Particle interaction model

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Contents

1 Introduction

Here I give a brief explanation of interaction model for dust particles in contact, used in our simulation. The concepts of our modeling are summarized as follows:

- Particles are hard spheres but can overlap each other when they are in contact. This overlapping creates various interactions between contact particles, i.e., repulsive and attractive forces in the normal direction, and resistance to sliding, rolling and twisting.
- Each particle consists of an elastic body with surface energy. Elastic behavior produces repulsive forces and surface energy is the source of attractive forces.
- In elastic regime, which means monomer's deformation is reversible and no energy dissipation occurs, i.e., spring-like behavior, we assume potentials for each degree of freedom of particle motion (Fig. 1). Forces and torques acting between contact particles are given by the derivative of those potentials.
- Initial contact points on particle surfaces are recorded and their motions are traced. Displacements necessary to calculate potentials of sliding and rolling motions are given by the change of those contact points.
- When the displacements become larger than critical values assumed, we consider inelastic deformations occur: excesses of the displacements are cut-off and energies corresponding to the displacement excesses are dissipated. Energies stored in the form of potentials are also dissipated when contact particles separate.
- These ideas are based on the previous works, such as Hertz (1881) (Hertzian contact elastic theory), Johnson, Kendall and Roberts (1971) (JKR theory for contact elastic bodies with surface energy), Johnson (1987) (contact elastic theory), Chokshi et al. (1993), and Dominik and Tielens (1995, 1996).

In the following, details of grain interaction model are described, considering two spheres (particle 1 and 2) in contact with each other, having radius r_1 and r_2, Young modulus E_1 and E_2, Poisson's ratio ν_1 and ν_2, (shear modulus G_1 and G_2), respectively. Surface energy between two spheres is γ. The position vectors of the two spheres' centers are $\boldsymbol{x}_1$ and $\boldsymbol{x}_2$, respectively.

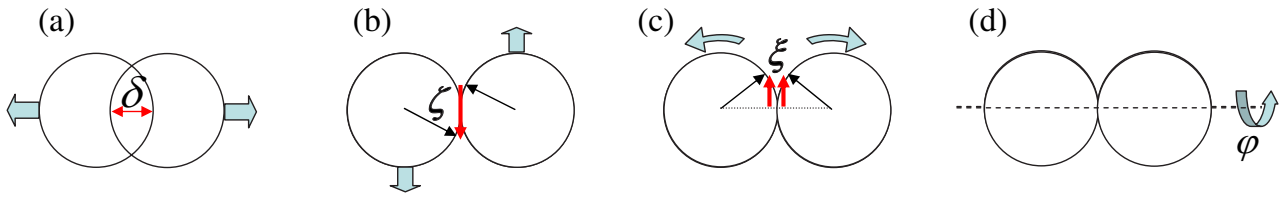

Figure 1: Degrees of freedom for two contact particles: (a) normal, (b) sliding, (c) rolling, (d) twisting.

2 Normal contact of elastic spheres with surface energy : JKR theory

Here, I summarize main consequences derived from JKR theory (Johnson, Kendall and Roberts, 1971; see also Johnson, 1987) for normal contact of elastic spheres having surface energy. It should be noted that variables described here are used in the following sections.

Two spheres in contact make a contact surface that is approximated by a flat disk with radius a. When no external forces are acting, the repulsive force due to elasticity and the attractive force due to surface energy are balanced, then a becomes equilibrium radius a_0 ;

$$a_0 = \left(\frac{9\pi\gamma R^2}{E^*}\right)^{\frac{1}{3}}, \tag{2.1}$$

where

$$\frac{1}{R} = \frac{1}{r_1} + \frac{1}{r_2}, \qquad \frac{1}{E^*} = \frac{1-\nu_1^2}{E_1} + \frac{1-\nu_2^2}{E_2}. \tag{2.2}$$

