elastic nonhomogeneous peridynamic body by the following mass density and body force density:

$$\rho(\mathbf{x}) = \sum_{i=1}^{N} M_i \Delta(\mathbf{x} - \mathbf{x}_i), \qquad \mathbf{b}(\mathbf{x}, t) = \sum_{i=1}^{N} \mathbf{F}_i^{\text{ext}}(t) \Delta(\mathbf{x} - \mathbf{x}_i) \tag{156}$$

and by the following strain energy density function:

$$\hat{W}(\underline{\mathbf{Y}}, \mathbf{x}) = \Delta(\mathbf{x} - \mathbf{x}_0) U(\mathbf{y}_1, \ldots, \mathbf{y}_N) \tag{157}$$

where Δ is the three dimensional Dirac delta function. To put (157) in a form whose right hand side depends explicitly on $\underline{\mathbf{Y}}$, recall the definition of the deformation state (55), and use the abbreviated notation

$$\mathbf{y} = \mathbf{y}(\mathbf{x}, t), \qquad \underline{\mathbf{Y}} = \underline{\mathbf{Y}}[\mathbf{x}, t]. \tag{158}$$

Then, for any $\mathbf{x}$,

$$\mathbf{y}_i = \mathbf{y} + \underline{\mathbf{Y}}\langle \mathbf{x}_i - \mathbf{x}\rangle, \qquad i = 1, \ldots, N.$$

Now we can rewrite $\hat{W}$ in terms of the deformation state:

$$\begin{aligned}\hat{W}(\underline{\mathbf{Y}}, \mathbf{x}) &= \Delta(\mathbf{x} - \mathbf{x}_0) U(\mathbf{y}_1, \ldots, \mathbf{y}_N) \\ &= \Delta(\mathbf{x} - \mathbf{x}_0) U(\mathbf{y} + \underline{\mathbf{Y}}\langle \mathbf{x}_1 - \mathbf{x}\rangle, \ldots, \mathbf{y} + \underline{\mathbf{Y}}\langle \mathbf{x}_N - \mathbf{x}\rangle) \\ &= \Delta(\mathbf{x} - \mathbf{x}_0) U(\underline{\mathbf{Y}}\langle \mathbf{x}_1 - \mathbf{x}\rangle, \ldots, \underline{\mathbf{Y}}\langle \mathbf{x}_N - \mathbf{x}\rangle). \end{aligned} \tag{159}$$

In the last step of (159), the translational invariance of U was used as stated in (152). Using (75), it is easily confirmed that the force state corresponding to this $\hat{W}$ is given by

$$\underline{\hat{\mathbf{T}}}(\underline{\mathbf{Y}}, \mathbf{x})\langle \boldsymbol{\xi}\rangle = \Delta(\mathbf{x} - \mathbf{x}_0) \sum_{i=1}^{N} \frac{\partial U}{\partial \mathbf{y}_i} \Delta(\boldsymbol{\xi} - (\mathbf{x}_i - \mathbf{x})).$$

It can also be confirmed directly that with ρ and $\mathbf{b}$ supplied by (156), the equation of motion (16), evaluated at any $\mathbf{x} = \mathbf{x}_i$, implies

$$M_i \ddot{\mathbf{y}}_i = -\frac{\partial U}{\partial \mathbf{y}_i} + \mathbf{F}_i^{\text{ext}}, \qquad i = 1, \ldots, N \tag{160}$$

which shows that the force on particle i due to interactions with other members of the N-tuple is $-\partial U/\partial \mathbf{y}_i$.

In subsequent discussion, it will be necessary to have the peridynamic description of the N-tuple of particles in the form (151). This can be accomplished by treating the reference point for the N-tuple, $\mathbf{x}_0$, as a particle with zero mass. Define

$$M_0 = 0, \qquad \mathbf{T}_{0j} = \frac{\partial U}{\partial \mathbf{y}_j}, \qquad j = 1, \ldots, N \tag{161}$$

and

$$\mathbf{T}_{00} = \mathbf{T}_{j0} = \mathbf{T}_{ij} = \mathbf{0}, \qquad i = 1, \ldots, N,\ j = 1, \ldots, N. \tag{162}$$

With these definitions, the equation of motion for peridynamic particles (147) implies (160). It also implies the additional relation

$$M_0 \ddot{\mathbf{y}}_0 = \sum_{j=1}^{N} \frac{\partial U}{\partial \mathbf{y}_j} = \mathbf{0}$$

which vanishes because of (153). With the definitions (161) and (162), the requirement for nonpolarity (146) is immediately seen to be implied by (154).

Several results have been obtained:

- This N-tuple of particles interacting through the multibody potential U can be described exactly as a peridynamic state-based constitutive model with a strain energy density function $\hat{W}(\cdot, \mathbf{x})$ that is nonzero at a *single arbitrary point* $\mathbf{x} = \mathbf{x}_0$.
- The bond force densities in the force state at this $\mathbf{x}_0$ involve only the partial derivatives of U.
- These bond force densities generate the correct expression for Newton's second law for the particles, (160).
- We did not need to identify the force that each particle exerts on the other, since the forces $\mathbf{T}_{0j}$ only involve the gradient of the N-body potential.
- Nonpolarity of the bond force densities is necessarily satisfied for any admissible U.

The primary limitation of the method presented here for treating molecular dynamics through the peridynamic equations is that the N-tuples that interact through the multibody potentials are defined in the reference configuration, so it is assumed that these sets of particles do not change over time. This would be a good approximation for solids, but not fluids, in which the sets of particles that interact would evolve over time. However, it may be possible to extend the peridynamic theory to an Eulerian framework, which would avoid this problem.

7.6 Peridynamic stress due to two discrete particles

Consider two distinct particles i and j with reference positions $\mathbf{x}_i$ and $\mathbf{x}_j$. Let the force state field be given by

$$\underline{\mathbf{T}}[\mathbf{x}]\langle\boldsymbol{\xi}\rangle = \mathbf{T}_{ij}\Delta(\mathbf{x} - \mathbf{x}_i)\Delta(\boldsymbol{\xi} - (\mathbf{x}_j - \mathbf{x}_i)). \tag{163}$$

One or both of these points may be a zero-mass reference point for a multibody potential, as discussed in the previous section, or they may both have positive mass. Recall from (120) that the peridynamic stress tensor field is given by

$$\boldsymbol{\nu}(\mathbf{x}) = \int_{\mathcal{U}} \int_0^\infty \int_0^\infty (y+z)^2 \underline{\mathbf{T}}[\mathbf{x} - z\mathbf{m}]\langle(y+z)\mathbf{m}\rangle \otimes \mathbf{m}\, dz\, dy\, d\Omega_{\mathbf{m}} \tag{164}$$

where $\mathcal{U}$ is the unit sphere and $d\Omega_{\mathbf{m}}$ is a differential solid angle in the direction of the unit vector $\mathbf{m}$. Let L denote the open line segment connecting $\mathbf{x}_i$ and $\mathbf{x}_j$. Comparing the last two equations, evidently the integrand in (164)

takes on nonzero values only if $\mathbf{x} \in L$ and only if $\mathbf{m} = \pm\mathbf{m}_{ij}$, where $\mathbf{m}_{ij}$ is the unit vector defined by

$$\mathbf{m}_{ij} = \frac{\mathbf{x}_j - \mathbf{x}_i}{|\mathbf{x}_j - \mathbf{x}_i|} \tag{165}$$

(see Figure 10). From this observation and the form of the integrand in (164), it follows that $\boldsymbol{\nu}$ can be expressed in the form

$$\boldsymbol{\nu}(\mathbf{x}) = \mathbf{S}(\mathbf{x}) \otimes \mathbf{m}_{ij} \tag{166}$$

where $\mathbf{S}$ is a vector-valued function that takes on non-null values only on L. Recall from the properties of the peridynamic stress tensor (123) that

$$\text{div } \boldsymbol{\nu}(\mathbf{x}) = \int_{\mathcal{H}} \left(\underline{\mathbf{T}}[\mathbf{x}]\langle \boldsymbol{\xi} \rangle - \underline{\mathbf{T}}[\mathbf{x} + \boldsymbol{\xi}]\langle -\boldsymbol{\xi} \rangle \right) dV_{\boldsymbol{\xi}}.$$

