Derivation of Interatomic Forces to Replicate an Elastica

Arman Guerra

February 22, 2021

1 Introduction

This document is made to supplement and explain some features of the code in this repository, specifically I derive the inter-particle potentials that I use in 1d and 2d simulations of beams and plates in LAMMPS.

LAMMPS is a particle dynamics simulator, and works by calculating the displacements of "particles" based on potentials that are applied to them. We will "glue" many particles together and determine their contact mechanics using three inter-particle potentials which serve three purposes:

- A potential which adds a stretching rigidity to the beam
- A potential which adds a bending rigidity to the beam
- A potential which dictates the contact between two beams or a beam and a wall.

I will discuss the last potential first, and then derive the first two. At the end, we will arrive at a Hertzian contact model for spheres, and an energy for 1d and 2d elastic structures respectively of

$$U_{1d} = \frac{\pi}{8} E d \sum_{ij} (q_{ij} - q_0)^2 + \frac{E \pi d^3}{64} \sum_{ijk} (1 + \cos \theta_{ijk}) \tag{1}$$

$$U_{2d} = \frac{\pi}{8} E d \sum_{ij} (q_{ij} - q_0)^2 + \frac{E \pi d^3}{64} \sum_{ijk} (1 + \cos \theta_{ijk}) \tag{2}$$

Where d is the diameter of particles glued together

2 Contact

In all of these simulations I have used the `pair_style granular` command with the `pair_coeff...hertz/material` contact model reference the documentation, and for any walls I have used `fix...wall/gran/region...hertz/material`. These two commands set up a standard Hertzian granular contact potential – for any overlap between two particles δ_g or a particle and a wall δ_w (Figure 1c or whatever) the force on each particle by the other grain or by the wall is given by

$$F_g = \frac{4}{3} E_{eff} r_{eff}^{1/2} \delta_g^{3/2} \tag{3}$$

$$F_w = \frac{4}{3} E r^{1/2} \delta_w^{3/2} \tag{4}$$

Where $E_{eff} = ((1 - \nu_1^2)/E_1 + (1 - \nu_2^2)/E_2)^{-1}$ and $r_{eff} = r_1 r_2/(r_1 + r_2)$. All of the settings that I use in these commands are explained in the documentation reference the documentation, but in general, if a particle comes into contact with another particle or a wall it acts like an elastic sphere. Note that I set the diameter of the particles to be the target width of the beam. Therefore, care must be taken that, for instance, if two beams come into contact, their contact point is at the center of one of the particles of each beams (Figure 1d or whatever). Otherwise there may be some overlap between the beams.

