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An Elastic Plastic Contact Model with Strain Hardening for the LAMMPS Granular Package

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Abstract

The following details the implementation of an analytical elastic plastic contact model with strain hardening for normal impacts into the LAMMPS granular package. The model assumes that, upon impact, the collision has a period of elastic loading followed by a period of mixed elastic plastic loading, with contributions to each mechanism estimated by a hyperbolic secant weight function. This function is implemented in the LAMMPS source code as the pair style gran/ep/history. Preliminary tests, simulating the pouring of pure nickel spheres, showed the elastic/plastic model took 1.66x as long as similar runs using gran/hertz/history.

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1. INTRODUCTION

This report describes the implementation of a new elastic-plastic contact model for spheres that can exhibit strain-hardening into the LAMMPS (Large-scale Atomistic/Molecular Massively Parallel Simulator) granular package. What follows is a brief description of the relevant portions of the LAMMPS granular package and the elastic-plastic contact model. For more detailed information, see the LAMMPS documentation and reference [1].

1.1. LAMMPS Granular Package

LAMMPS includes a "granular" package for the simulation of macro-scale spherical particles. This package accounts for the diameter and mass of each particle in addition to their angular and linear velocities when solving Newton's equations of motion in a given simulation domain. Accordingly, the particle-particle interactions can be based oncontinuum models for contact mechanics and frictional effects. The current LAMMPS distribution includes three granular pair styles: gran/hooke, gran/hooke/history and gran/hertz history. These pair styles model the normal elastic contact force between two particles as either linearly proportional to the overlap distance (the Hookean model) or via a nonlinear spring (the Hertz contact model). The tangential force is calculated via a columbic friction model with the option of tangential elastic contact. Each pair style allows for velocity damping, wherein a viscoelastic damping constant is specified for normal and tangential contact. The overall force acting on the point of contact between two particles is thus

$$F = F_{n(elas)} + F_{n(damp)} + F_{t(fric)} + F_{t(damp)}. \tag{1}$$

This force calculation is detailed below for the gran/hertz/history pair style as that is the basis for the current work.

1.1.1. Hertzian Contact

The gran/hertz/history pair style models the normal contact force of any two particles via

$$F_{n(elas)} = \sqrt{\delta}\sqrt{\frac{R_i R_j}{R_i + R_j}}\left(k_n \delta \mathbf{n}_{ij}\right) = \frac{4}{3} E \sqrt{r_{eff}}\,\delta^{3/2}\mathbf{n}_{ij}, \tag{2}$$

where δ is the overlap distance between two particles, R_i and R_j are the non-deformed radii of the particles, k_n is the elastic constant specified by the user and n_{ij} is the unit vector between the particle centers. Some may be more familiar with the expression on the right side of the equation where E is the elastic modulus, and r_{eff} is the effective radius of the particle pair,

$$r_{eff} = \frac{R_i R_j}{R_i + R_j}. \tag{3}$$

1.1.2. Frictional Forces.

Friction is calculated in gran/hertz/history using a piecewise definition

$$F_{t(fric)} = \begin{cases} -\sqrt{\delta r_{eff}}k_t \Delta s_t & \sqrt{\delta r_{eff}}|k_t \Delta s_t| < \mu \|F_n\| \\ -\mu \|F_n\| \widehat{v_t} & \sqrt{\delta r_{eff}}|k_t \Delta s_t| \geq \mu \|F_n\| \end{cases}, \tag{4}$$

with elastic constant k_t, tangential displacement vector between particles Δs_t, friction coefficient μ, and tangential component of the particles' relative velocity v_t. Of these properties, k_t and μ are specified by the user. This is one of two ways that energy is dissipated in these simulations.

1.1.3. Velocity Damping

A second method that can dissipate energy in the system is via the inclusion of viscoelastic damping. This is handled in LAMMPS by additional terms in the calculation of normal and tangential velocity with normal damping coefficient γ_n and tangential damping coefficient γ_t

$$F_{n(damp)} = -\sqrt{\delta r_{eff}} m_{eff} \gamma_n \mathbf{v}_n \tag{5}$$
$$F_{t(damp)} = -\sqrt{\delta r_{eff}} m_{eff} \gamma_t \mathbf{v}_t. \tag{6}$$

The effective mass of the two particles is based on the mass of each of the particles (m_i and m_j)

$$m_{eff} = \frac{m_i m_j}{m_i + m_j}. \tag{7}$$

Figure 1 shows the effects of various damping parameters on the normal contact force of two particles colliding "head-on".