The compression length between two contact spheres, δ, is defined as

$$\delta = r_1 + r_2 - |\boldsymbol{x}_1 - \boldsymbol{x}_2|. \tag{2.3}$$

As particles considered in our simulation are hard, i.e, non-deformable, two contact spheres overlap when $\delta > 0$. In that sense, δ can be considered to be overlapping length. It should be noted that negative value of δ is possible. $\delta < 0$ means that a neck-like structure is formed between the contact particles. The equilibrium compression, δ_0, at which $a = a_0$, is given by

$$\delta_0 = \frac{a_0^2}{3R}. \tag{2.4}$$

The force necessary to separate two spheres in contact quasi-statically is given by

$$F_c = 3\pi\gamma R. \tag{2.5}$$

At the moment of separation, δ becomes $-\delta_c$, where

$$\delta_c = \frac{3}{2}\left(\frac{1}{6}\right)^{\frac{1}{3}}\delta_0 \simeq 0.825\delta_0. \tag{2.6}$$

The relations between the force acting between two contact particles, F, the contact disk radius a, and the compression length δ are given by

$$\frac{F}{F_c} = 4\left[\left(\frac{a}{a_0}\right)^3 - \left(\frac{a}{a_0}\right)^{\frac{3}{2}}\right] \tag{2.7}$$

$$\frac{\delta}{\delta_c} = 6^{\frac{1}{3}}\left[2\left(\frac{a}{a_0}\right)^2 - \frac{4}{3}\left(\frac{a}{a_0}\right)^{\frac{1}{2}}\right] \tag{2.8}$$

3 Potentials, forces and torques in elastic regime

3.1 Potentials

A total potential U for contact two particles is given by the sum of potential for each degree of freedom :

$$U = U_n(\delta) + U_{slide}(\boldsymbol{\zeta}) + U_{roll}(\boldsymbol{\xi}) + U_{twist}(\boldsymbol{\phi}), \tag{3.1}$$

where

- $U_n(\delta)$: Normal direction potential as a function of overlapping length (or compression) δ. Details on the form of $U_n(\delta)$ are described in the next section.
- $U_{slide}(\boldsymbol{\zeta})$: Potential stored by tangentially sliding motion as a function of sliding displacement $\boldsymbol{\zeta}$. The definition of $\boldsymbol{\zeta}$ is described later. $U_{slide}(\boldsymbol{\zeta})$ is given by

  $$U_{slide}(\boldsymbol{\zeta}) = \frac{1}{2} k_s |\boldsymbol{\zeta}|^2, \tag{3.2}$$

  where k_s is a constant (like a spring constant) given by the elastic contact theory (Johnson, 1987) as follows[1];

  $$k_s = 8 a_0 G^*, \quad \textit{where} \ \frac{1}{G^*} = \frac{2-\nu_1}{G_1} + \frac{2-\nu_2}{G_2}. \tag{3.3}$$

- $U_{roll}(\boldsymbol{\xi})$: Potential stored by rolling motion as a function of rolling displacement $\boldsymbol{\xi}$. The definition of $\boldsymbol{\xi}$ is described later. $U_{roll}(\boldsymbol{\xi})$ is given by

  $$U_{roll}(\boldsymbol{\xi}) = \frac{1}{2} k_r |\boldsymbol{\xi}|^2, \tag{3.4}$$

  where k_r is a constant given by Dominik and Tielens (1995) as follows[2];

  $$k_r = \frac{4F_c}{r_1}. \tag{3.5}$$

- $U_{twist}(\boldsymbol{\phi})$: Potential stored by twisting motion as a function of twisting angular displacement $\boldsymbol{\phi}$. The definition of $\boldsymbol{\phi}$ is described later. $U_{twist}(\boldsymbol{\phi})$ is given by

  $$U_{twist}(\phi) = \frac{1}{2} k_t \boldsymbol{\phi}^2, \tag{3.6}$$

  where k_t is a constant given gym the contact elastic theory (Johnson, 1987) as follows[1];

  $$k_t = \frac{16}{3} G a_0^3, \quad \textit{where} \ \frac{1}{G} = \frac{1}{G_1} + \frac{1}{G_2}. \tag{3.7}$$

It should be noted that these potentials, in reality, would not be independent of each other. In the above equations, however, we assume them as independent functions just for simplicity.