Applying this to (163) leads to

$$\text{div } \boldsymbol{\nu}(\mathbf{x}) = \big(\Delta(\mathbf{x} - \mathbf{x}_i) - \Delta(\mathbf{x} - \mathbf{x}_j) \big) \mathbf{T}_{ij}. \tag{167}$$

Let $\mathcal{R}$ be a sphere centered at $\mathbf{x}_i$ with radius $r < |\mathbf{x}_j - \mathbf{x}_i|$ (so that its boundary $\partial\mathcal{R}$ intersects L). By (167) and the properties of the delta function,

$$\int_{\mathcal{R}} \text{div } \boldsymbol{\nu}(\mathbf{x}) \, dV = \mathbf{T}_{ij}.$$

From this, (166), and the divergence theorem,

$$\mathbf{T}_{ij} = \int_{\partial\mathcal{R}} \boldsymbol{\nu}(\mathbf{x})\mathbf{n} \, dA = \int_{\partial\mathcal{R}} (\mathbf{S}(\mathbf{x}) \otimes \mathbf{m}_{ij})\mathbf{n} \, dA$$

where $\mathbf{n}$ is the outward-directed unit normal vector to $\partial\mathcal{R}$. But since $\mathbf{S}$ is non-null only on L, it follows that $\mathbf{n} = \mathbf{m}_{ij}$ there. Therefore,

$$\mathbf{T}_{ij} = \left(\int_{\partial\mathcal{R}} \mathbf{S}(\mathbf{x}) \, dA \right) \mathbf{m}_{ij} \cdot \mathbf{m}_{ij} = \int_{\partial\mathcal{R}} \mathbf{S}(\mathbf{x}) \, dA$$

since $\mathbf{m}_{ij}$ is a unit vector. Since this must hold for every choice of r such that $0 < r < |\mathbf{x}_j - \mathbf{x}_i|$, it follows from (166) that

$$\int_P \boldsymbol{\nu}(\mathbf{x}) \, dA = \mathbf{T}_{ij} \otimes \mathbf{m}_{ij} \tag{168}$$

for every plane P normal to L that intersects L. Thus, $\boldsymbol{\nu}$ has the structure of a two-dimensional Dirac delta function. Another way to state this is as follows:

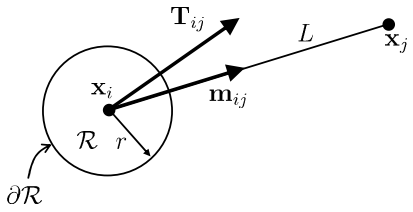

Figure 10: Interacting particles at $\mathbf{x}_i$ and $\mathbf{x}_j$.

- $\boldsymbol{\nu} = \mathbf{0}$ on $\mathbb{R}^3 - L$.
- For any function γ on $\mathbb{R}^3$, using (168),

$$\int_{\mathbb{R}^3} \gamma \boldsymbol{\nu} \, dV = \int_L \int_{P_s} \gamma \boldsymbol{\nu} \, dA \, ds = \mathbf{T}_{ij} \otimes \mathbf{m}_{ij} \int_L \gamma \, ds \tag{169}$$

  where s is path length along L, and P_s is the plane normal to L that intersects L at s. This relation will be used in the next section in computing the average stress among many particles.

7.7 Average stress due to many discrete particles

Now consider a system of many particles. These may include zero-mass reference points for multibody potentials (Figure 11), as discussed in Section 7.5. From the results of the previous section, the peridynamic stress tensor field $\boldsymbol{\nu}$ is non-null only on the line segments L_{ij} connecting pairs of particles that interact with each other. (This is unrelated to whether the particles interact through a pair potential or a multibody potential.) To make this stress more useful, an averaging function is now introduced. First, the mechanical significance of an averaged stress field is investigated.

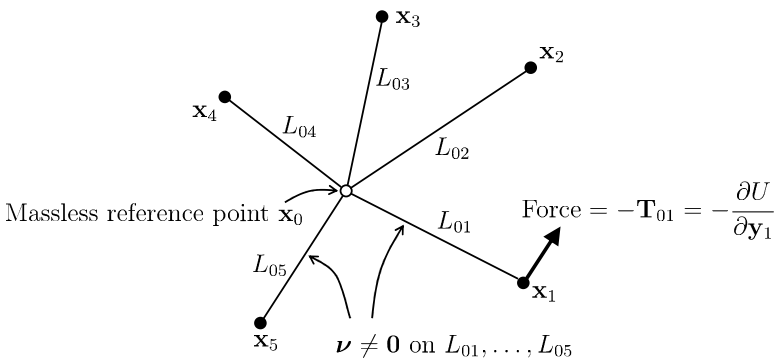

Figure 11: Peridynamic particles interacting through a 5-body potential with reference point $\mathbf{x}_0$.

Let ϕ be an averaging function on $\mathbb{R}^3$ such that $\int \phi = 1$. A typical choice of ϕ would be

$$\phi(\mathbf{q}) = c\exp(-|\mathbf{q}|^2/a^2) \tag{170}$$

where a and c are constants. Let $\boldsymbol{\nu}$ be the peridynamic stress tensor field. Recall the local equation of motion in terms of the stress tensor (122):

$$\rho(\mathbf{x})\ddot{\mathbf{y}}(\mathbf{x},t) = \text{div}\ \boldsymbol{\nu}(\mathbf{x},t) + \mathbf{b}(\mathbf{x},t). \tag{171}$$

Evaluate this equation at $\mathbf{x}+\mathbf{q}$, multiply both sides by $\phi(\mathbf{q})$ and integrate over $\mathbb{R}^3$:

$$\int \phi(\mathbf{q})\rho(\mathbf{x}+\mathbf{q})\ddot{\mathbf{y}}(\mathbf{x}+\mathbf{q},t)\ dV_{\mathbf{q}} = \int \phi(\mathbf{q})\text{div}\ \boldsymbol{\nu}(\mathbf{x}+\mathbf{q},t)\ dV_{\mathbf{q}} + \int \phi(\mathbf{q})\mathbf{b}(\mathbf{x}+\mathbf{q},t)\ dV_{\mathbf{q}}.$$

Define the following averaged quantities:

$$\begin{aligned}
\bar{\rho}(\mathbf{x}) &= \int \phi(\mathbf{q})\rho(\mathbf{x}+\mathbf{q})\ dV_{\mathbf{q}},\\
\bar{\mathbf{y}}(\mathbf{x},t) &= \frac{1}{\bar{\rho}(\mathbf{x})}\int \phi(\mathbf{q})\rho(\mathbf{x}+\mathbf{q})\mathbf{y}(\mathbf{x}+\mathbf{q},t)\ dV_{\mathbf{q}},\\
\bar{\boldsymbol{\nu}}(\mathbf{x},t) &= \int \phi(\mathbf{q})\boldsymbol{\nu}(\mathbf{x}+\mathbf{q},t)\ dV_{\mathbf{q}},\\
\bar{\mathbf{b}}(\mathbf{x},t) &= \int \phi(\mathbf{q})\mathbf{b}(\mathbf{x}+\mathbf{q},t)\ dV_{\mathbf{q}}.
\end{aligned} \tag{172}$$

Note that $\bar{\mathbf{y}}$ is a mass-weighted average deformed position vector. In terms of these quantities, (171) becomes

$$\bar{\rho}(\mathbf{x})\ddot{\bar{\mathbf{y}}}(\mathbf{x},t) = \text{div}\ \bar{\boldsymbol{\nu}}(\mathbf{x},t) + \bar{\mathbf{b}}(\mathbf{x},t).$$

This is the peridynamic equation of motion in terms of the averaged quantities.