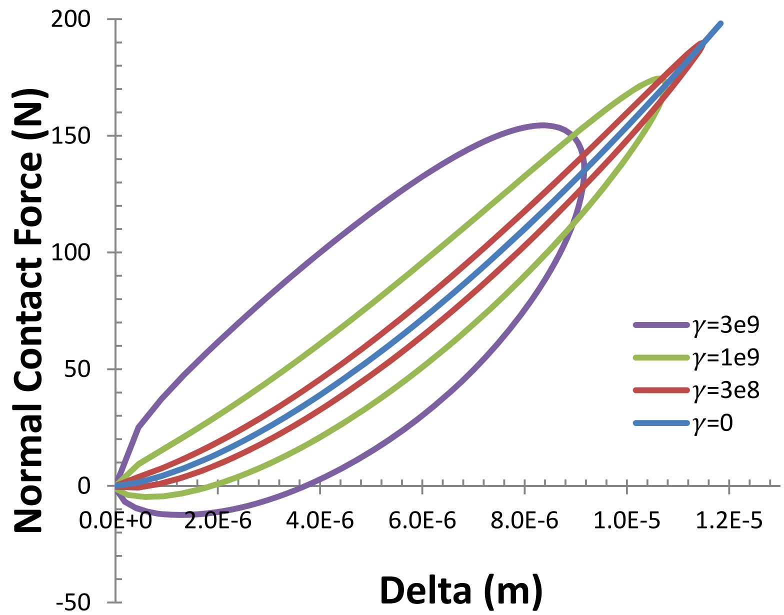


Figure 1: Effects of various damping coefficients ($m^{-1}s^{-1}$) on a simulated Ni-WC collision.

Table 1: Inputs for gran/hertz/history.

Input:	k_n	k_t	γ_n	γ_t	μ	Dampflag
Description:	Normal elastic constant	Tangential elastic constant	Normal damping parameter	Tangential damping parameter	Coulombic friction coefficient	Include or exclude $F_{t(damp)}$
SI Units:	Pa	Pa	1/m/s	1/m/s	None	None
Relevant Equation:	(2)	(4)	(5)	(6)	(4)	(1)

This can be a useful representation of soft, viscous materials, but is phenomenologically incorrect for harder materials, such as metals, that deform plastically upon such impacts.

1.1.4 Input Syntax

LAMPPS requires the inputs detailed in Table 1 to use gran/hertz/history. The following command calls the pair style gran/hertz/history

```
pair_style gran/hertz/history Kn Kt gamma_n gamma_t xmu dampflag
```

1.2. Elastic-Plastic Contact Model

A new model for contact force between spherical particles that accounts for plastic deformation and strain hardening is developed in [1]. This model poses that, like tensile behavior, as contact between two particles is initiated it enters a period of recoverable elastic deformation, followed by a period of mixed elastic/plastic deformation. The following is a brief summary of the relationships derived in that model.

1.2.1. The Elastic Regime

It is accepted that the load reaction follows the Hertzian relationship described in Eq. 2 from the initiation of contact until the onset of yield ($0 < \delta \leq \delta_y$), defined as

$$\delta_y = \frac{r_{eff}}{A(\nu)}\left(\frac{\pi\sigma_y}{2E}\right)^2. \tag{8}$$

From [2], the maximum amplitude of the stress field $A(\nu)$ in the more compliant material during contact as function of its Poisson ratio ν is defined by

$$A(\nu) = \max_{z/a\,\geq\,0}\left(-(1+\nu)\left(1-\frac{z}{a}\tan^{-1}\left(\frac{a}{z}\right)\right)+\frac{3}{2}\frac{1}{1+(z/a)^2}\right)^2, \tag{9}$$

where z/a is the ratio of the depth below the contact point to the radius of the contact area.

