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Statistical Coarse-Graining of Molecular Dynamics into Peridynamics

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Abstract

This paper describes an elegant statistical coarse-graining of molecular dynamics at finite temperature into peridynamics, a continuum theory. Peridynamics is an efficient alternative to molecular dynamics enabling dynamics at larger length and time scales. In direct analogy with molecular dynamics, peridynamics uses a nonlocal model of force and does not employ stress/strain relationships germane to classical continuum mechanics. In contrast with classical continuum mechanics, the peridynamic representation of a system of linear springs and masses is shown to have the same dispersion relation as the original spring-mass system.

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1 Introduction

The recent paper [10] observes that the differential equations of classical linear elasticity break down at length scales up to about 100 angstroms due to the local force assumption. In contrast, the peridynamic [11] theory of continuum mechanics is based on *nonlocal* force interactions, and it belongs to the class of microcontinuum theories defined by generalizing the local force assumption to allow force at a distance. However all such theories achieve nonlocality, except for peridynamics, by 1) augmenting the displacement field with supplementary fields (e.g. rotations) to provide information on fine-scale kinematics, 2) using higher order gradients of the displacement field, or 3) averaging the local strains and/or stresses (see [1, 2, 3] for a general discussion and references). In contrast, peridynamics employs an integral operator to *sum* forces and so obviates the need for strain; hence peridynamics is well aligned with molecular dynamics.

This paper describes an elegant statistical coarse-graining of molecular dynamics at finite temperature into peridynamics, a continuum theory. Peridynamics is an efficient alternative to molecular dynamics enabling dynamics at larger length and time scales. The coarse-graining avoids the use of a unit cell typical of homogenization approaches [4, 6], and any reliance upon the Cauchy-Born rule [5].

Our coarse graining proceeds in three steps: 1) representation of a collection of interacting atoms at finite temperature as a peridynamic body, 2) homogenization of the peridynamic body, 3) rescaling of the homogenized peridynamic equation of motion to a larger length scale. For ease of exposition, our coarse graining uses pairwise force interactions but we remove this restriction at the end of our paper with a peridynamic notion of multibody potentials. We show that the homogenized peridynamic equation of motion for a linear mass-spring model results in the same acoustic and optical phonon dispersion relationships of the lattice. Hence peridynamic reproduces the short-wavelength behavior associated with lattice dynamics, in contrast to classical continuum mechanics. We also show that a continuum mechanics notion of stress for the statistical representation of atoms can be defined.

Molecular dynamics requires only the current positions of atoms to determine the internal forces on the atoms. In contrast, in continuum mechanics, the internal forces are not, in general, determined by the current positions of the points alone (an exception to this is a static homogeneous fluid). Continuum mechanics relates internal forces on points in a body to the *deformation* of the body in the macroscopic sense. The current positions must be compared with the positions of the same points in a reference configuration, otherwise concepts such as deformation, stretch, and strain are meaningless. The need to define a reference configuration, which is concept foreign to molecular dynamics, is one of the fundamental challenges in making the transition to a continuum model for solids.

Continuum mechanics posits a *reference configuration* that may be thought of as the position of the body at $t = 0$. The location of a point of the body in the reference configuration is generically called $\mathbf{x}$; any such $\mathbf{x}$ provides a label for a certain piece of continuous matter. At any time $t \geq 0$, the position of the body is given by the map $\mathbf{\Phi}_t$ called the *deformation*, and the deformed image of the body under $\mathbf{\Phi}_t$ is called the *deformed configuration*. The vector $\mathbf{\Phi}_t(\mathbf{x}) - \mathbf{\Phi}_0(\mathbf{x}) = \mathbf{u}(\mathbf{x}, t)$ is the *displacement* of $\mathbf{x}$. In contrast to classical continuum mechanics, it is not assumed that the deformation is continuous, let alone differentiable.