If the distance between interacting particles, *i.e.,* the horizon, is small compared to the length scale of the averaging function (such as a in (170)), then it is a good approximation to assume that ϕ is constant along any of the bonds. Neglecting the resulting error term, from (169) and (172), for any pair of particles i and j,

$$\bar{\boldsymbol{\nu}}(\mathbf{x}) = (\mathbf{T}_{ij}\otimes\mathbf{m}_{ij})\big(|\mathbf{x}_j-\mathbf{x}_i|\phi(\mathbf{x}_i-\mathbf{x})\big)$$

Using (165), this can also be written as

$$\bar{\boldsymbol{\nu}}(\mathbf{x}) = \phi(\mathbf{x}_i-\mathbf{x})\mathbf{T}_{ij}\otimes(\mathbf{x}_j-\mathbf{x}_i).$$

For the system with many particles, this becomes

$$\bar{\boldsymbol{\nu}}(\mathbf{x}) = \sum_i \sum_{j\neq i} \phi(\mathbf{x}_i - \mathbf{x})\mathbf{T}_{ij} \otimes (\mathbf{x}_j - \mathbf{x}_i). \tag{173}$$

Since ϕ has dimensions of 1/volume and $\mathbf{T}_{ij}$ has dimensions of force, $\bar{\boldsymbol{\nu}}$ has dimensions of force/area. By (149) and the first of (172), the averaged density for many particles is given by

$$\bar{\rho}(\mathbf{x}) = \sum_i M_i \phi(\mathbf{x}_i - \mathbf{x}).$$

If $\bar{\boldsymbol{\nu}}$ is evaluated in the reference configuration, in which $\mathbf{y}_i = \mathbf{x}_i$, then the requirement (146) for nonpolarity implies that $\bar{\boldsymbol{\nu}}$ is symmetric. To confirm this, let $\mathbf{a}$ be any vector, and note that (146) implies

$$\sum_i \phi_i \sum_{j\neq i} \boldsymbol{\xi}_{ij} \times \mathbf{T}_{ij} = \mathbf{0}, \qquad \boldsymbol{\xi}_{ij} = \mathbf{x}_j - \mathbf{x}_i, \qquad \phi_i = \phi(\mathbf{x}_i - \mathbf{x}).$$

Then, using the BAC-CAB rule and (173),

$$\begin{aligned}
\mathbf{0} &= \sum_i \phi_i \sum_{j\neq i} (\boldsymbol{\xi}_{ij} \times \mathbf{T}_{ij}) \times \mathbf{a} \\
&= \sum_i \phi_i \sum_{j\neq i} \mathbf{a} \times (\mathbf{T}_{ij} \times \boldsymbol{\xi}_{ij}) \\
&= \sum_i \phi_i \sum_{j\neq i} \big[\mathbf{T}_{ij}(\mathbf{a}\cdot\boldsymbol{\xi}_{ij}) - \boldsymbol{\xi}_{ij}(\mathbf{a}\cdot\mathbf{T}_{ij})\big] \\
&= \sum_i \phi_i \sum_{j\neq i} \big[(\mathbf{T}_{ij}\otimes\boldsymbol{\xi}_{ij})\mathbf{a} - (\boldsymbol{\xi}_{ij}\otimes\mathbf{T}_{ij})\mathbf{a}\big] \\
&= 2\,\mathrm{skw}\left[\sum_i \phi_i \sum_{j\neq i} (\mathbf{T}_{ij}\otimes\boldsymbol{\xi}_{ij})\right]\mathbf{a} \\
&= 2\big[\mathrm{skw}\,\bar{\boldsymbol{\nu}}(\mathbf{x})\big]\mathbf{a}
\end{aligned}$$

where "skw" means the skew-symmetric part of a tensor. Since this must hold for any $\mathbf{a}$, it follows that skw $\bar{\boldsymbol{\nu}}(\mathbf{x}) = \mathbf{0}$; hence $\bar{\boldsymbol{\nu}}$ is symmetric.

Thus, nonpolarity of forces implies the symmetry of the averaged peridynamic stress tensor, prior to significant deformation of the system. After deformation, the stress tensor is no longer symmetric except in special cases. This is comparable to the asymmetry of the classical Piola stress tensor in a body undergoing large deformation.

Our expression for $\bar{\boldsymbol{\nu}}$ in (173) performs the averaging in the reference configuration, because the reference position vector $\mathbf{x}$ is the spatial variable.

Because of this, the weighting for a particle does not change as the particle moves. This means that if the particles are highly mobile, as in a gas, the expression (173) for stress is not very useful, because its status as an observable quantity depends on the assumption that the particles always remain close together. In this case, it is more useful to perform the averaging in the deformed configuration, so that the weighting of each particle varies as it moves closer to or farther from an observation point. To derive the effect of this change on the averaged stress, define the momentum density at any point $\mathbf{x}$ in space by

$$\bar{\mathbf{p}} = \sum_i M_i \phi_i \dot{\mathbf{y}}_i, \qquad \phi_i = \phi(\mathbf{y}_i - \mathbf{x}).$$

Define a function Φ by

$$\Phi(\mathbf{z}, \mathbf{x}) = \phi(\mathbf{z} - \mathbf{x}),$$

thus

$$\bar{\mathbf{p}} = \sum_i M_i \Phi(\mathbf{y}_i, \mathbf{x}) \dot{\mathbf{y}}_i.$$

Observe that

$$\frac{\partial \Phi}{\partial \mathbf{z}} = -\frac{\partial \Phi}{\partial \mathbf{x}}. \tag{174}$$

Evaluating the time derivative of $\bar{\mathbf{p}}$ holding $\mathbf{x}$ fixed, while using (174) and temporarily neglecting body forces, leads to

$$\begin{aligned}
\dot{\bar{\mathbf{p}}} &= \sum_i M_i \Big[\phi_i \ddot{\mathbf{y}}_i + (\dot{\mathbf{y}}_i \cdot \frac{\partial \Phi}{\partial \mathbf{z}}(\mathbf{y}_i, \mathbf{x})) \dot{\mathbf{y}}_i \Big] \\
&= \sum_i M_i \Big[\phi_i \ddot{\mathbf{y}}_i - (\dot{\mathbf{y}}_i \cdot \frac{\partial \Phi}{\partial \mathbf{x}}(\mathbf{y}_i, \mathbf{x})) \dot{\mathbf{y}}_i \Big] \\
&= \sum_i M_i \Big[\phi_i \ddot{\mathbf{y}}_i - \text{div } \big(\Phi(\mathbf{y}_i, \mathbf{x}) \dot{\mathbf{y}}_i \otimes \dot{\mathbf{y}}_i \big) \Big] \\
&= \sum_i M_i \Big[\phi_i \ddot{\mathbf{y}}_i - \text{div } \big(\phi_i \dot{\mathbf{y}}_i \otimes \dot{\mathbf{y}}_i \big) \Big] \\
&= \sum_i M_i \phi_i \ddot{\mathbf{y}}_i - \text{div } \sum_i M_i \phi_i \dot{\mathbf{y}}_i \otimes \dot{\mathbf{y}}_i.
\end{aligned}$$

We are free to choose any reference configuration that is convenient. In this case, choose it to be the configuration at any time t. Then the peridynamic stress tensor is given by (173) with $\mathbf{x}_i = \mathbf{y}_i$, so that

$$\dot{\bar{\mathbf{p}}} = \text{div } \bar{\boldsymbol{\nu}} + \text{div } \boldsymbol{\kappa} + \bar{\mathbf{b}}$$

where the *kinetic stress tensor* is defined by

$$\boldsymbol{\kappa} = -\sum_i M_i \phi_i \dot{\mathbf{y}}_i \otimes \dot{\mathbf{y}}_i.$$

The kinetic stress tensor accounts for the transport of momentum due to the motion of particles into or out of a region that is fixed in space. In contrast, the peridynamic stress tensor accounts only for the acceleration of particles. Kinetic stress is the primary contributor to pressure in gases, in which interactions between particles are weak but velocities, including thermal velocities, are significant. The idea of kinetic stress is not new and not particular to the peridynamic model, but it is included here to show that it can be included in the peridynamic concept of momentum balance in a straightforward way.

The averaged peridynamic stress given by (173) is similar to Hardy's expression for the potential contribution to the stress tensor [37], which is obtained by averaging a large number of particles interacting through pair potentials. Hardy also discusses the relation of this stress tensor to the virial stress. The present approach applies to multibody potentials, while ensuring that the average stress satisfies balance of angular momentum (in the sense of producing symmetric $\bar{\boldsymbol{\nu}}$ in the reference configuration, as shown above).

8 Damage and fracture

This section presents the peridynamic view of damage and its incorporation into a material model. This is presented within a thermodynamic framework that highlights the role of irreversibility of damage. Various damage evolution laws and their implications are described, the simplest being independent bond breakage. The energy balance for moving defects is investigated, leading to peridynamic expressions for the J-integral, surface energy, and the Griffith criterion for crack growth.