1.2.2. The Mixed Elastic-Plastic Regime

After the onset of yield, the model hypothesizes that deformation has both elastic and plastic contributions, with the elastic contribution decaying as the plastic contribution increases. The normal force on the point of contact then becomes

$$F_n = \phi_1(\delta)F_{n(elas)} + \phi_2(\delta)F_{n(plas)} \tag{10}$$

With transitionary functions ϕ_1 and ϕ_2 that determine the contribution of each deformation mechanism. If a uniform pressure distribution during plastic flow is assumed, the contact force is

$$F_{n(plas)} = p_0\pi \frac{a^n}{a_p^{n-2}}\mathbf{n}_{ij}. \tag{11}$$

where the exponent n is the Meyer Hardness, a is the instantaneous contact radius, and p_0 and a_p are the contact pressure and contact area radius at which fully developed plastic flow occurs. Given the relationship

$$a^2 = \big(1 + \phi_2(\delta)\big)r_{eff}\delta, \tag{12}$$

then

$$a_p^2 = 2r_{eff}\delta_p. \tag{13}$$

Without strain hardening, p_0 can be calculated given the Brinnel Hardness H via

$$p_o = Hg10^6. \tag{14}$$

Here, The acceleration due to gravity g is needed for unit conversion from the units of Brinell Hardness (kgf/mm^2) to Pa. In [1], ϕ_1 and ϕ_2 are derived to be

$$\phi_1(\delta) = \begin{cases} \operatorname{sech}\left((1+\xi)\frac{\delta-\delta_y}{\delta_p-\delta_y}\right) & \delta > \delta_y \\ 1 & \delta \le \delta_y \end{cases} \tag{15}$$

$$\phi_2(\delta) = \begin{cases} 1 - \operatorname{sech}\left((1-\xi)\frac{\delta-\delta_y}{\delta_p-\delta_y}\right) & \delta > \delta_y \\ 0 & \delta \le \delta_y \end{cases}. \tag{16}$$

These functions are scaled by ξ, an empirical constant that is shown to agree well with the data given $\xi = n - 2$, and are dependent on δ_p, which is derived along with ϕ_1 and ϕ_2

$$\delta_p = \left(\frac{3\pi p_0}{2E}\right)^2 r_{eff}. \tag{17}$$

1.2.3. The Restitution Phase

This model accepts the well-established rule that unloading is an elastic process, with no reverse yielding. The normal force during restitution follows

$$F_{n(rest)} = \begin{cases} \frac{4}{3}E\sqrt{\bar{r}_{eff}}\left(\delta - \bar{\delta}\right)^{3/2} & \delta > \bar{\delta} \\ 0 & \delta \le \bar{\delta} \end{cases}, \tag{18}$$

using $\bar{r}_{eff}$ and $\bar{\delta}$, which are the deformed radius of curvature and residual deformation, respectively, that result from contact. These values can be obtained by continuity and are given as

$$\bar{\delta} = \delta_m\left(1 - \frac{F_m}{4/3E\sqrt{r_{eff}}\delta_m^{3/2}}\right) \tag{19}$$

$$\bar{r}_{eff} = \frac{F_m^2}{(4/3E)^2\left(\delta_m - \bar{\delta}\right)^3} \tag{20}$$

where δ_m and F_m are the maximum displacement and normal force, respectively, achieved during contact prior to restitution. Equation 19 is a proposed relationship that specifies $\bar{\delta}$ is proportional to $F_m/F_{n(elas)}(\delta_m)$, and Eq. 20 is derivable from continuity. This model results in a loading curve such as shown in Figure 2.

