PDLAMMPS - made easy

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1 Peridynamic theory of solids

The peridynamic theory of solid mechanics (S. Silling, 2000; S. Silling, Zimmermann, & Abeyarante, 2003; S. A. Silling, Epton, Weckner, Xu, & Askari, 2007) has been proposed as an alternative to the classical theory, and is offered as a mathematically consistent technique for modeling solid bodies with continuous and discontinuous displacements as well as a method that unifies the mechanics of particles and continuum bodies through the utilization of long-range forces.

The balance equation between rate of change of linear momentum and applied force on a deformable body Ω develops the fundamental equation in classical continuum mechanics is written in Eq. (1)

$$\rho(x)\,\ddot{u}(x,t) = \nabla\cdot\sigma + \mathbf{b}(x,t)\,. \tag{1}$$

where, $x \in \Omega$, t is the time, ρ is the mass density, $\ddot{u}$ is the accelaration, σ is the stress tensor and b is the body force. This differential equation is not well defined at the discontinuities. The PD formulation of a continuum introduces integral form of kinematic equation in order to mitigate this issue by calculating the force density on each material point as

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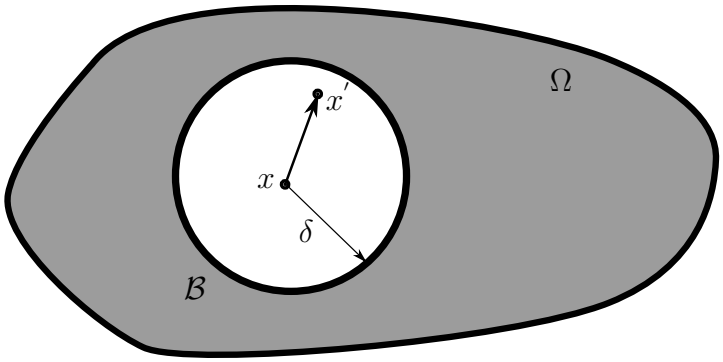

Figure 1: Schematic of peridynamic body.

$$\rho(x)\,\ddot{\mathbf{u}}(x,t) = \int_{\mathcal{B}} \mathbf{f}(\eta,\xi)\,dV + \mathbf{b}(x,t)\,. \tag{2}$$

where, deformable body Ω is represented with respect to an arbitrary frame of reference, $\mathbf{f}$ is the pairwise force applied on particle at x by a neighborhood particle at $x^{'}$ and $\mathcal{B}$ is a spherical region in the neighborhood of x with radius δ, ξ=$x^{'}$-x and η=$\mathbf{u}\left(x^{'},t\right)-\mathbf{u}(x,t)$ are relative position and displacement vectors, respectively (Fig 1) . For a certain $\delta>0$, $\mathbf{f}(\eta,\xi)=0$ for all η when $\|\xi\|>\delta$. This equation may be written more elaborately in terms of bond between x and $x^{'}$ as

$$\rho(x)\,\ddot{\mathbf{u}}(x,t) = \int_{\mathcal{B}} \left\{\underline{\mathbf{T}}[x,t]\left\langle x^{'}-x\right\rangle - \underline{\mathbf{T}}\left[x^{'},t\right]\left\langle x-x^{'}\right\rangle\right\} dV_{x^{'}} + \mathbf{b}(x,t)\,. \tag{3}$$

Equation. 3 is Newton,s equation of motion for continuum node x. The left hand side of Eq. 3 is $MassDensity \times Acceleration$ and the right hand side of Eq. 3 corresponds to force density. Equation. 3 can be written in discretized form as (Parks, Lehoucq, Plimpton, & Silling, 2008)

$$\rho_i\ddot{\mathbf{u}}_i = \sum_{j\neq i}^{\mathcal{M}_\delta}\{\underline{\mathbf{T}}[x_i,t]\langle x_j-x_i\rangle - \underline{\mathbf{T}}[x_j,t]\langle x_i-x_j\rangle\}\Delta V_{x_i} + \mathbf{b}_i. \tag{4}$$