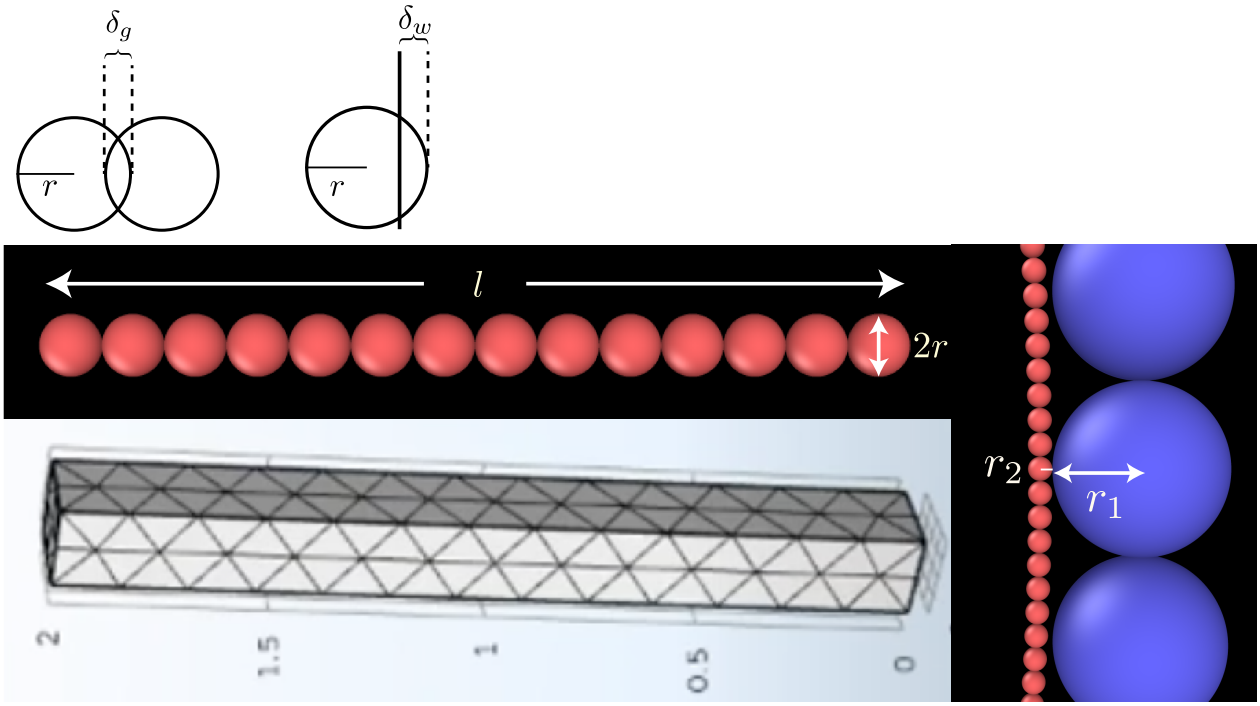

Figure 1: Hello

3 1d Beams

We would like to replicate the physics of a thin ($l/R < something$) cylindrical beam, with Young's modulus E, length l, and cross sectional radius r (Figure 1). I will do this by gluing particles or diameter d in a straight line with the following potentials.

3.1 Stretching

To add a stretching rigidity to the beams I will apply a harmonic "Bond" between adjacent particles in the beam using the `bond_style harmonic` pair potential. I define an equilibrium distance between adjacent particles, or equilibrium Bond length q_0 and calculate the energy of a Bond between particle i and particle j which has a Bond length q_{ij} as

$$U_s = K(q_{ij} - q_0)^2 = K(\Delta q_{ij})^2 \tag{5}$$

Where I define Δq_{ij} to be the change from equilibrium of the Bond length. The force on the particles are as such $F = dU_s/dq = 2K\Delta q_{ij}$. In all of the simulations that I have run, I have set q_0 equal to the diameters of the particles d, that is, the potential acts to keep the particles of the beam just touching. This is not necessary, one could imagine a beam made up of more spherical particles with some neighbor overlap, or fewer spherical particles with a larger distance between each pair.

To continue the derivation, we can take the definition of the Young's modulus $E = \sigma/\epsilon = (F/A)/(\Delta l/l_0)$ where A is the cross sectional area of the beams $\pi(d/2)^2$. If we statically compress or stretch a beam, the force on the ends will be equal to the force between any adjacent particle, which we found above to be $F = 2K\Delta q$ (I have dropped the subscript of q because the Bond lengths will all be the same). The strain of the whole beam $\Delta l/l_0$ will be equal to the strain of each Bond $\Delta q/q_0$ so we have

$$E = \frac{F/A}{\Delta l/l_0} = \frac{2K\Delta q}{\pi(d/2)^2}\frac{d}{\Delta q} = K\frac{8}{\pi d} \implies K = \frac{\pi}{8}Ed \tag{6}$$

Where I have used the fact that $q_0 = d$.