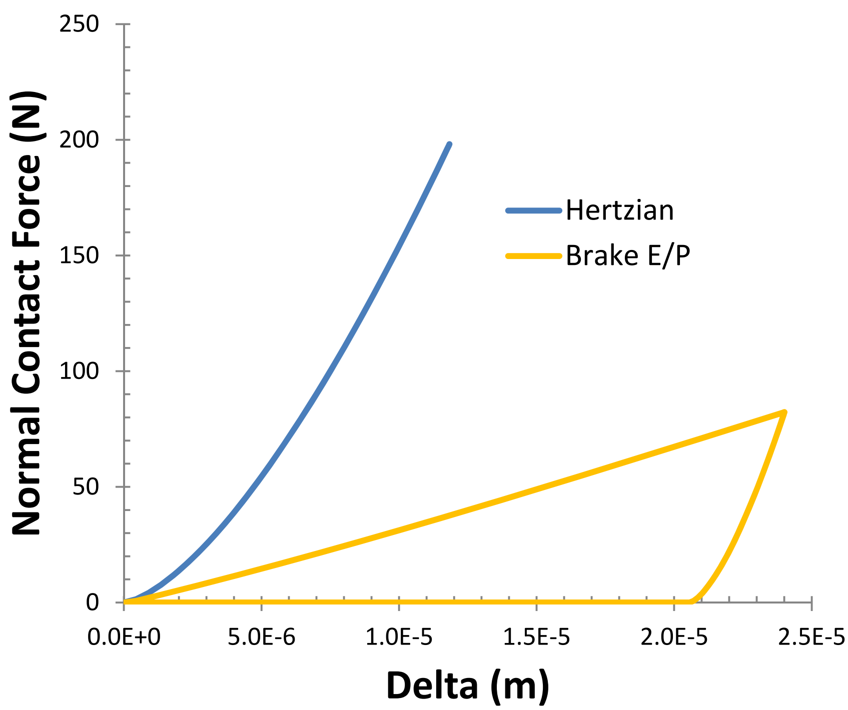


Figure 2: Normal force reaction for Hertzian, Brake Elastic/Plastic Model for a 4.5m/s collision between 3.18mm spheres of Ni and WC.

2. NEW LAMMPS MODEL

To incorporate the elastic-plastic contact model into LAMMPS, a new pair style is used. To allow high levels of user control, only neccessary features of the contact model are implemented into the pair style while the remaining features are included in an initialization script, which allows users to estimate inputs from experimental data. These programs are described in what follows.

2.1 Pair Style gran/ep/history

The new pair style is called gran/ep/history, "ep" being an abbreviation for "elastic-plastic" and history denoting the capability to use shear history to calculate frictional effects. The handing of friction is the same in gran/ep/history as it is in gran/hertz/history, although the observed magnitude of the frictional force will be different due to the new calculation of the normal force. The damping forces are also calculated the same way, but are implemented slightly differently as noted in Eqs. 5 and 6. The new pair style accepts all the inputs that gran/hertz/history accepts and five additional terms to define the plastic behavior.

2.1.1 Addition of plastic terms

In order to implement the elastic-plastic contact model, the overall force on a spherical particle (Eq. 1 for gran/hertz/history) becomes

$$F = \begin{cases} \phi_1(\delta)\left(F_{n(elas)} + F_{n(damp)}\right) + \phi_2(\delta)F_{n(plas)} + F_{t(fric)} + F_{t(damp)}: & \delta > \delta_m \\ F_{n(rest)} + F_{n(damp)} + F_{t(fric)} + F_{t(damp)}: & \delta \leq \delta_m \end{cases}. \quad (21)$$

The inputs described in Table 1 are used to calculate $F_{n(elas)}$, $F_{n(damp)}$, $F_{t(fric)}$ and $F_{t(damp)}$ in exatly the same way as gran/hertz/history. Additional inputs, detailed in Table 2 are necessary to calculate $\phi_1(\delta)$, $\phi_2(\delta)$ and $F_{n(plas)}$.

2.1.2 Input Syntax

To model a single material using gran/ep/history, insert the following lines into the input script:

```
pair_style gran/ep/history &
Kn Kt gamma_n gamma_t xmu dampflag weight cy cp p0 n
pair_coeff * *
```

Table 2: Additional inputs for gran/ep/history.

Input:	ξ	c_y	c_p	p_0	n
Description:	Weight constant	Proportionality constant such that $\delta_y = c_y r_{eff}$	Proportionality constant such that $\delta_p = c_p r_{eff}$	Plastic flow pressure	Meyer's Hardness exponent
SI Units:	None	None	None	Pa	None
Relevant Equation:	(15), (16)	(15), (16)	(15), (16)	(11)	(11)