2 Peridynamics

The peridynamic formulation of continuum mechanics [11] was introduced as a way to model deformation with no assumptions (e.g. continuity, differentiability) on the displacement field, so that discontinuities (e.g. cracks) can be modeled. The peridynamic equation of motion is

$$\rho(\mathbf{x})\ddot{\mathbf{u}} = \int \mathbf{f}\left(\mathbf{u}' - \mathbf{u}, \mathbf{x}' - \mathbf{x}, \mathbf{x}\right) dV_{\mathbf{x}'} + \mathbf{b}, \tag{1}$$

where $\mathbf{u} \equiv \mathbf{u}(\mathbf{x}, t), \mathbf{u}' = \mathbf{u}(\mathbf{x}', t)$, $\mathbf{b} \equiv \mathbf{b}(\mathbf{x}, t)$ is a prescribed body force density field, ρ is mass density in the reference configuration, and $\mathbf{f}$ is a *pairwise force function* whose value is the force vector (per unit volume squared) that the point $\mathbf{x}'$ exerts on the point $\mathbf{x}$. In (1), and throughout this paper, all volume integrals are taken over $\mathbb{R}^3$.

All constitutive information about a material is contained in $\mathbf{f}$. We assume that there exists a scalar-valued function w called the *micropotential* such that

$$\mathbf{f}(\boldsymbol{\eta}, \boldsymbol{\xi}, \mathbf{x}) = \nabla_{\boldsymbol{\eta}} w(\boldsymbol{\eta}, \boldsymbol{\xi}, \mathbf{x}), \tag{2}$$

where $\boldsymbol{\xi} = \mathbf{x}' - \mathbf{x}$ and $\boldsymbol{\eta} = \mathbf{u}' - \mathbf{u}$, so that $\boldsymbol{\eta} + \boldsymbol{\xi}$ represents the *current* relative position vector. The concept of a *bond*, denoted by $\boldsymbol{\xi}$, that extends over a finite distance is a fundamental difference between peridynamics and classical continuum mechanics. The latter is based on the idea of contact forces (interactions between points that are in direct contact with each other). $\mathbf{f}$ contains a length scale δ that represents the cutoff distance (or *horizon*) for interactions.

Balance of linear and angular momenta [11] imply that w depends only on $|\boldsymbol{\eta} + \boldsymbol{\xi}|$; thus $w = w_0(|\boldsymbol{\eta} + \boldsymbol{\xi}|, \boldsymbol{\xi}, \mathbf{x})$ for some scalar valued function w_0. For a peridynamic body at a given time, the strain energy density W and total strain energy U are given by

$$W(\mathbf{x}, t) = \frac{1}{2} \int w(\boldsymbol{\eta}, \boldsymbol{\xi}, \mathbf{x})\, dV_{\boldsymbol{\xi}}, \quad U(t) = \int W(\mathbf{x}, t)\, dV_{\mathbf{x}}. \tag{3}$$

Peridynamics has been implemented in a computational model called EMU [12] that is being applied to a variety of problems across a wide range of length scales, for example [13].

The peridynamic equation of motion (1) is an integro-differential equation that can be recast so that it is formally identical to the classical equation of motion. This is accomplished by defining the *peridynamic stress tensor* [9]

$$\boldsymbol{\nu}(\mathbf{x}, t) = \frac{1}{2} \int_{\mathcal{S}} \int_0^\infty \int_0^\infty (y + z)^2 \mathbf{g} \otimes \mathbf{m}\, dz\, dy\, d\Omega_{\mathbf{m}}, \tag{4a}$$

$$\mathbf{g} = \mathbf{f}(\mathbf{u}(\mathbf{x} + y\mathbf{m}) - \mathbf{u}(\mathbf{x} - z\mathbf{m}), (y + z)\mathbf{m}, \mathbf{x}) \tag{4b}$$

where $\mathcal{S}$ is the unit sphere, $d\Omega_{\mathbf{m}}$ is a differential solid angle in the direction of unit vector $\mathbf{m}$, and $\otimes$ indicates the dyadic product of two vectors. The peridynamic stress tensor field is a solution to differential equation

$$\nabla_{\mathbf{x}} \cdot \boldsymbol{\nu}(\mathbf{x}, t) = \int \mathbf{f}\left(\mathbf{u}' - \mathbf{u}, \mathbf{x}' - \mathbf{x}, \mathbf{x}\right) dV_{\mathbf{x}'} \tag{5}$$

where $\nabla_{\mathbf{x}}\cdot$ is the divergence operator. The peridynamic stress satisfies $\boldsymbol{\nu}\cdot\mathbf{n} = 0$ on the convex hull of the body where $\mathbf{n}$ is the outward unit normal.