8.1 Damage as part of a constitutive model

Suppose that a material has a free energy function ψ and entropy function η that depend not only on the deformation state and temperature, but also on a scalar state $\underline{\phi}$ called the *damage state*. We write

$$\psi(\underline{\mathbf{Y}}, \theta, \underline{\phi}), \qquad \eta(\underline{\mathbf{Y}}, \theta, \underline{\phi}). \tag{175}$$

The damage state is special in that it cannot decrease over time, thus

$$\dot{\underline{\phi}} \geq 0, \quad \textit{i.e.,} \qquad \dot{\underline{\phi}}\langle\boldsymbol{\xi}\rangle \geq 0 \quad \forall\, \boldsymbol{\xi} \in \mathcal{H}. \tag{176}$$

It is also assumed that

$$0 \leq \underline{\phi} \leq 1, \quad \textit{i.e.,} \qquad 0 \leq \underline{\phi}\langle\boldsymbol{\xi}\rangle \leq 1 \quad \forall\, \boldsymbol{\xi} \in \mathcal{H}. \tag{177}$$

The damage state is determined by the deformation and by other variables through a prescribed *damage evolution law* of the form

$$\underline{\phi} = \underline{D}(\underline{\mathbf{Y}}, \dot{\underline{\mathbf{Y}}}, \dots)$$

or alternatively in terms of the rate of damage growth:

$$\dot{\underline{\phi}} = \dot{\underline{D}}(\underline{\mathbf{Y}}, \dot{\underline{\mathbf{Y}}}, \dots).$$

A material model such that, for any $\boldsymbol{\xi} \in \mathcal{H}$,

$$\underline{\phi}\langle\boldsymbol{\xi}\rangle = 1 \quad \Longrightarrow \quad \underline{\mathbf{T}}\langle\boldsymbol{\xi}\rangle = \mathbf{0} \tag{178}$$

is said to have *strong* damage dependence. All other material models have *weak* damage dependence.

8.2 Irreversibility of damage growth

Recall the inequality (69) derived from the first and second laws in terms of free energy:

$$\underline{\mathbf{T}} \bullet \dot{\underline{\mathbf{Y}}} - \dot{\theta}\eta - \dot{\psi} \geq 0.$$

We now repeat the Coleman and Noll method [15] used previously in Section 4.5 to obtain restrictions on the constitutive response in the presence of evolving damage. Differentiating the first of (175) with respect to time yields

$$\dot{\psi} = \psi_{\underline{\mathbf{Y}}} \bullet \dot{\underline{\mathbf{Y}}} + \psi_\theta \dot{\theta} + \psi_{\underline{\phi}} \bullet \dot{\underline{\phi}}, \tag{179}$$

where $\psi_{\underline{\mathbf{Y}}}$ and $\psi_{\underline{\phi}}$ are the Fréchet derivatives of ψ with respect to $\underline{\mathbf{Y}}$ and $\underline{\phi}$ respectively, and $\psi_\theta = \partial\psi/\partial\theta$. Combining the last two expressions yields

$$\big[\underline{\mathbf{T}} - \psi_{\underline{\mathbf{Y}}}\big] \bullet \dot{\underline{\mathbf{Y}}} - \big[\eta + \psi_\theta\big]\dot{\theta} - \psi_{\underline{\phi}} \bullet \dot{\underline{\phi}} \geq 0. \tag{180}$$

As in Section 4.5, assume that $\dot{\underline{\mathbf{Y}}}$ and $\dot{\theta}$ can be varied independently and arbitrarily in (180), hence

$$\underline{\mathbf{T}} = \psi_{\underline{\mathbf{Y}}}, \qquad \eta = -\psi_\theta. \tag{181}$$

In view of (176), $\dot{\underline{\phi}}$ cannot be set arbitrarily in (180), leading to the conclusion

$$\psi_{\underline{\phi}} \leq \underline{0}\,, \tag{182}$$

which is the second law restriction on the dependence of free energy on the damage. Using (181), (179) takes the form

$$\dot{\psi} = \underline{\mathbf{T}} \bullet \dot{\underline{\mathbf{Y}}} - \dot{\theta}\eta + \psi_{\underline{\phi}} \bullet \dot{\underline{\phi}}. \tag{183}$$

Now assume an adiabatic process, so that $h = r = 0$. Subtracting (68), which continues to hold in the presence of damage, from (183) leads to the conclusion

$$\dot{\eta} = \frac{\dot{\psi}^d}{\theta}, \qquad \dot{\psi}^d := -\psi_{\underline{\phi}} \bullet \dot{\underline{\phi}} \tag{184}$$

where $\dot{\psi}^d$ is the rate of energy dissipation. The first of (184) gives the entropy production due to damage evolution.

8.3 Bond breakage

Recall the definition of the scalar extension state $\underline{e}$,

$$\underline{e} = |\underline{\mathbf{Y}}| - |\underline{\mathbf{X}}| \tag{185}$$

where $\underline{\mathbf{X}}$ is the identity state defined in (49). A useful example of a damage evolution law is given by the following model:

$$\underline{\phi}\langle\boldsymbol{\xi}\rangle = \underline{D}(\underline{\mathbf{Y}},\boldsymbol{\xi})\langle\boldsymbol{\xi}\rangle = \max_t f(\underline{e}\langle\boldsymbol{\xi}\rangle,\boldsymbol{\xi}) \tag{186}$$

where $f(e,\boldsymbol{\xi})$ is a nondecreasing function of e, $0 \le f \le 1$, and the maximum is taken over all times up to t. Assume for simplicity that for a given motion, $\underline{e}$ is a nondecreasing function of time. Observing from (185) that

$$\dot{\underline{e}} = \underline{\mathbf{M}} \cdot \underline{\mathbf{Y}}, \qquad \underline{\mathbf{M}} = \frac{\underline{\mathbf{Y}}}{|\underline{\mathbf{Y}}|}, \tag{187}$$

differentiating (186) with respect to time yields an equivalent damage evolution law in terms of the rate:

$$\dot{\underline{\phi}}\langle\boldsymbol{\xi}\rangle = \dot{\underline{D}}(\underline{\mathbf{Y}},\dot{\underline{\mathbf{Y}}},\boldsymbol{\xi}) = f_e(\underline{e}\langle\boldsymbol{\xi}\rangle,\boldsymbol{\xi})\underline{\mathbf{M}}\langle\boldsymbol{\xi}\rangle \cdot \dot{\underline{\mathbf{Y}}}\langle\boldsymbol{\xi}\rangle \tag{188}$$

where f_e denotes the partial derivative of f with respect to e. It is helpful to introduce a vector state $\underline{\mathbf{r}}$ defined by

$$\underline{\mathbf{r}}\langle\boldsymbol{\xi}\rangle = f_e(\underline{e}\langle\boldsymbol{\xi}\rangle,\boldsymbol{\xi})\underline{\mathbf{M}}\langle\boldsymbol{\xi}\rangle \tag{189}$$

so that (188) can be written as

$$\dot{\underline{\phi}} = \underline{\mathbf{r}} \cdot \dot{\underline{\mathbf{Y}}} \tag{190}$$

provided $\underline{e}$ is nondecreasing. A specific case of such a damage model is *bond breakage* in tension, in which

$$f(e,\boldsymbol{\xi}) = H\big(e - e_b(\boldsymbol{\xi})\big) \tag{191}$$

where H is the Heaviside step function and $e_b(\boldsymbol{\xi})$ is the prescribed *bond breakage extension* for the bond $\boldsymbol{\xi}$. In this case

$$f_e(e,\boldsymbol{\xi}) = \Delta\big(e - e_b(\boldsymbol{\xi})\big)$$

and from (188),

$$\dot{\underline{\phi}} = \Delta(\underline{e} - e_b)\underline{\mathbf{M}} \cdot \dot{\underline{\mathbf{Y}}}$$

Alternatively, the same damage evolution law can be defined in terms of the rate through (190) with

$$\underline{\mathbf{r}} = \Delta(\underline{e} - e_b)\underline{\mathbf{M}}.$$

Bond breakage in compression can be treated in a similar way.