[1] According to the elastic contact theory (Johnson, 1987), a is used instead of a_0 in the formula of k_s and k_t. We use, however, a_0 so that U_{slide} and U_{twist} should be independent of the normal direction displacement, $\delta(a)$.

[2] According to the theory proposed by Dominik and Tielens (1995), the resistance torque for rolling motion is given by $M_r = -4F_c \left(\frac{a}{a_0}\right)^{\frac{3}{2}} \xi$. Here, by the same reason as described in giving k_s, we assume that $a = a_0$, so that we obtain $M_r = -4F_c\xi$ and then $k_s = \frac{4F_c}{r_1}$.

3.2 Contact point vector

An initial contact point on particle surfaces are recorded. We define unit contact point vectors $\boldsymbol{n}_1$ and $\boldsymbol{n}_2$ as vectors originated from the center of each particle and oriented to the initial contact point. The directions of $\boldsymbol{n}_1$ and $\boldsymbol{n}_2$ are changed only by the rotation of each particle.

3.3 General formulae of forces and torques

Force acting on particle 1 is given by

$$\boldsymbol{F}_1 = -\frac{\partial U}{\partial \boldsymbol{x}_1}. \tag{3.8}$$

Torque acting on particle 1 is given by

$$\boldsymbol{M}_1 = -\frac{\partial U}{\partial \boldsymbol{\theta}_1}, \tag{3.9}$$

where $\boldsymbol{\theta}_1$ is the rotational angle vector of particle 1 around its center.

Considering the infinitesimal rotation of $\boldsymbol{n}_1$,

$$\delta \boldsymbol{n}_1 = \delta \boldsymbol{\theta}_1 \times \boldsymbol{n}_1, \tag{3.10}$$

the infinitesimal change of potential δU due to $\delta \boldsymbol{n}_1$ is given by

$$\begin{aligned} \delta U &= \frac{\partial U}{\partial \boldsymbol{n}_1} \cdot \delta \boldsymbol{n}_1 = \frac{\partial U}{\partial \boldsymbol{n}_1} \cdot (\delta \boldsymbol{\theta}_1 \times \boldsymbol{n}_1) = \delta \boldsymbol{\theta}_1 \cdot \left(\boldsymbol{n}_1 \times \frac{\partial U}{\partial \boldsymbol{n}_1} \right) \\ &= \left(\boldsymbol{n}_1 \times \frac{\partial U}{\partial \boldsymbol{n}_1} \right) \cdot \delta \boldsymbol{\theta}_1. \end{aligned} \tag{3.11}$$

Comparing this equation with the formula of infinitesimal change of potential δU due to $\delta \boldsymbol{\theta}_1$

$$\delta U = \frac{\partial U}{\partial \boldsymbol{\theta}_1} \cdot \delta \boldsymbol{\theta}_1, \tag{3.12}$$

we obtain

$$\frac{\partial U}{\partial \boldsymbol{\theta}_1} = \boldsymbol{n}_1 \times \frac{\partial U}{\partial \boldsymbol{n}_1}. \tag{3.13}$$

Therefore, the torque formula (3.9) can be expressed by

$$\boldsymbol{M}_1 = -\boldsymbol{n}_1 \times \frac{\partial U}{\partial \boldsymbol{n}_1}. \tag{3.14}$$

3.4 Normal direction

The force acting on the particle 1 by the normal direction interaction between particle 1 and 2 is given by

$$\boldsymbol{F}_{n,1} = -\frac{\partial U_n}{\partial \boldsymbol{x}_1} = -\frac{\partial U_n}{\partial \delta}\frac{\partial \delta}{\partial \boldsymbol{x}_1}. \tag{3.15}$$

According to the JKR theory, normal direction potential $U_n(\delta)$ is given through the contact disk radius a as follows;

$$\frac{U_n(\delta(a))}{F_c\delta_c} = 4\times 6^{\frac{1}{3}}\left\{\frac{4}{5}\left(\frac{a}{a_0}\right)^5 - \frac{4}{3}\left(\frac{a}{a_0}\right)^{\frac{7}{2}} + \frac{1}{3}\left(\frac{a}{a_0}\right)^2\right\} \tag{3.16}$$

with

$$\frac{\delta(a)}{\delta_c} = 6^{\frac{1}{3}}\left\{2\left(\frac{a}{a_0}\right)^2 - \frac{4}{3}\left(\frac{a}{a_0}\right)^{\frac{1}{2}}\right\}. \tag{3.17}$$

Thus, $\dfrac{\partial U_n}{\partial \delta}$ can be numerically calculated from $U_n(\delta)$ shown in Fig. 2. In addition, we ignore the potential in the region $\delta < 0$ before particles contact, that is, particles contact initially at $\delta = 0$.