Here, $\|x_j-x_i\|\leq\delta$. $\mathcal{M}_\delta$ correspond to number of peridynamic nodes within the horizon δ. The force vector state $\underline{\mathbf{T}}[x,t]$ is interpreted in terms

of mapping the bond between x_i and x_j to a force per volume which has a cutoff range. Each particle experiences two types of forces: short range forces and long range forces i.e. bond-forces. Short range forces are repulsive in nature. The bond-force on each particle is generated from the bonds it shares with the neighboring particles. Here, the $\underline{\mathbf{T}}$ is an infinite dimensional vector operator that maps the deformed image of the vector contained in the angle brackets, $\langle\rangle$, into the force acting on x. $\underline{\mathbf{T}} = \underline{t}\underline{\mathbf{M}}$ is defined as a *force vector-state*. $\underline{t}$ and $\underline{\mathbf{M}}$ are the scalar force state and deformed state, respectively. In PDLAMMPS the bond based peridynamics is implemented as prototype microelastic brittle model (**PMB**). The scalar force state for *PMB* is written as (Parks et al., 2008; S. Silling, 2000)

$$\underline{t}_{PMB} = \frac{1}{2}\frac{18K}{\pi\delta^4}\frac{\|\eta+\xi\| - \|\xi\|}{\|\xi\|}. \tag{5}$$

For the state-based peridynamic linearly elastic (**LPS**), elastic-plastic (**EPS**) and viscoelastic (**VES**) solids the scaler force state is written as (Parks et al., 2008; S. A. Silling et al., 2007)

$$\underline{t}_{Elastic} = -\frac{3K\theta}{m}\underline{\omega x} + \alpha\underline{\omega e}^d, \tag{6}$$

$$\underline{t}_{Plastic} = -\frac{3K\theta}{m}\underline{\omega x} + \alpha\underline{\omega}\left(\underline{e}^d - \underline{e}^{dp}\right), \tag{7}$$

$$\underline{t}_{Viscoelastic} = -\frac{3K\theta}{m}\underline{\omega x} + (\alpha_\infty + \alpha_i)\,\underline{e}^d - \alpha_i\underline{\omega e}^{db(i)}. \tag{8}$$

In Eq. 6 $\underline{\omega}\langle\xi\rangle$, $\underline{x}\langle\xi\rangle = \|\xi\|$ where $\xi = \mathbf{x}' - \mathbf{x}$. m, θ, $\underline{e}$ and $\underline{e}^d$ are the influence function, reference state, weighted volume, dilatation, extension state and deviatoric extension state respectively . The bulk modulus is K and the shear modulus (G) related term $\alpha = \frac{15G}{m}$ (S. A. Silling et al., 2007). In the above equations $\underline{e}^{dp}$ is the plastic component of the extension state, $\underline{e}^{db(i)}$ is the back extension state. For viscoelasticity model $\alpha = \alpha_\infty + \alpha_i$ and $0 < \alpha_i < \frac{15\mu}{m}$ (Parks et al., 2008; Mitchell, 2011a, 2011b). The detail about the peridynamic models implemented in PDLAMMPS can be found in the PDLAMMPS-documentation (Parks et al., 2008) and EPS and VES documentations (Rahman & Foster, 2013a, 2013b).

2 Implementation of peridynamics in LAMMPS

As the discretized version of the governing equation in peridynamics (Eq. 4) is a Newton's equation of motion, peridynamics was implemented in the classical molecular dynamics package LAMMPS (Parks et al., 2008; Plimpton, 1995). The peridynamics implementation in LAMMPS is known as *PDLAMMPS*. The package *PERI* in the LAMMPS *src* directory contains four peridynamic pair-styles: pmb, lps, eps and ves. *PERI* can be compiled as follows

```
$ make yes-peri
$ make foo
```

Here, *foo* corresponds to the machine name you are building LAMMPS for. For more information please look at the LAMMPS compilation instructions at `http://lammps.sandia.gov/docSection_start.html#start_2`.