8.4 Ordinary material models with strong damage dependence

Suppose an elastic material model is defined by

$$\hat{W}(\underline{\mathbf{Y}}) = W^0(\underline{e}) \tag{192}$$

where W^0 is a function and $\underline{e}$ is the scalar extension state, defined by (185). Because of (187), the chain rule implies

$$\nabla \hat{W}(\underline{\mathbf{Y}}) = \nabla W^0(\underline{e})\underline{\mathbf{M}}.$$

Now we will modify the material model (192) to include damage. To do this, define a free energy density function by

$$\psi(\underline{\mathbf{Y}}, \underline{\phi}) = W^0\big((\underline{1} - \underline{\phi})\underline{e}\big). \tag{193}$$

The first of (181) and the chain rule provide the following force state:

$$\underline{\mathbf{T}} = \psi_{\underline{\mathbf{Y}}} = (\underline{1} - \underline{\phi})\underline{t}^0\underline{\mathbf{M}}, \qquad \underline{t}^0 = \nabla W^0\big((\underline{1} - \underline{\phi})\underline{e}\big). \tag{194}$$

Because of the $(\underline{1} - \underline{\phi})$ term in this expression for $\underline{\mathbf{T}}$, evidently (178) holds for this material, so it has strong damage dependence. By (193),

$$\psi_{\underline{\phi}} = -\underline{t}^0\underline{e}. \tag{195}$$

So, the second law requirement (182) holds provided

$$\underline{t}^0\underline{e} \geq 0. \tag{196}$$

This asserts that the scalar bond force density in each bond has the same sign as the bond's scalar extension.

8.5 Bond-based constitutive models with bond breakage

An important special case of the ordinary material with strong damage dependence is obtained if the bond breakage model for evolution of damage is combined with a bond-based constitutive model. Following (78), choose

$$W^0(\underline{e}) = \int_{\mathcal{H}} w(\underline{e}\langle\boldsymbol{\xi}\rangle, \boldsymbol{\xi})\, dV_{\boldsymbol{\xi}}$$

where $w(e, \boldsymbol{\xi})$ is the differentiable bond potential function. Let the damage evolution be described by the bond breakage model in (191). Following the method of the previous section, modify W^0 to include damage by defining the following free energy function:

$$\psi(\underline{\mathbf{Y}}, \underline{\phi}) = W^0\big((\underline{1} - \underline{\phi})\underline{e}\big) = \int_{\mathcal{H}} w\big((1 - \underline{\phi}\langle\boldsymbol{\xi}\rangle)\underline{e}\langle\boldsymbol{\xi}\rangle, \boldsymbol{\xi}\big)\, dV_{\boldsymbol{\xi}}. \tag{197}$$

From (194), the force state is given by

$$\underline{\mathbf{T}} = (1 - \underline{\phi})\underline{t}^0\underline{\mathbf{M}}, \qquad \underline{t}^0\langle\boldsymbol{\xi}\rangle = w_e\big((1 - \underline{\phi}\langle\boldsymbol{\xi}\rangle)\underline{e}\langle\boldsymbol{\xi}\rangle, \boldsymbol{\xi}\big).$$

The Fréchet derivative of ψ with respect to $\underline{\phi}$ is supplied by (195), thus

$$\psi_{\underline{\phi}}\langle\boldsymbol{\xi}\rangle = -\underline{e}\langle\boldsymbol{\xi}\rangle w_e\big((1 - \underline{\phi}\langle\boldsymbol{\xi}\rangle)\underline{e}\langle\boldsymbol{\xi}\rangle, \boldsymbol{\xi}\big) \tag{198}$$

for all $\boldsymbol{\xi} \in \mathcal{H}$. The second law condition is given by (196). The important distinction between this material and more general ordinary materials is that here, $\underline{t}^0\langle\boldsymbol{\xi}\rangle$ and $\underline{\phi}\langle\boldsymbol{\xi}\rangle$ for a given bond $\boldsymbol{\xi}$ are determined independently of whatever happens in all the other bonds.

It is of interest to compute the dissipated energy at a point $\mathbf{x}$ up to time t. To do this, use the second of (184) and (198), assuming for simplicity that $\underline{e}$ is nondecreasing:

$$\psi^d = -\int_0^t \psi_{\underline{\phi}} \bullet \dot{\underline{\phi}}\, dt = \int_0^t \int_{\mathcal{H}} \underline{e}\langle\boldsymbol{\xi}\rangle w_e\big((1 - \underline{\phi}\langle\boldsymbol{\xi}\rangle)\underline{e}\langle\boldsymbol{\xi}\rangle, \boldsymbol{\xi}\big)\dot{\underline{\phi}}\langle\boldsymbol{\xi}\rangle\, dV_{\boldsymbol{\xi}}\, dt.$$

Recalling that, by definition, $\psi_{\underline{\phi}}$ refers to the derivative of ψ holding $\underline{\mathbf{Y}}$, and therefore $\underline{e}$, constant, it follows that

$$\psi^d = -\int_{\mathcal{H}} \int_0^{\phi\langle\boldsymbol{\xi}\rangle} \frac{d}{d\sigma} w\big((1 - \sigma)\underline{e}\langle\boldsymbol{\xi}\rangle, \boldsymbol{\xi}\big)\, d\sigma\, dV_{\boldsymbol{\xi}}.$$

Combining this with (186) and (191), because $\underline{\phi}\langle\boldsymbol{\xi}\rangle$ changes discontinuously when the extension reaches the bond breakage extension $e_b(\boldsymbol{\xi})$, it follows that

$$\psi^d = \int_{\mathcal{H}} w_b(\boldsymbol{\xi})\underline{\phi}\langle\boldsymbol{\xi}\rangle\, dV_{\boldsymbol{\xi}}$$

where the *bond breakage energy* is defined by

$$w_b(\boldsymbol{\xi}) = w(e_b(\boldsymbol{\xi}), \boldsymbol{\xi}) - w(0, \boldsymbol{\xi}).$$

In this material, the dissipated energy is simply the integral of the bond breakage energies over all the broken bonds in the family.

In this material, ψ^d depends only on the current value of $\underline{\phi}$. This is not true for most other materials; a counterexample is the separable damage model discussed in the next section.

8.6 Separable damage models

The previous section showed how damage can be introduced into a bond-based material model simply by modifying the bond potential function with a term that depends on bond damage, as indicated in (197). The present

section deals with incorporation of damage into more general elastic consitutive models. Assume that such an "undamaged" model is provided, and let $W^0(\underline{\mathbf{Y}})$ be its strain energy density function. Let $\underline{\mathbf{T}}^0 = \nabla W^0$. Further assume that

$$W^0(\underline{\mathbf{X}}) = 0 \qquad \text{and} \qquad W^0(\underline{\mathbf{Y}}) \geq 0 \quad \forall\, \underline{\mathbf{Y}} \in \mathcal{V}. \tag{199}$$

Define a free energy density function by

$$\psi(\underline{\mathbf{Y}}, \underline{\phi}) = \Phi(\underline{\phi}) W^0(\underline{\mathbf{Y}}) \tag{200}$$

where

$$\Phi(\underline{\phi}) = \frac{1}{V} \int_{\mathcal{H}} (1 - \underline{\phi}\langle \boldsymbol{\xi} \rangle)^2 \, dV_{\boldsymbol{\xi}}, \qquad V = \int_{\mathcal{H}} dV_{\boldsymbol{\xi}}. \tag{201}$$

Because the damage state and the deformation state appear in separate terms in (200), this type of damage model will be called *separable*. After evaluating the Fréchet derivatives and using the first of (181), the force state including damage is found to be

$$\underline{\mathbf{T}}\langle \boldsymbol{\xi} \rangle = \psi_{\underline{\mathbf{Y}}}\langle \boldsymbol{\xi} \rangle = \Phi(\underline{\phi}) \underline{\mathbf{T}}^0\langle \boldsymbol{\xi} \rangle. \tag{202}$$

This means that all the bonds have their force reduced by the same scalar $\Phi(\underline{\phi})$. Φ decreases monotonically with time because, by the assumption (176), $\underline{\phi}$ increases monotonically. From (200) and (201), the Fréchet derivative of free energy with respect to $\underline{\phi}$ is given by

$$\psi_{\underline{\phi}}\langle \boldsymbol{\xi} \rangle = -\frac{2W^0(\underline{\mathbf{Y}})}{V} (1 - \underline{\phi}\langle \boldsymbol{\xi} \rangle). \tag{203}$$