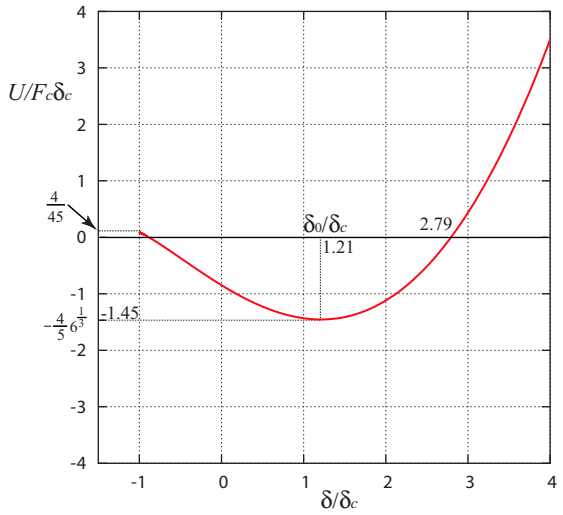

Figure 2: Potential U_n as a function of δ.

$\dfrac{\partial \delta}{\partial \boldsymbol{x}_1}$ can be derived from Eq. (2.3), $\delta = r_1 + r_2 - |\boldsymbol{x}_1 - \boldsymbol{x}_2|$, and we obtain

$$\frac{\partial \delta}{\partial \boldsymbol{x}_1} = -\frac{\boldsymbol{x}_1 - \boldsymbol{x}_2}{|\boldsymbol{x}_1 - \boldsymbol{x}_2|} \tag{3.18}$$

As a result, we obtain

$$\boldsymbol{F}_{n,1} = \frac{\partial U_n}{\partial \delta}\frac{\boldsymbol{x}_1 - \boldsymbol{x}_2}{|\boldsymbol{x}_1 - \boldsymbol{x}_2|}. \tag{3.19}$$

For example, when compression occurs over equilibrium (i.e., $\delta > \delta_0$), $\dfrac{\partial U_n}{\partial \delta}$ becomes positive as shown in Fig. 2 and thus the direction of normal force $\boldsymbol{F}_{n,1}$ becomes the same as $\boldsymbol{x}_1 - \boldsymbol{x}_2$, that is, repulsive.

It is obvious that any torques cannot be generated from U_n, because U_n is not a function of $\boldsymbol{n}_1$.

3.5 Resistance to sliding motion

For the definition of slide displacement $\boldsymbol{\zeta}$, we consider a vector $\boldsymbol{\zeta}_0$ as follows;

$$\boldsymbol{\zeta}_0 = r_1\boldsymbol{n}_1 - r_2\boldsymbol{n}_2 + (r_1 + r_2)\boldsymbol{n}_c, \tag{3.20}$$

where

$$\boldsymbol{n}_c = \frac{\boldsymbol{x}_1 - \boldsymbol{x}_2}{|\boldsymbol{x}_1 - \boldsymbol{x}_2|} \ (\equiv \frac{\boldsymbol{r}_c}{r_c}). \tag{3.21}$$

$\boldsymbol{\zeta}_0$ is nearly equal to the vector originated from the initial contact point of particle 2 to that of particle 1. We define $\boldsymbol{\zeta}$ as the component of $\boldsymbol{\zeta}_0$ perpendicular to the vector $\boldsymbol{n}_c$ (see Fig. 3),

$$\boldsymbol{\zeta} = \boldsymbol{\zeta}_0 - (\boldsymbol{\zeta}_0 \cdot \boldsymbol{n}_c)\,\boldsymbol{n}_c. \tag{3.22}$$