2.1 Linear peridynamic soild: LPS

The formulation for *peri-lps* (Eq.6) was applied in PDLAMMPS. The pair style for *lps* is

```
pair_style peri/lps
pair_coeff * * K G horizon s00 Constant_alpha
```

Here, K, G, Constant-s_{00} and Constant-α are the bulk modulus, shear modulus and bond-breaking constants, respectively. [1] The unit for K and G is $\frac{Force}{Area}$. Constant-s_{00} and Constant-α are ***unit-less***. The horizon δ is in the unit of *Length*.

2.2 Peridynamic elastic-plastic soild: EPS

The formulation for *peri-eps* (Eq.7) was applied in PDLAMMPS. The pair style for *eps* is (Rahman & Foster, 2013a)

```
pair_style peri/eps
pair_coeff * * K G horizon s00 alpha YieldStress
```

[1] The user must not get confused with the completely different parameters: Constant-α and $\alpha = \frac{15G}{m}$.

Here, K, G, Constant-s_{00} and Constant-α are the bulk modulus, shear modulus and bond-breaking constants, respectively. *YieldStress* is the material's yield stress σ_Y. The unit for K, G and σ_Y is $\frac{Force}{Area}$. Constant-s_{00} and Constant-α are ***unit-less***. The horizon δ is in the unit of *Length*.

2.3 Peridynamic visco-elastic soild: VES

The formulation for *peri-ves* (Eq.8) was applied in PDLAMMPS. The pair style for *ves* is (Rahman & Foster, 2013b)

```
pair_style peri/ves
pair_coeff * * K G horizon s00 alpha lambda_i tau_i
```

Here, K, G, Constant-s_{00} and Constant-α are the bulk modulus, shear modulus and bond-breaking constants, respectively. Constant-λ_i and Constant-τ_i are the viscoelastic relaxation parameter and time constant, respectively. The unit for K and G is $\frac{Force}{Area}$. Constant-s_{00}, Constant-α, Constant-λ_i and Constant-τ_i are ***unit-less***. The horizon δ is in the unit of *Length*.

2.4 Peridynamic prototype microelastic brittle solid: PMB

The formulation for *peri-pmb* (Eq.5) was applied in PDLAMMPS. The pair style for *pmb* is

```
pair_style peri/pmb
pair_coeff * * c horizon s00 alpha
```

Here, $c = \frac{18K}{\pi\delta^4}$, Constant-$s_{00}$ and Constant-α are the spring constant and bond-breaking constants, respectively. The unit for c is $\frac{Energy}{Length^7}$. Constant-s_{00} and Constant-α are ***unit-less***. The horizon δ is in the unit of *Length*.

3 Consistent units in PDLAMMPS

In PDLAMMPS the units must be consistent with the available LAMMPS units. Let, K, G, δ are the bulk-modulus, shear modulus and horizon, respectively. $\tilde{\mathbf{f}}$ and $\mathbf{r}_{IJ}$ are the force density vector at a node and distance between I^{th} and J^{th} peridynamic nodes, respectively. These later two parameters can be obtained after running PDLAMMPS (e.g. *LAMMPS dump file*).

For an example, in ***si*** and ***metal*** units the set of consists units are shown in Table. 1. For other LAMMPS units the user must follow the required unit consistency in LAMMPS. [2]

	Metal	Si
K	eV/$\mathring{A}^3$	Pascals
G	eV/$\mathring{A}^3$	Pascals
δ	$\mathring{A}$	Meters
$\tilde{\mathbf{f}}$	eV/$\mathring{A}^4$	Newtons/Cubic meters
$\mathbf{r}_{IJ}$	$\mathring{A}$	Meters