The second law requirement (182) is necessarily satisfied because of (177), (199), and (203). The energy dissipation rate is found from (184) and (203) to be

$$\begin{aligned} \dot{\psi}^d = -\psi_{\underline{\phi}} \bullet \dot{\underline{\phi}} &= \frac{2W^0(\underline{\mathbf{Y}})}{V} \int_{\mathcal{H}} (1 - \underline{\phi}\langle \boldsymbol{\xi} \rangle) \dot{\underline{\phi}}\langle \boldsymbol{\xi} \rangle \, dV_{\boldsymbol{\xi}} \\ &= -W^0(\underline{\mathbf{Y}}) \dot{\Phi}. \end{aligned}$$

The dissipated energy up to time t is therefore given by

$$\psi^d(t) = \int_0^t \dot{\psi}^d(\tau) \, d\tau = -\int_0^t W^0(\underline{\mathbf{Y}}[\tau]) \dot{\Phi}(\tau) \, d\tau.$$

The separable damage model results in a material characterization with weak dependence on damage (see Section 8.1), because (202) does not necessarily imply that bonds with $\underline{\phi}\langle \boldsymbol{\xi} \rangle = 1$ have $\underline{\mathbf{T}}\langle \boldsymbol{\xi} \rangle = \mathbf{0}$. This is in contrast to the materials discussed in Section 8.4, which exhibit strong damage dependence.

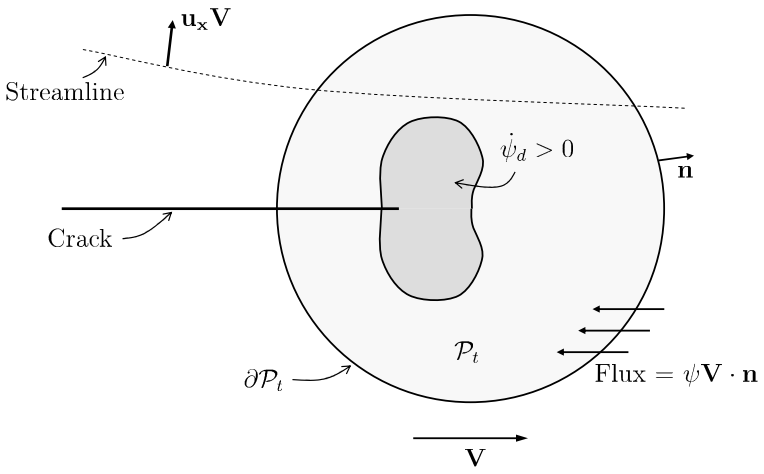

Figure 12: Subregion $\mathcal{P}_t$ containing points where there is energy dissipation moves to the right with velocity $\mathbf{V}$.

8.7 Energy balance in progressive damage

Consider a closed, bounded subregion $\mathcal{P}_t$ with constant shape that translates through the reference configuration $\mathcal{B}$ with velocity $\mathbf{V}$; thus there is a flux of material through its boundary $\partial\mathcal{P}_t$. Assume a *steady-state* motion of the form

$$\mathbf{y}(\mathbf{x}, t) = \mathbf{x} + \mathbf{u}(\mathbf{x} - \mathbf{V}t) \tag{204}$$

where $\mathbf{u}$ is some differentiable function (Figure 12).

Assume that body force, kinetic energy, heat transport, and heat sources are all negligible. Additionally assume an isothermal process, so that $\dot{\theta} = 0$. These assumptions along with the local first law expression (65) and (183) imply

$$\dot{\psi} = \dot{\varepsilon} + \psi_{\underline{\phi}} \bullet \dot{\underline{\phi}}. \tag{205}$$

Recalling the shorthand notation in (12), the global first law (35) in this case has the form

$$\int_{\mathcal{P}_t} \dot{\varepsilon}\, dV = \int_{\mathcal{P}_t} \int_{\mathcal{B}\setminus\mathcal{P}_t} (\mathbf{t}\cdot\dot{\mathbf{y}}' - \mathbf{t}'\cdot\dot{\mathbf{y}})\, dV'\, dV. \tag{206}$$

Because the motion is steady state, the total time derivative of any intensive quantity over $\mathcal{P}_t$ vanishes. The Reynolds transport theorem therefore

implies, for the free energy ψ,

$$\frac{d}{dt}\int_{\mathcal{P}_t}\psi\,dV=\int_{\mathcal{P}_t}\dot{\psi}\,dV+\int_{\partial\mathcal{P}_t}\psi\mathbf{V}\cdot\mathbf{n}\,dA=0$$

where $\mathbf{n}$ is the outward-directed unit normal to $\partial\mathcal{P}_t$. Using this and (205),

$$\int_{\mathcal{P}_t}\left(\dot{\varepsilon}+\psi_{\underline{\phi}}\bullet\dot{\underline{\phi}}\right)dV+\int_{\partial\mathcal{P}_t}\psi\mathbf{V}\cdot\mathbf{n}\,dA=0.$$

From this and (206),

$$\int_{\mathcal{P}_t}\int_{\mathcal{B}\setminus\mathcal{P}_t}(\mathbf{t}\cdot\dot{\mathbf{y}}'-\mathbf{t}'\cdot\dot{\mathbf{y}})\,dV'\,dV+\int_{\mathcal{P}_t}\psi_{\underline{\phi}}\bullet\dot{\underline{\phi}}\,dV+\int_{\partial\mathcal{P}_t}\psi\mathbf{V}\cdot\mathbf{n}\,dA=0.$$

Evaluating $\dot{\mathbf{y}}$ and $\dot{\mathbf{y}}'$ using (204), therefore

$$\int_{\mathcal{P}}\int_{\mathcal{B}\setminus\mathcal{P}}\left(\mathbf{t}'\cdot(\mathbf{u}_{\mathbf{x}}\mathbf{V})-\mathbf{t}\cdot(\mathbf{u}'_{\mathbf{x}}\mathbf{V})\right)dV'\,dV+\int_{\mathcal{P}}\psi_{\underline{\phi}}\bullet\dot{\underline{\phi}}\,dV+\int_{\partial\mathcal{P}}\psi\mathbf{V}\cdot\mathbf{n}\,dA=0\quad(207)$$

where the t subscript has been dropped from $\mathcal{P}_t$ and

$$\mathbf{u}_{\mathbf{x}}=\text{grad}\,\mathbf{u}(\mathbf{x}-\mathbf{V}t),\qquad\mathbf{u}'_{\mathbf{x}}=\text{grad}\,\mathbf{u}(\mathbf{x}'-\mathbf{V}t).$$

(Note that (207) has the same structure as the master balance law discussed in Section 2.5.) Using the second of (184), this result can be expressed in the form

$$\mathbf{J}\cdot\mathbf{V}=\int_{\mathcal{P}}\dot{\psi}^d\,dV,\qquad\dot{\psi}^d=-\psi_{\underline{\phi}}\bullet\dot{\underline{\phi}}\quad(208)$$

where

$$\mathbf{J}=\int_{\mathcal{P}}\int_{\mathcal{B}\setminus\mathcal{P}}\left(\mathbf{u}_{\mathbf{x}}^T\mathbf{t}'-(\mathbf{u}'_{\mathbf{x}})^T\mathbf{t}\right)dV'\,dV+\int_{\partial\mathcal{P}}\psi\mathbf{n}\,dA.\quad(209)$$

This provides the peridynamic equivalent of the J-integral in the standard theory [57]. (208) and (209) relate the free energy lost in some dissipative process to quantities along the surface of a subregion $\mathcal{P}$ that contains the material where the dissipation is occurring. This dissipative region can be much smaller than $\mathcal{P}$. The required quantities on the surface $\partial\mathcal{P}$ can be evaluated if the deformation is known near this surface. Thus, we can "measure" the dissipation based on these far-field quantities without knowing the details of what happens in the dissipative region. Recall that (176) and (182), which are consequences of the second law, together with (208), ensure that

$$\mathbf{J}\cdot\mathbf{V}\geq 0$$

for any $\mathbf{V}$; in other words the rate of energy dissipation is always nonnegative.