3 Peridynamic probabilistic distribution

Consider a set of N atoms with mass m_i with positions in a reference configuration $\{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N\}$. Suppose these atoms interact through a pair potential v. Let $dV_{\mathbf{x}}$ denote a volume element at a point $\mathbf{x}$ in the reference configuration. Let $\mathbf{y} = \mathbf{\Phi}_t(\mathbf{x})$, and at some given $t \geq 0$, let $dV_{\mathbf{y}}$ denote the image of $dV_{\mathbf{x}}$ under the deformation $\mathbf{\Phi}_t$. Let $\Gamma_i(\mathbf{y}, t)$ denote the probability density of finding atom i at the point $\mathbf{y}$ in the deformed configuration at time t. Assume that

$$\Gamma_i(\mathbf{y}, t)\; dV_{\mathbf{y}} = \gamma_i(\mathbf{x})\; dV_{\mathbf{x}}, \qquad \gamma_i(\mathbf{x}) \equiv \Gamma_i(\mathbf{y}, 0), \tag{6}$$

the latter of which defines the function γ_i on the reference configuration. In words, the probability of finding atom i in $dV_{\mathbf{y}}$ is independent of time as the volume element deforms under Φ_t, e.g. the probability is conserved. (Note that (6) is a condition on the mapping $\mathbf{\Phi}_t$.) An example of a γ_i is given by the marginal density obtained by integrating out all momentum and all but the i-th position degrees of freedom of phase space density.

The potential energy between volume elements $dV_{\mathbf{y}}$ and $dV_{\mathbf{y}'}$ is

$$dU = \sum\sum v(|\mathbf{y}' - \mathbf{y}|)\Gamma_j(\mathbf{y}')\Gamma_i(\mathbf{y})\; dV_{\mathbf{y}'}\; dV_{\mathbf{y}} \tag{7}$$

in which the sum $\sum$ is over the N atoms. In the (7) and the remainder of this paper, double sums do not include $i = j$, and for ease of notation denote $\Gamma_i(\mathbf{y}) = \Gamma_i(\mathbf{y}, t)$. Define a peridynamic body, in the reference configuration, by

$$\rho(\mathbf{x}) = \sum m_i\gamma_i(\mathbf{x}), \tag{8a}$$

$$w(\boldsymbol{\eta}, \boldsymbol{\xi}, \mathbf{x}) = \sum\sum v(|\boldsymbol{\xi} + \boldsymbol{\eta}|)\gamma_j(\mathbf{x} + \boldsymbol{\xi})\gamma_i(\mathbf{x}), \tag{8b}$$

where $\boldsymbol{\xi} + \boldsymbol{\eta} = \mathbf{\Phi}_t(\mathbf{x} + \boldsymbol{\xi}) - \mathbf{\Phi}_t(\mathbf{x})$. As an example, the change of variables $\mathbf{x}' = \mathbf{x} + \boldsymbol{\xi}$ and $\mathbf{y}' = \mathbf{\Phi}_t(\mathbf{x}')$ gives the N atom total strain energy (3) of (8b) as

$$U = \frac{1}{2}\int\int v(|\mathbf{y}' - \mathbf{y}|)\sum\sum \gamma_i(\mathbf{x}')\gamma_j(\mathbf{x}) dV_{\mathbf{x}'} dV_{\mathbf{x}}.$$

Hence, the assumption (6) gives the total strain energy as

$$U = \frac{1}{2}\int\int v(|\mathbf{y}' - \mathbf{y}|)\sum\sum \Gamma_i(\mathbf{y}')\Gamma_j(\mathbf{y})\; dV_{\mathbf{y}'}\; dV_{\mathbf{y}}$$

in agreement with (7). This result establishes that any deformation of the peridynamic body (8) has the correct total strain energy. The special case of atoms with positions $\mathbf{y}_i(t)$ corresponds to $\Gamma_i(\mathbf{y}) = \Delta(\mathbf{y} - \mathbf{y}_i(t))$, where $\Delta(\cdot)$ is the Dirac delta function. Hence, for an N atom system, $U = \frac{1}{2}\sum\sum v(|\mathbf{y}_j - \mathbf{y}_i|)$. Departures of the γ_i from delta functions encompass probabilistic behavior of atoms at the small scale due to random thermal motions and the inherently chaotic motion of particles in a nonlinear system. It is also possible to identify the γ_i with probabilities arising from quantum mechanical wave functions, *i.e.*, $\gamma_i = \psi_i^*\psi_i$.