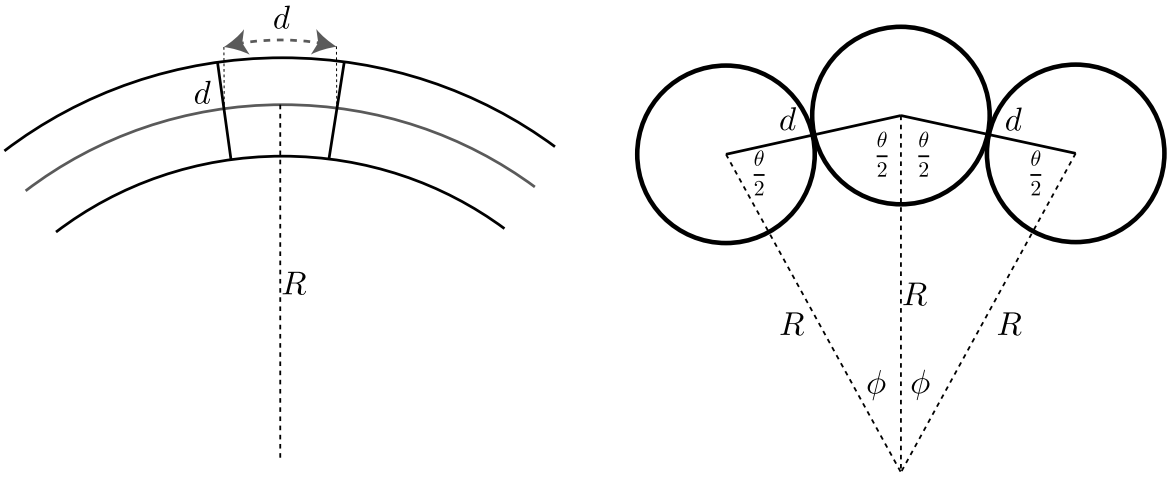

Figure 2: Hello

3.2 Bending

To derive the pair potential needed to induce the correct bending rigidity in our LAMMPS beams we will consider two beams, a continuous beam and a discrete beam, and do an imaginary experiment on both of them. Then we will find the energy in each beam and set them equal to one another, and the parameters that we need for our LAMMPS simulations will drop out.

For a continuous elastic beam with a moment I, the energy of bending is

$$U_b^c = \frac{EI}{2} \int \kappa^2 ds \tag{7}$$

Where κ is the curvature of the beam, I have used the superscript c to indicate that the beam is continuous. To achieve an energy of bending in LAMMPS I will use what is called an "Angle" (Figure something something). A LAMMPS Angle is like a Bond (which I used in the previous section on the stretching potential) except instead of considering the interaction between two particles, each Angle applies a potential based on the positions of three particles. The specific Angle potential that I will use is `angle_style cosine` which applies a potential

$$U_b^d = B(1 + \cos\theta) \tag{8}$$

Where θ is the angle between the three particles and I have used the superscript d to indicate that this is a discrete beam. Our imaginary experiment will be to statically bend each beam to a radius of curvature R such that $\kappa = 1/R$ everywhere (Figure something). The energy in a chunk of the continuous beam of width d will be

$$U_b^c = \frac{EI}{2R^2} \int ds = \frac{EI}{2R^2} d = \frac{E\pi d^5}{128R^2} \tag{9}$$

Where I have taken the moment of the cylindrical beam $I = \pi d^4/64$. Moving to the discrete case, in a chunk of width d in the bulk of the beam there is one particle (since the particles have width d). The energy assigned to that particle because of the bending of the beam can be found by summing up the contributions of each of the Angles that it is a part of. There are three particles in each Angle, so to each constituent

particle we will assign one third of the energy in that Angle. Furthermore each particle is a part of three angles, so the energy in each particle in the column due to bending, and therefore the energy in a chunk of the beam of width d is $3*(1/3)B(1+\cos\theta) = B(1+\cos\theta)$. This may seem like a large fuss to make over such a simple conclusion, but this argument will be essential when we move to 2 dimensional elastic structures.

The only thing that is left is to connect $(1+\cos\theta)$ to the radius of curvature R. I will do this geometrically referring to the angles and lengths defined in Figure 2. By the law of cosines, we have that

$$d^2 = 2R^2 - 2R^2\cos\phi = 2R^2(1-\cos\phi) \tag{10}$$

Since the interior angles in the triangles in Figure 2 must sum to 180 degrees, we have that $\phi = 180 + \theta/2 + \theta/2 \implies \theta = 180 - \phi$ so $1+\cos\theta = \frac{d^2}{2R^2}$. Setting the energies equal we have

$$U_b = \frac{Bd^2}{2R^2} = \frac{E\pi d^5}{128R^2} \implies B = \frac{E\pi d^3}{64} \tag{11}$$