Although it was assumed that $\mathbf{u}$ is differentiable (with respect to all spatial coordinates), it is only the directional derivative $\mathbf{u_x V}$ in the direction of motion that is used. Therefore, it is permissible to have discontinuities parallel to the direction of propagation, as would be the case with a crack. As in the classical development of the J-integral [57], the assumption of a steady motion excludes curved or oscillatory cracks. However, the peridynamic method can nevertheless be applied in these cases, as demonstrated by the numerical studies summarized in Section 1.2.

Evidently, if there is no dissipation within the closed surface $\partial\mathcal{P}$, then $\mathbf{J} = \mathbf{0}$. So, $\mathcal{P}$ can be deformed to include any amount of additional material in which there is no dissipation occurring without changing the value of $\mathbf{J}$. In this sense, $\mathbf{J}$ is "path independent."

8.8 Relation to the Griffith criterion

A good approximation in many solids is to assume that a crack will grow if a definite amount of energy G, called the *critical energy release rate*, is available to it per unit area of crack advance. The critical energy release rate is often thought of as being consumed in separating atoms to create new surface area, but it can include other processes as well, such as plastic work in the vicinity of the crack tip. Plasticity in peridynamic materials, although not treated in the present article, is discussed in [67]. Like the rate dependence discussed in Section 4.5 (see (73)), plasticity represents a mechanism whose energy dissipation rate can be included through terms similar to $\dot{\psi}^d$ discussed here for damage evolution.

The Griffith concept of crack growth can be related to the peridynamic model as follows. In (208), suppose $\dot{\underline{\phi}}$ scales with $\mathbf{V}$. In other words, assume that the damage model is such that there exists a vector state valued function $\underline{\mathbf{r}}(\underline{\phi})$ such that

$$\dot{\underline{\phi}} = \underline{\mathbf{r}} \bullet \dot{\underline{\mathbf{Y}}}.$$

(189) is an example of such an $\mathbf{r}$. From (204),

$$\dot{\underline{\mathbf{Y}}}[\mathbf{x}]\langle \mathbf{x}' - \mathbf{x}\rangle = -(\mathbf{u}'_{\mathbf{x}} - \mathbf{u}_{\mathbf{x}})\mathbf{V}.$$

Combining the last two equations,

$$\dot{\underline{\phi}} = -(\underline{\mathbb{G}} \bullet \underline{\mathbf{r}}) \cdot \mathbf{V} \tag{210}$$

where the double state field $\underline{\mathbb{G}}$ is defined by

$$\underline{\mathbb{G}}[\mathbf{x}]\langle \boldsymbol{\xi}, \boldsymbol{\zeta}\rangle = \big(\mathbf{u}^T_{\mathbf{x}}(\mathbf{x}+\boldsymbol{\xi}) - \mathbf{u}^T_{\mathbf{x}}(\mathbf{x})\big)\Delta(\boldsymbol{\zeta} - \boldsymbol{\xi}).$$

for all bonds $\boldsymbol{\xi}, \boldsymbol{\zeta} \in \mathcal{H}$. From (208) and (210),

$$\mathbf{J} \cdot \mathbf{V} = \left(\int_{\mathcal{P}} \underline{\psi}_{\underline{\phi}} \bullet \underline{\underline{\mathbb{G}}} \bullet \underline{\mathbf{r}} \, dV \right) \cdot \mathbf{V}$$

from which it follows that

$$\mathbf{J} = \int_{\mathcal{P}} \underline{\psi}_{\underline{\phi}} \bullet \underline{\underline{\mathbb{G}}} \bullet \underline{\mathbf{r}} \, dV. \tag{211}$$

If the direction of propagation is parallel to a unit vector $\mathbf{a}$, then $\mathbf{J} \cdot \mathbf{a}$ is the energy dissipation (with units of energy/length). If the body is a plate of thickness β containing a crack through its thickness, and if $\mathcal{P}$ is a cylinder through the thickness containing the crack tip, then the energy dissipated per unit crack area is

$$G_{\mathbf{a}} = \frac{\mathbf{J} \cdot \mathbf{a}}{\beta}.$$

Under the assumptions of the present analysis, we have arrived at the Griffith model for crack growth: energy is dissipated at a constant rate per unit crack area, independent of time and propagation speed. Of course, the integrand in (211) depends on all the details of the deformation and the material model, including the damage model.

8.9 Surface energy

The results of the previous section show that, under certain conditions, a crack growing in a peridynamic solid consumes a fixed amount of energy per unit area of crack growth. This energy can be computed, in a numerical model of a growing crack, either by evaluating $\mathbf{J}$ directly from (211) or using the expression (209) that was derived from an energy balance on a moving subregion containing the crack tip. By carrying out this calculation for different choices of parameters in the damage evolution law $\underline{D}$ or $\dot{\underline{D}}$, these parameters can be calibrated to experimental data on critical energy release rate.

In this section, a simpler but approximate procedure is presented for accomplishing the same thing. This procedure assumes that the energy consumed by a growing crack equals the work required, per unit crack area, to separate two halves of a body across a plane (Figure 13). Suppose a plane $\mathcal{A}$ separates a large homogeneous body $\mathcal{B}$ into two subsets $\mathcal{B}_+$ and $\mathcal{B}_-$, where $\mathcal{B}_-$ includes $\mathcal{A}$. Consider a small patch on $\mathcal{A}$ with area a. Let $\mathcal{P}$ be the cylinder normal to $\mathcal{A}$, extending infinitely in both directions from it, whose cross-section is this small patch. Also define $\mathcal{P}_+ = \mathcal{P} \cap \mathcal{B}_+$ and $\mathcal{P}_- = \mathcal{P} \cap \mathcal{B}_-$.

Consider a motion with velocity field $\mathbf{v}$ given by

$$\mathbf{v} = \begin{cases} \mathbf{c}/2 & \text{on } \mathcal{B}_+ \\ -\mathbf{c}/2 & \text{on } \mathcal{B}_- \end{cases}$$

where $\mathbf{c}$ is a constant vector. Now compute the total energy E absorbed by $\mathcal{P}$ in this motion. By (34),

$$E = \int_0^t \mathcal{W}_{\text{abs}}(\mathcal{P})\, dt' = \int_0^\infty \int_{\mathcal{P}} \int_{\mathcal{B}} \mathbf{t} \cdot (\mathbf{v}' - \mathbf{v})\, dV'\, dV\, dt$$

where $\mathbf{t} = \mathbf{t}(\mathbf{x}', \mathbf{x}, t)$, $\mathbf{v} = \mathbf{v}(\mathbf{x})$, and $\mathbf{v}' = \mathbf{v}(\mathbf{x}')$. In this discussion, t serves as a convenient parameter although dynamics is not considered. Because the body is homogeneous, the energies absorbed by $\mathcal{P}_+$ and by $\mathcal{P}_-$ must be equal. Also, bonds that do not cross $\mathcal{A}$ do not contribute to the integrand, since $\mathbf{v} = \mathbf{v}'$ for these bonds. With these simplifications,

$$E = 2 \int_0^\infty \int_{\mathcal{P}_-} \int_{\mathcal{B}_+} \mathbf{t} \cdot \mathbf{c}\, dV'\, dV\, dt, \tag{212}$$

in which the factor of 2 appears because the integral over $\mathcal{P}_+$ is not included explicitly. Assume that the material is characterized by a free energy density function with damage. By (181),

$$\mathbf{t} = \mathbf{t}(\mathbf{x}', \mathbf{x}, t) = \psi_{\underline{\mathbf{Y}}}(\underline{\mathbf{Y}}, \underline{\phi})\langle \mathbf{x}' - \mathbf{x} \rangle.$$

Following [26], assume that the material model is such that each bond consumes a prescribed amount of work (per unit volume squared) w_0 as the two parts of the body are separated out to a large distance:

$$\int_0^\infty \mathbf{t} \cdot \mathbf{c}\, dt = w_0 \qquad \forall\, \mathbf{x} \in \mathcal{B}_-, \quad \forall\, \mathbf{x}' \in \mathcal{B}^+.$$

An example of such a material model is one in which each bond breaks at the time $\tau(\mathbf{x}', \mathbf{x})$ at which the net work done on it up to that time equals w_0, thus

$$\underline{\phi}[\mathbf{x}, t]\langle \mathbf{x}' - \mathbf{x} \rangle = H(t - \tau(\mathbf{x}', \mathbf{x}))$$

where τ is defined by

$$\int_0^{\tau(\mathbf{x}', \mathbf{x})} \mathbf{t} \cdot \mathbf{c}\, dt = w_0.$$