Table 1: Difference between consistent units in PDLAMMPS

4 Additional features in PDLAMMPS

In PDLAMMPS there are three *compute* commands available. The command ***compute damage/atom*** calculates the damage $\phi(\mathbf{x},t)$ at each peridynamic node (Parks et al., 2008). The peridynamic damage can be expressed as

$$\phi(\mathbf{x},t) = 1 - \frac{\int_{\mathcal{H}} \mu(t,\eta,\xi)\, dV_{x'}}{\int_{\mathcal{H}} dV_{x'}} \tag{9}$$

$$s_0(t,\eta,\xi) = s_{00} - \alpha s_{min}(t,\eta,\xi) \tag{10}$$

$$s_{min}(t) = \min_{\xi} s(t,\eta,\xi) \tag{11}$$

Here, $\mu(t,\eta,\xi)$ is a binary function.

$\mu(t,\eta,\xi) = 1$ if $s'\left(t',\eta,\xi\right) < \min\left(s_0\left(t',\eta,\xi\right), s_0\left(t',\eta',\xi\right)\right)$ for $0 \le t' \le t$. Otherwise, $\mu(t,\eta,\xi) = 0$. And, ξ'=x''-x' and η'=$\mathbf{u}\left(x'',t\right) - \mathbf{u}\left(x',t\right)$. The Eq. 9 refers to the accumulation of damages at a node while each bond stretch exceeds the critical bond stretch $s_0(t,\eta,\xi)$. The material dependent parameters Constant-s_{00} and Constant-α are used in Eq. 11. During the simulation the values for $\phi(\mathbf{x},t)$ varies within the interval $[0,1]$

[2]For detail information the user is referred to *http://lammps.sandia.gov/doc/units.html.*

Another compute command is ***compute dilatation/atom***. The dilatation $\theta(\mathbf{x},t)$ is written as (S. A. Silling et al., 2007)

$$\theta(\mathbf{x},t) = \frac{3}{m(\mathbf{x},t)}\int_{\mathcal{B}} \underline{\omega}\langle\xi\rangle \underline{x}\langle\xi\rangle \underline{e}\langle\xi\rangle dV_\xi \tag{12}$$

$$m(\mathbf{x},t) = \int_{\mathcal{B}} \underline{\omega}\langle\xi\rangle \underline{x}\langle\xi\rangle \underline{x}\langle\xi\rangle dV_\xi \tag{13}$$

It is observed from Eq. 12 and 13 that $\theta(\mathbf{x},t)$ is ***unit-less*** and it is varies within the interval $[0,\infty)$. This compute command is applicable to *peri-lps*, *peri-eps* and *peri-ves*.

The third compute is ***compute plasticity/atom***. This compute is applicable to only *peri-eps*. At each time-step ***compute plasticity/atom*** calculates and stores the plasticity parameter λ for each peridynamic node. λ refers to the plasticity consistency parameter. From Eq. 7 the deviatoric component of the scalar force state is $\underline{t}^d_{Plastic} = \alpha\underline{\omega}\left(\underline{e}^d - \underline{e}^{dp}\right)$. In order to obtain the constitutive model based on plasticity the f allowable deviatoric force state $\underline{t}^d_{Plastic}$ satisfies the inequality $\psi\left(\underline{t}^d_{Plastic}\right) - \psi_0 \leq 0$. Preferably, $\psi\left(\underline{t}^d_{Plastic}\right) = \frac{\|\underline{t}^d_{Plastic}{}^2\|}{2}$. Here, $\psi_0 \leq 0$ is the yield point of the material. Based on the plastic flow rule $\dot{e}^{dp} = \lambda\nabla^d\psi$. $\nabla^d\psi$ is the constrained Frèchet derivative of ψ while the previously mentioned inequality is satisfied. For detail derivations please look at the document provided by John Mitchell at Sandia national lab (Mitchell, 2011a). λ is ***unit-less*** and varies within the interval $[0,\infty)$. All three of these computes store the values in C++ one dimensional arrays or vectors.

References

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