3.3 Rectangular Beams

If the beams are rectangular instead of cylindrical with a square cross section of side lengths d, the derivation for the bending and the stretching are slightly different. The stretching constant K can be found as

$$E = \frac{F/A}{\Delta l/l_0} = \frac{2K\Delta q q_0}{dq_0^2\Delta q} = \frac{2K}{q_0} \implies K = \frac{Ed}{2} \tag{12}$$

And for bending, the discrete case stays the same but the bending moment of inertia changes for the continuous case, which leads to

$$U_b^c = \frac{EId}{2R^2} = \frac{Ed^5}{24R^2}, U_b^d = \frac{Bd^2}{2R^2} \implies B = \frac{Ed^3}{12} \tag{13}$$

4 2d Plates

We would like to replicate the physics of a thin ($w/t > something, h/t > something$) plate with Young's modulus E, width w, height h, and thickness t (Figure **??**). I will do this by gluing particles of diameter d in a triangular lattice. I will use the fact that, because of the symmetry of the triangular lattice, the energy of stretching and bending does not depend on the direction of stretching or bending (find the reference for this, and maybe also do simulations or derivations to show it). Therefore I will, without loss of generality, select the orientation of bending and stretching that leads to the simplest derivation

4.1 Stretching

For a continuous 2d plate, the energy of stretching can be found as the integral of the force

$$U_s^c = \int F d\Delta l = \int EA\epsilon d\Delta l = \int Eht\frac{\Delta l}{l_0}d\Delta l = \frac{Eht}{2}\frac{\Delta l^2}{l_0} \tag{14}$$

To make a 2d plate, I will use the same Bond style as in the 1d case (Equation 3.1) but I will glue the particles together in a triangular lattice. Take the lattice shown in Figure 3a. If this lattice is stretched in the direction indicated by the black arrows, some of the Bonds will be put in tension (the axial Bonds, blue) and others will be put in compression (the transverse Bonds, red). In a triangular lattice with harmonic bonds, the poissons ratio is 1/3 (reference) so if the strain in the axial direction is $\Delta l/l_0$ then the strain in the transverse direction will be $\Delta l/3l_0$

We will find the total energy in stretching by counting up the energy in each Bond. We can find this as the total area, multiplied by the energy in each Bond, times the number of Bonds per unit area ($A * U_{Bond} * \frac{\#Bonds}{area}$). The total area of the plate we will consider will be the width times the height $A = wh$. The number of Bonds per unit area we can find from Figure 3 – there is 1 axial and 2*1/4=1/2 a transverse Bond in an area of $d^2\sqrt{3}/4$.

The energy in an axial bond can be found by finding Δq_a with the pythagorean theorem

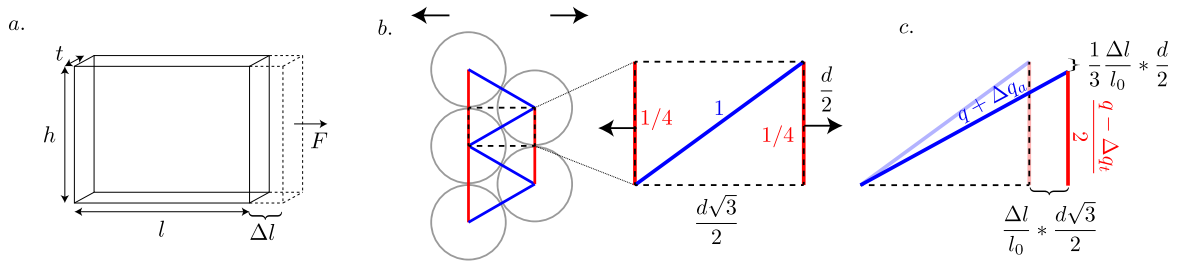

Figure 3: Hello

$$(q+\Delta q_a)^2 = \left[\frac{d\sqrt{3}}{2}\left(1+\frac{\Delta l}{l_0}\right)\right]^2 + \left[\frac{d}{2}\left(1+\frac{\Delta l}{3l_0}\right)\right]^2 \tag{15}$$