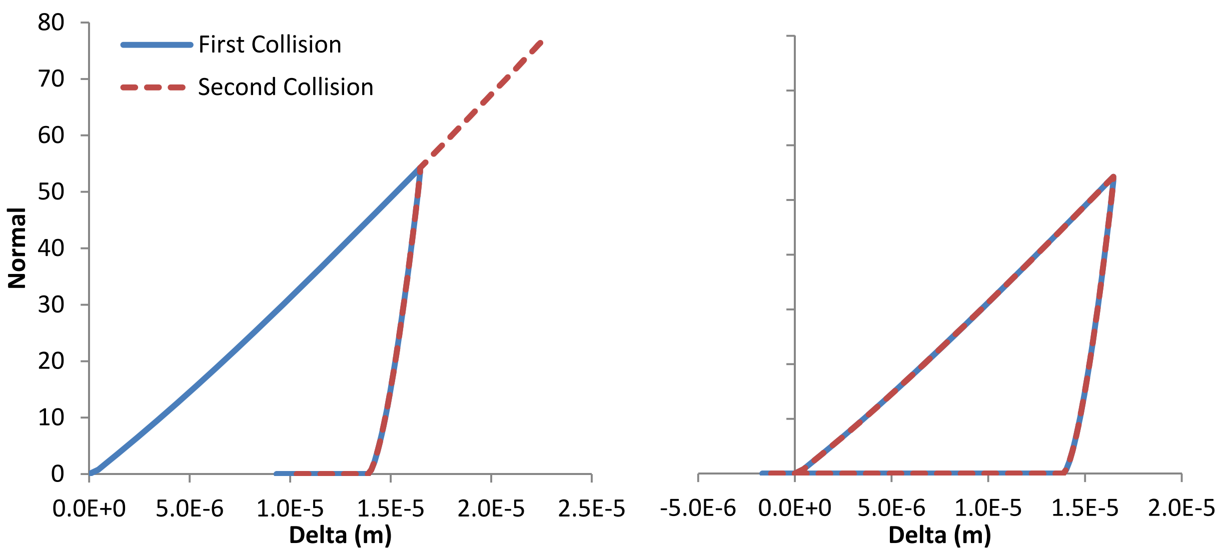
To model two different materials, the following syntax can be used:

```
pair_style hybrid &
gran/ep11/history Kn Kt gamma_n gamma_t xmu dampflag weight cy cp p0 n &
gran/ep12/history Kn Kt gamma_n gamma_t xmu dampflag weight cy cp p0 n &
gran/ep22/history Kn Kt gamma_n gamma_t xmu dampflag weight cy cp p0 n
pair_coeff 1 1 gran/ep11/history
pair_coeff 1 2 gran/ep12/history
pair_coeff 2 2 gran/ep22/history
```

The arguments following “gran/ep11/history” are those governing a collision between two particles of material type “1”, and those following “gran/ep12/history” govern a collision between a particle of type “1” and a particle of type “2”, etc. This method can currently be used for up to four material types. It is important that every material interaction possible in a simulation is defined.

2.1.3 Handling of multiple load cycles

During a simulation, a pair of spheres may collide multiple times. Several different loading curves can result, depending on the relative positions of the spheres. Consider the following scenarios for a pair of strain-hardenable spheres. Case I, They undergo a collision, restitution, then a second collision at the same point of impact. Case II, They undergo a collision, restitution, then a second collision at a new point not affected by the first. Case III, They undergo a collision, restitution, then a second collision in a region of the sphere that has been deformed by the first.



(a) (b)

Figure 3: Second Collision load curves when (a) δ remains positive and (b) δ reaches a negative value.

Table 3: Pair style time comparison.

Pair Style	Average Total Simulation Time (min)	Average Pair Calculation Time (min)
gran/hertz/history	67.52	10.01
gran/ep/history	111.83	28.86

For simplicity, the model is implemented under the assumption that each subsequent impact between two spheres that have already come in contact is one of the first two cases (Case I or Case II) and not among the numerous potential configurations that arise when considering Case III. An example of Case I and Case II collisions are illustrated in Fig. 3. If the distance between sphere centers is smaller than it would be undeformed, the first scenario (Case I) is assumed. The loading curve of the second collision then follows the restitution curve of the first collision until the maximum force of that collision is reached, and then continues on the loading curve of the first collision (see Fig. 3a). If at any point the distance between sphere centers is larger than it would be undeformed, the second scenario (Case II) is assumed and loading begins as it did in the first collision (see Fig. 3b).

2.1.4 Timing Benchmark and Comparison

For algorithmic timing comparisons, small benchmark simulations are used that model 2000 pure nickel particles of 5mm diameter poured into a cylindrical drum of 10cm diameter from a height of 10 cm over 0.5 sec using both gran/hertz/history and gran/ep/history. Table 3 documents the computational times for 500 simulations run on four processors for both impact models. The use of gran/ep history contributed to a 1.66x increase in computation time, largely due to a 2.88x increase in computation time spent on pair calculations.