By using the above formula of $\boldsymbol{\zeta}$, we can obtain the force $\boldsymbol{F}_{s,1}$ and the torque $\boldsymbol{M}_{s,1}$ acting on the particle 1 due to sliding motion between particle 1 and 2 as follows:

$$\begin{aligned} \boldsymbol{F}_{s,1} &= -\frac{\partial U_{slide}(\boldsymbol{\zeta})}{\partial \boldsymbol{x}_1} = -\frac{\partial}{\partial \boldsymbol{x}_1}\left(\frac{1}{2}k_s\boldsymbol{\zeta}^2\right) = -k_s\boldsymbol{\zeta}\cdot\frac{\partial \boldsymbol{\zeta}}{\partial \boldsymbol{x}_1} \\ &= -k_s\boldsymbol{\zeta}\frac{r_1 + r_2 - \boldsymbol{\zeta}_0\cdot\boldsymbol{n}_c}{|\boldsymbol{x}_1 - \boldsymbol{x}_2|}, \end{aligned} \tag{3.23}$$

$$\begin{aligned} \boldsymbol{M}_{s,1} &= -\boldsymbol{n}_1 \times \frac{\partial U_{slide}(\boldsymbol{\zeta})}{\partial \boldsymbol{n}_1} = -\boldsymbol{n}_1 \times \frac{\partial}{\partial \boldsymbol{n}_1}\left(\frac{1}{2}k_s\boldsymbol{\zeta}^2\right) = -k_s\boldsymbol{n}_1 \times \left(\boldsymbol{\zeta}\cdot\frac{\partial \boldsymbol{\zeta}}{\partial \boldsymbol{n}_1}\right) \\ &= -r_1 k_s \boldsymbol{n}_1 \times \boldsymbol{\zeta}. \end{aligned} \tag{3.24}$$

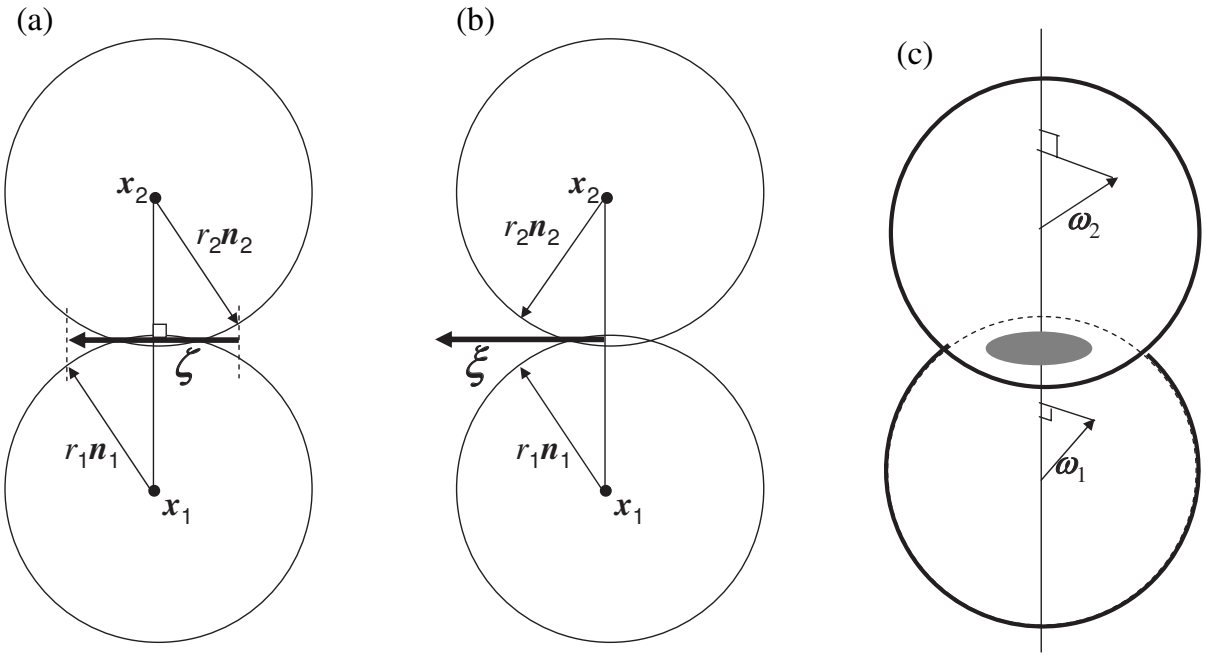

Figure 3: Schematic views of (a) sliding, (b) rolling, and (c)twisting for the definition of each displacement.