The purpose of the γ_i is to create a precise connection between the basic kinematical concept in continuum mechanics, the deformation, and quantities relevant at the small scale. Hence, the peridynamic equation of motion describes the evolution of mass, force and body force densities associated with a probabilistic representation of atoms. The γ_i are not the localization functions considered by Hardy [7] because the γ_i's are not assumed to be peaked about any location, and they are assumed to satisfy the kinematic constraint (6). They are also different from the interpolation functions applied by Kunin [8, pp. 12] to develop a class of continuous functions with a 1-to-1 correspondence to a discrete lattice.

4 Homogenization

We have derived a continuum model capable of representing the deformation of a set of atoms whose positions are given by probabilities. To make this model more useful for traditional continuum mechanics applications, we *homogenize* the peridynamic fields over space. Let ϕ be a non-negative function on $\mathbb{R}^3$ such that

$$\phi(\mathbf{q}) = \phi(-\mathbf{q}), \qquad \int \phi(\mathbf{q})\, dV_{\mathbf{q}} = 1. \tag{9}$$

For a given peridynamic material with density ρ and micropotential w, define a homogenized peridynamic material with density $\bar{\rho}$ and micropotential $\bar{w}$ by

$$\bar{\rho}(\mathbf{x}) = \int \phi(\mathbf{q})\rho(\mathbf{x}+\mathbf{q})\, dV_{\mathbf{q}} \tag{10a}$$

$$\bar{w}(\boldsymbol{\eta},\boldsymbol{\xi},\mathbf{x}) = \int \phi(\mathbf{q})w(\boldsymbol{\eta},\boldsymbol{\xi},\mathbf{x}+\mathbf{q})\, dV_{\mathbf{q}}. \tag{10b}$$

Suppose the body is subjected to a *uniform deformation*, *i.e.*, for some constant tensor $\mathbf{H}$, $\mathbf{u}(\mathbf{x},t) = \mathbf{H}\mathbf{x}$ for all $\mathbf{x}$ and all t. The total strain energy (3) in the homogenized body is

$$\begin{aligned} \bar{U} &= \frac{1}{2}\int\int\int \phi(\mathbf{q})w(\mathbf{H}\boldsymbol{\xi},\boldsymbol{\xi},\mathbf{x}+\mathbf{q})\, dV_{\mathbf{q}}\, dV_{\boldsymbol{\xi}}\, dV_{\mathbf{x}} \\ &= \frac{1}{2}\int\int w(\mathbf{H}\boldsymbol{\xi},\boldsymbol{\xi},\mathbf{z})\, dV_{\boldsymbol{\xi}}\, dV_{\mathbf{z}} = U \end{aligned} \tag{11}$$

where the change of variables $\mathbf{z} = \mathbf{x}+\mathbf{q}$, and the second of (9) were used. This result shows that for any uniform deformation, the total strain energy is invariant under the homogenization.

To illustrate the properties of a homogenized atomic system, we derive acoustic and optical peridynamic phonon dispersion relationships for a 1D linear spring-mass system. For the acoustic relationships, it is suffices to consider a 1D lattice with spring constant, mass, and spacing k, m, and $a(= x_{i+1} - x_i)$. The resulting equation of motion and the strain energy in each spring are given by

$$m\ddot{u}_i = k(u_{i+1} - 2u_i + u_{i-1}), \quad v = \frac{k}{2}(u_{i+1} - u_i)^2. \tag{12}$$