We will expand and simplify, take that $q_0 = d$ and, assuming the strains are small, drop any terms of order Δq_a^2 and $(\Delta l/l_0)^2$, which brings us to

$$\Delta q_a = \frac{2\Delta l}{3l_0} d \tag{16}$$

The change in the bond length in the transverse direction is simply 2 times the reduction in height of the triangle in Figure 3a:

$$\Delta q_t = \frac{\Delta l}{3l_0} d \tag{17}$$

The energy in a discrete plate is therefore

$$U_s^d = U_a^d + U_t^d = AK\Delta q_a^2 \frac{1}{d^2\sqrt{3}/4} + AK\Delta q_t^2 \frac{1/2}{d^2\sqrt{3}/4} \tag{18}$$

Where we have inserted our numerical findings for $A * U_{Bond} * \frac{\#Bonds}{area}$ for each type of bond. Expanding and simplifying we get

$$U_s^d = \frac{4AK}{d^2\sqrt{3}}\left[\left(\frac{2\Delta l}{3l_0}d\right)^2 + \frac{1}{2}\left(\frac{\Delta l}{3l_0}d\right)^2\right] = \frac{4whK}{d^2\sqrt{3}}\frac{1}{2}\left(\frac{\Delta l}{l_0}\right)^2 d^2 \tag{19}$$

If we set this equal to the continuous case, take that $w = l_0$ and solve for K we get

$$K = \frac{\sqrt{3}}{4} Et \tag{20}$$

Which is the same as the value in (REFERENCE).

4.2 Bending

Just like in the 1d case of bending, we will perform an imaginary bending experiment for both a continuous and a discrete plate, and set the energies equal to one another. We will bend the plates such that they have a radius of curvature R on one axis (which we will align with the x axis), and 0 on the axis perpendicular to it (the y axis), that is, we will bend them into a cylinder, as shown in Figure whatever. We can find the energy in this plate as

$$U_b^c = \frac{\widetilde{B}}{2}\int\int\left(\frac{d^2w}{dx^2} + \frac{d^2w}{dy^2}\right)^2 dxdy = \frac{\widetilde{B}}{2}\int\int\left(\frac{1}{R}+0\right)^2 dxdy = \frac{\widetilde{B}A}{2R^2} \tag{21}$$

Just like in the 1d case, we will find the product of the energy in each bent Angle, the number of bent Angles per area, and the area. We will use the same Angle style as in the 1d case (Equation 3.2). I will

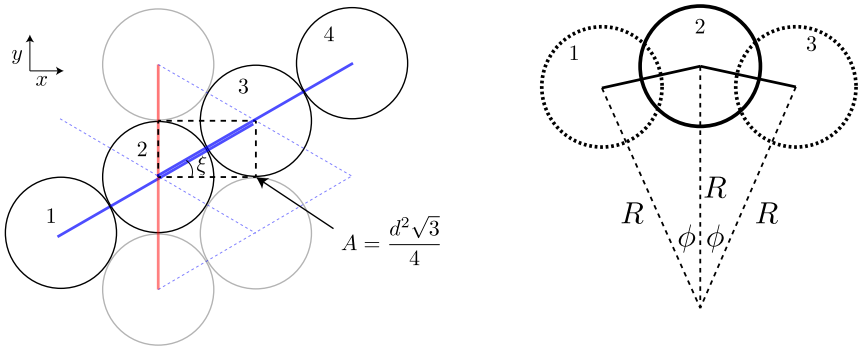

Figure 4: Hello

orient the lattice as we see in Figure 4, such that one of the three orientations of Angles runs parallel to the y axis. Since there is no bending along the y axis, all of those Angles do not bend (red). To find the number of bonds per unit area, we can look at the box shown in that lattice, which has an area of $d^2\sqrt{3}/4$ and which contains two half-Angles, that is, it contains half of the Angle between particles 1 2 and 3, and half of the Angle between particles 2 3 and 4. Therefore there is a total of one Angle associated to that area, so the energy can be found as

$$U_b^d = AB[1 + \cos\theta]\frac{4}{d^2\sqrt{3}} \tag{22}$$

Now we must find the angle θ that each of the bending Angles will bend to given the radius of curvature R. This will not be as simple in the 1d case mostly because of one major difference – if we bend along the x axis, it will bend all of the blue Angles the same amount. But since these bonds are not oriented in the x direction, the amount of bending will not only depend on R but also on the angle ξ that the bonds make with the direction of curvature.