2.2 Initialization script

An initialization script is used to generate appropriate LAMMPS commands as described in Section *2.1.2* using the material properties and relationships described in Section 1.2. For efficiency, Eq. 9 is replaced by the quadratic fit

$$A(\nu) = 0.381981\nu^2 - 0.804221\nu + 0.591121. \quad (22)$$

This equation has a correlation of $R^2 = 0.999987$. The initialization script requires the properties detailed in Table 4.

Table 4: Properties required for use of gran_ep_initialize.py.

Property:	E	ν	σ	n	H
Description:	Young's Moduls	Poisson's Ratio	Yield Stress	Meyer's Hardness	Brinell Hardness
Units:	Pa	None	Pa	None	kgf/mm^2
Relevant Eauation:	8, 18, 19, 20	9, 22	8	11, 23	14

To use this code, the user enters the relevant properties into the section labeled "## List of material properties" then executes the calculation. The output will contain the commands that must be copied and pasted into the LAMMPS input script. Substituting the string 'unknown' for yield stress and Meyer's hardness has two effects: 1) the code assumes other materials yield first, and 2) the code generates an elastic-only command for interactions between two spheres of that type. This is appropriate in the case of one ceramic interacting with metals. For instance, if one were to run gran_ep_initialize.py with

```
# Properties for material 1
name =          'Pure Nickel'
Emod =          159e9          # Pa  % Young's modulus
nu =            0.3            # Poisson's ratio
SY =            159e6          # Pa % Yield strength
Meyer =         2.21           # Meyer's Hardness
rho =           8880           # density, kg/m^3
HB =            90             # Brinell Hardness, kgf/mm^2

# Properties for material 2
name =          'WC-10Co'
Emod =          475e9
nu =            0.22
SY =            'unknown'
Meyer =         'unknown'
rho =           14500
HB =            1167
```

the output would look like:

```
units si

pair_stlye hybrid &
gran/ep11/history 1.165e+11 0 0 0 0 0 2.100e-01 3.140e-06 1.418e-04 2.207e+08
2.210e+00   &
gran/ep12/history 1.726e+11 0 0 0 0 0 2.100e-01 1.431e-06 2.227e-04 4.098e+08
2.210e+00   &
gran/ep22/history 3.328e+11 0 0 0 0 0 0 1 1 0 2 # elastic interaction only

pair_coeff 1 1 gran/ep11/history  #Pure Nickel/Pure Nickel interaction:
pair_coeff 1 2 gran/ep12/history  #Pure Nickel/WC-10Co interaction:
pair_coeff 2 2 gran/ep22/history  #WC-10Co/WC-10Co interaction:

set type 1 density 8880
set type 2 density 14500
```

The "elastic interaction only" command is functionally equivalent to

```
gran/hertz/history 3.328e+11 0 0 0 0 0 0
```

The weight constant ξ is calculated by the empirical relationship

$$\xi = \begin{cases} n-2 & n > 2 \\ \delta_y/\delta_p & n \le 2 \end{cases} \tag{23}$$

and is subject to the constraints $0.01 < \xi < 0.5$ and $F_{n(ElasticPlastic)}(\delta_y) < F_{n(Elastic)}(\delta_p)$. If these are not met, ξ is assumed to be 0.1 and iteratively increased by 1% until they are.

Note that these commands are for frictionless collisions with no viscoelastic damping. They would have to be edited to include these effects. Up to four materials can be modeled this way in LAMMPS, but an unlimited number of input lines can be generated in a single run.

3. DISCUSSION

3.1. Limitations

The new pair style gran/ep/history accounts for normal plastic deformation via a model that assumes collision on a single point of contact. It does not account for changes to the normal force reaction due to small amounts of tangential sliding around deformed areas. It also does not account for plastic deformation that has occurred due to frictional forces. This model does not include temperature calculation, and therefore cannot adjust parameters due to temperature changes that would result from high energy impacts. However, this new model does include strain hardening, plasticity, and other effects as documented in [1]. For low to moderate energy impacts of metallic volumes, this is an appropriate model to use.

3.2. Future Work

This project could continue in a number of ways. First, the model should be validated with comparison to experimental systems, such as the drop experiments in [3]. Should the current model prove insufficient, it may be useful for the next generation of these codes to address the issues described in 3.1. This would give insight into the predictive usefulness of these factors on real systems. One physical phenomenonthat could be implemented in the short term is the elastic-plastic microslip friction model in [1]. Finally, it would be useful to compare the current model to atomistic simulations to see how each model predicts parameters such as δ_y and to compare the compliance curves.

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