Assume continuous and discrete waves $e^{\iota(\kappa x - \omega t)}$, where $\iota = \sqrt{-1}$, κ is the wave number, and ω is the angular frequency of the wave. Substitution of the discrete wave into (12) yields the well-known discrete dispersion relationship

$$\omega_d^2(\kappa) = \frac{2k}{m}(1 - \cos\kappa a). \tag{13}$$

Recall that $\Delta(\cdot)$ is the Dirac delta function, and so the peridynamic density and micropotential are given by

$$\rho(x) = m\sum \Delta(x - x_i), \tag{14a}$$

$$w(\eta, \xi, x) = \frac{k}{2}\eta^2 \sum \Delta(x - x_i)\Delta(|\xi| - a), \tag{14b}$$

so that homogenizing using (10) leads to

$$\bar{\rho}(x) = m\sum \phi(x - x_i), \tag{15a}$$

$$\bar{f}(\eta, \xi, x) = k\eta \sum \phi(x - x_i)\Delta(|\xi| - a). \tag{15b}$$

Substitution of the continuous wave into the peridynamic equation of motion (1) with (15) results in

$$m\ddot{u}(x,t)\sum \phi(x - x_i) = k(u(x + a, t) - 2u(x,t) + u(x - a, t))\sum \phi(x - x_i),$$

where the first of (9) has been used. The sums cancel, yielding a continuous dispersion relationship that is identical to (13). Hence, we have demonstrated that for this system, the homogenized peridynamic continuum model gives the same dispersion relation as the original lattice.

We now derive the optical phonon dispersion relationships for a one-dimensional diatomic lattice in which the spring constants are all the same, but the masses alternate between m_0 and m_1. Define separate density and displacement fields ρ_α, u_α, $\alpha = 0, 1$. Let x_i^α and $\eta_\alpha = u_{1-\alpha}(x + \xi) - u_\alpha(x)$ denote the positions of the atoms with mass m_α, and their relative displacement. In an analogous fashion to (15), homogenization yields the mass and force densities

$$\bar{\rho}_\alpha = m_\alpha \sum \phi(x - x_i^\alpha), \qquad \bar{f}_\alpha = k\eta_\alpha \sum \phi(x - x_i^\alpha)\Delta(|\xi| - a).$$

The assumption $u_\alpha = A_\alpha e^{\iota(\kappa x - \omega t)}$, where A_α are the amplitudes, results in two coupled homogeneous algebraic equations:

$$m_\alpha A_\alpha \omega^2 = 2k(A_\alpha - A_{1-\alpha}\cos\kappa a), \qquad \alpha = 0, 1.$$

This is identical to the secular equation for the original discrete diatomic lattice that leads to the well-known dispersion relations

$$\frac{\omega^2}{k} = \left(\frac{1}{m_0} + \frac{1}{m_1}\right) \pm \sqrt{\left(\frac{1}{m_0} + \frac{1}{m_1}\right)^2 - \frac{4\sin^2\kappa a}{m_0 m_1}}.$$

The two roots in this equation correspond to the two branches of the dispersion relation.

Our conclusion is that the peridynamic continuum model with two displacement fields, after homogenization, preserves the dispersion relation of the original system, including both the acoustic and optical branches. In contrast, classical continuum mechanics results in a linear dispersion curve.

5 Rescaling

The peridynamic equations contain a length scale, or horizon, δ, as explained in the discussion following (2). Let the micropotentials w, w' correspond to peridynamic materials with horizon δ, δ', respectively, and define the relationship between the two micropotentials as

$$w'(\boldsymbol{\eta}, \boldsymbol{\xi}, \mathbf{x}) = \epsilon^3 w(\epsilon\boldsymbol{\eta}, \epsilon\boldsymbol{\xi}, \mathbf{x}), \quad \epsilon = \frac{\delta}{\delta'} \leq 1. \tag{16}$$

Consider a body subjected to a uniform deformation $\mathbf{H}$, and let $\boldsymbol{\xi} = \epsilon\boldsymbol{\xi}'$ so that $dV_{\boldsymbol{\xi}} = \epsilon^3 dV_{\boldsymbol{\xi}'}$. Using (3) and (16), the strain energy density W' corresponding to w' is

$$\begin{aligned} W' &= \frac{1}{2}\int w'(\mathbf{H}\boldsymbol{\xi}', \boldsymbol{\xi}', \mathbf{x})\, dV_{\boldsymbol{\xi}'} \\ &= \frac{1}{2}\int \epsilon^3 w(\epsilon\mathbf{H}\boldsymbol{\xi}, \epsilon\boldsymbol{\xi}, \mathbf{x})\, (\epsilon^{-3} dV_{\boldsymbol{\xi}}) \\ &= \frac{1}{2}\int_H w(\mathbf{H}\boldsymbol{\xi}, \boldsymbol{\xi}, \mathbf{x})\, dV_{\boldsymbol{\xi}} = W. \end{aligned} \tag{17}$$