Also, assume that in such a material model, $\mathbf{t} = \mathbf{0}$ for $t > \tau$. The function τ is not known in advance, but this does not matter; it can be computed in a numerical simulation "on the fly." Under these assumptions about the material, (212) becomes

$$E = 2w_0 \int_{\mathcal{P}_-} \int_{\mathcal{B}_+} \underline{\phi}[\mathbf{x}, \infty]\langle \mathbf{x}' - \mathbf{x} \rangle\, dV'\, dV. \tag{213}$$

To evaluate this double integral, observe that $\underline{\phi}[\mathbf{x},\infty]\langle\mathbf{x}'-\mathbf{x}\rangle = 1$ for bonds that connect points $\mathbf{x}\in\mathcal{P}_-$ to points $\mathbf{x}'\in\mathcal{B}_+$. Referring to Figure 14, any point $\mathbf{x}$ on the lower vertical axis with $0\le z\le\delta$ is connected to points $\mathbf{x}'$ within the spherical cap $\mathcal{H}\cap\mathcal{B}_+$. Working in a spherical coordinate system with elevation angle φ, azimuthal angle ϑ, and radius ξ, (213) reduces to

$$E = 2w_0 a\int_0^{2\pi}\int_0^{\delta}\int_z^{\delta}\int_0^{\cos^{-1}(z/\xi)} \xi^2\,\sin\varphi\,d\varphi\,d\xi\,dz\,d\vartheta = \frac{\pi w_0\delta^4 a}{2}. \quad (214)$$

Assuming that this surface energy equals the critical energy release rate G for the material times the area of the patch a,

$$G = E/a.$$

From this and (214), solving for w_0 yields

$$w_0 = \frac{2G}{\pi\delta^4}.$$

Thus, the critical value of work on a bond for bond breakage has been determined from the measurable quantity G. This result is independent of the details of the constitutive model.

9 Discussion

The development of the peridynamic theory presented above has emphasized the unifying aspect of the theory: the same field equations can be applied directly to traditional continua, to continua with emerging and propagating defects, and to discrete particles. Does such a unified treatment have any advantages over standard methods? One possible benefit is that since all these regimes satisfy the same field equations, it may not be necessary to devise coupling methods to connect disparate mathematical systems. For example, communication between an atomistic and a continuous region does not require coupling between a set of ODEs describing the particles and PDEs describing the continuum, since both regimes obey the same integro-differential equations in peridynamics. Development of such an atomistic-to-continuum coupling within the peridynamic framework is a current area of research.

Similarly, because the same field equations within the peridynamic model apply to points either on or off of a discontinuity, cracks and other defects grow autonomously. Their nucleation and progression are determined by the equation of motion and the material model, which may include damage evolution. It is not necessary to provide a supplemental kinetic relation that dictates the evolution of cracks, as is needed in traditional fracture

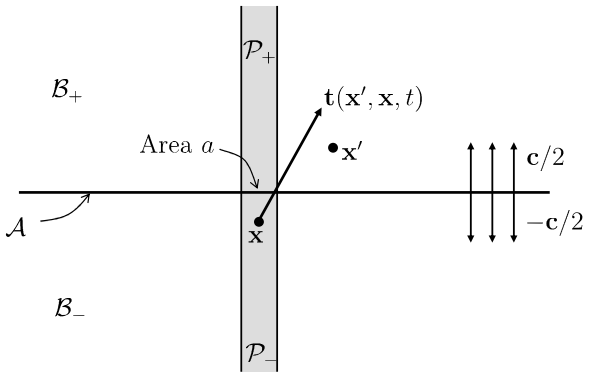

Figure 13: Computation of surface energy by the total work absorbed by $\mathcal{P}_-$ as it separates from $\mathcal{B}_+$.

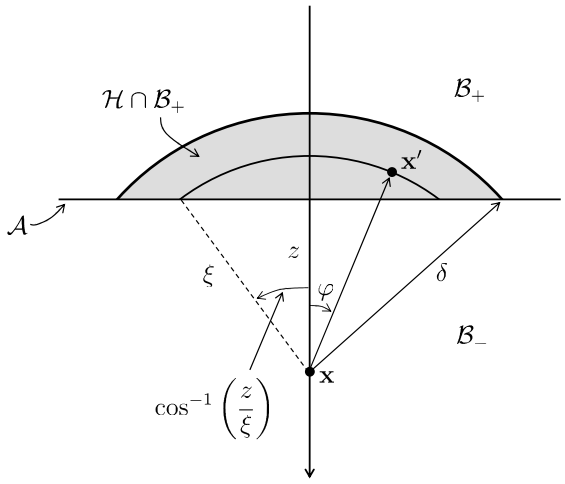

Figure 14: Computation of surface energy by the total work absorbed by $\mathcal{P}_-$ as it separates from $\mathcal{B}_+$.

mechanics. Instead, cracks appear and grow spontaneously depending on conditions.

It is worthwhile to compare the peridynamic approach to fracture against variational approaches [28, 12, 13] in which the growth of a crack is determined by energy minimization, including contributions from continuous parts of the body and from energy consumed by the crack. Like traditional fracture mechanics, this variational approach treats cracks as separate entities from the continuous parts of the deformation, hence the need to include their energy consumption through separate terms in the variational statement. Thus, the variational approach to fracture has fundamentally different purposes and characteristics from the peridynamic approach, which treats damage only through the material model and does not distinguish between cracked and continuous parts of the body.

A question of fundamental interest is the extent to which the peridynamic approach to damage can qualitatively and quantitatively reproduce the phenomena of fracture, particularly in complex materials and geometries. A closely related question is how the details of the constitutive model, including the damage evolution law, influence predicted fracture and failure of materials. As noted in Section 1.2, there are many encouraging numerical results available that apply peridynamic modeling to a variety of problems in fracture and fragmentation, including dynamic fracture. In most cases, these simulations rely on the simplest possible assumptions about material response and damage. A more comprehensive approach is needed to learn what insights can be gained from the peridynamic method for fracture, and what types of material models lead to the best agreement with experimental data.

As remarked in Section 3, the peridynamic theory uses vector states, rather than second order tensors, as the fundamental quantities that a constitutive model deals with. These states are infinite dimensional objects, unlike tensors, which are 9-dimensional. This suggests that there may be a potentially larger and richer environment provided by the peridynamic theory in material modeling. This environment includes, as discussed in the present article, the ability to treat discontinuities and long-range forces directly. But there may also be other avenues of material modeling in the peridynamic theory that remain to be explored. For example, it is demonstrated in [69] that peridynamics reveals a condition for a particular type of material instability, interpreted as the nucleation of a crack, that is not necessarily well described by mathematical conditions such as loss of ellipticity in the classical theory. It is shown in [79] that a peridynamic micromodulus function in one dimension can be obtained from experimental measurements of wave dispersion data. Material response within peridynamics, including its implications for material stability and generation of defects, is an open

and promising area of research.

As noted in Section 7.5, the representation of a system of a discrete particles within the peridynamic theory is at present limited by the interactions are defined in the reference configuration due to the Lagrangian nature of the method. The generality of the treatment could be improved by developing an Eulerian version of the model that would allow changing interactions. This would also permit a number of other applications to be modeled, notably those involving fluids.

Future development of the peridynamic theory will include multiscale applications. It may be possible to construct a consistent multiscale method within peridynamics, that is, a rigorously coupled set of models at different length scales that all have the same mathematical structure. Such a multiscale method has been proposed in [62]. In this approach, a set of reduced, or *coarsened*, degrees of freedom is chosen from a detailed linearized model at the smallest length scale. This detailed description could represent a linearized molecular dynamics model since, subject to the assumptions in Section 7.4, discrete particles are a special case of a peridynamic continuum. It is possible to evaluate the *coarsened micromodulus* function such that the forces within the coarsened model agree with what would have been evaluated from the full, detailed model, even though the coarsened model excludes many of the original degrees of freedom. The resulting coarsened model has the same mathematical structure as the detailed model, *i.e.,* linear peridynamics. Therefore, the coarsening process can be repeated over and over hierarchically, leading to successively more economical computational models.

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