This result shows that under uniform deformation, the strain energy density is invariant under rescaling. Thus, for purposes of macroscopic modeling, the rescaled material model has properties similar to those of the original model. From (16), we have that

$$\mathbf{f}' = \nabla_{\boldsymbol{\eta}} w'(\boldsymbol{\eta}, \boldsymbol{\xi}, \mathbf{x}) = \epsilon^4 \nabla_{\boldsymbol{\eta}} w(\epsilon\boldsymbol{\eta}, \epsilon\boldsymbol{\xi}, \mathbf{x}).$$

An immediate conclusion is that rescaled pairwise peridynamic forces are attenuated by $\epsilon^4 < 1$ when $\delta' > \delta$. Moreover, a non-local interaction with respect to the δ length scale becomes weaker for the larger length scale as the ratio ϵ decreases. An important practical implication is that the numerically stable time step associated with explicit time integration of the rescaled peridynamic equations of motion can be increased over that in the original small scale model.

6 Peridynamic states

An extension [14] of the peridynamic model allows for material models in which the potential due to interactions between an atom at $\mathbf{y}$ and all other atoms is in general given by $v(\mathbf{y}_1 - \mathbf{y}, \mathbf{y}_2 - \mathbf{y}, \ldots, \mathbf{y}_N - \mathbf{y})$. In this model, the strain energy density at $\mathbf{x}$ is expressed as

$$W = \hat{W}(\underline{\mathbf{Y}}), \qquad \underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle = \Phi_t(\mathbf{x} + \boldsymbol{\xi}) - \Phi_t(\mathbf{x}) \tag{18}$$

where $\underline{\mathbf{Y}}$ is a function called the *deformation state* that maps any bond $\boldsymbol{\xi}$ into its deformed image. The notation $\underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle$ refers to the value of the function $\underline{\mathbf{Y}}$ evaluated at the bond vector $\boldsymbol{\xi}$. To obtain the bond forces, (2) is replaced by

$$\mathbf{f} = \underline{\mathbf{T}}[\mathbf{x}]\langle\boldsymbol{\xi}\rangle - \underline{\mathbf{T}}[\mathbf{x} + \boldsymbol{\xi}]\langle-\boldsymbol{\xi}\rangle, \quad \underline{\mathbf{T}} = \nabla_{\underline{\mathbf{Y}}} W(\underline{\mathbf{Y}})$$

where $\underline{\mathbf{T}}[\mathbf{x}]$ is the *force state* at $\mathbf{x}$, and $\nabla_{\underline{\mathbf{Y}}} W$ denotes the Frechet derivative of W with respect to $\underline{\mathbf{Y}}$. The essential difference in this generalization is that in (18), W depends not only on the deformation of individual bonds, but on the *collective* deformation of *all* the bonds connected to $\mathbf{x}$.

In this generalized, or *state-based*, peridynamic model, the homogenization (10b) and rescaling technique (16) can be applied if the associated expressions are replaced by

$$\begin{aligned} \bar{W}(\underline{\mathbf{Y}})[\mathbf{x}] &= \int \phi(\mathbf{q}) W(\underline{\mathbf{Y}})[\mathbf{x}+\mathbf{q}]\; dV_{\mathbf{q}}, \\ W'(\underline{\mathbf{Y}}') &= W(\underline{\mathbf{Y}}), \quad \epsilon \underline{\mathbf{Y}}'\langle \boldsymbol{\xi}' \rangle = \underline{\mathbf{Y}}\langle \epsilon \boldsymbol{\xi}' \rangle. \end{aligned}$$

The first equation says that for any deformation state $\underline{\mathbf{Y}}$, $\bar{W}$ is the volume average of W weighted by ϕ holding $\underline{\mathbf{Y}}$ constant. The definition of the peridynamic stress tensor (5) still applies, provided (4b) is replaced by

$$\mathbf{g} = 2\underline{\mathbf{T}}[\mathbf{x} - z\mathbf{m}]\langle (y+z)\mathbf{m} \rangle.$$

Therefore, (5) defines a rigorous stress that can be associated to a multibody potential.

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