3.6 Resistance to rolling motion

As shown in see Fig. 3, we define the rolling displacement $\boldsymbol{\xi}$ by

$$\boldsymbol{\xi} = r_1\boldsymbol{n}_1 + r_2\boldsymbol{n}_2. \tag{3.25}$$

Since $U_{roll}(\boldsymbol{\xi})$ is obviously independent of $\boldsymbol{x}_1$, i.e., $\dfrac{\partial U_{roll}}{\partial \boldsymbol{x}_1} = 0$, therefore, no forces are generated by the rolling motion.

On the other hand, by using the above formula of ξ, we can obtain the resistant torque due to rolling motion (so-called 'rolling resistance') acting on the particle 1 as follows;

$$\begin{aligned} \boldsymbol{M}_{r,1} &= -\boldsymbol{n}_1 \times \frac{\partial U_{roll}(\boldsymbol{\xi})}{\partial \boldsymbol{n}_1} = -\boldsymbol{n}_1 \times \frac{\partial}{\partial \boldsymbol{n}_1}\left(\frac{1}{2}k_r\boldsymbol{\xi}^2\right) = -k_r\boldsymbol{n}_1 \times \left(\boldsymbol{\xi} \cdot \frac{\partial \boldsymbol{\xi}}{\partial \boldsymbol{n}_1}\right) \\ &= -r_1 k_r \boldsymbol{n}_1 \times \boldsymbol{\xi}. \end{aligned} \tag{3.26}$$

3.7 Resistance to twisting motion

The twisting angular displacement $\boldsymbol{\phi}$ is defined as

$$\boldsymbol{\phi} = \boldsymbol{n}_c \int_0^t (\boldsymbol{\omega}_1 - \boldsymbol{\omega}_2) \cdot \boldsymbol{n}_c dt, \tag{3.27}$$

where $\boldsymbol{\omega}_1$ and $\boldsymbol{\omega}_2$ are angular velocities of the particle 1 and 2, respectively (see Fig. 3). t is the time counted from the beginning of contact.

Then, the resistant torque due to twisting motion acting on the particle 1 is given by

$$\begin{aligned} \boldsymbol{M}_{t,1} &= -\frac{\partial U_{twist}(\boldsymbol{\phi})}{\partial \boldsymbol{\phi}} = -\frac{\partial}{\partial \boldsymbol{\phi}}\left(\frac{1}{2}k_t\boldsymbol{\phi}^2\right) \\ &= -k_t\boldsymbol{\phi} \end{aligned} \tag{3.28}$$

3.8 Description of particle rotation

We introduce Eulerian parameters (or quaternion) to describe the particle rotation;

$$e_0, \quad \boldsymbol{e} = (\, e_1,\ e_2,\ e_3\,), \quad with\ \ e_0^2 + e_1^2 + e_2^2 + e_3^3 = 1. \tag{3.29}$$

Rotation of a vector $\boldsymbol{p}$ around an arbitrary axis can be expressed by using the Eulerian parameters as follows: Considering $\boldsymbol{\psi}$ as the rotation angle vector (i.e., vectors are rotated by ψ in anticlockwise direction around the axis along $\boldsymbol{\psi}$) , Eulerian parameters are given by

$$e_0 = \cos\frac{\psi}{2} \tag{3.30}$$

$$\boldsymbol{e} = \hat{\boldsymbol{\psi}}\sin\frac{\psi}{2}, \tag{3.31}$$

where $\hat{\boldsymbol{\psi}}$ is the unit vector of $\boldsymbol{\psi}$. By using these Eulerian parameters, the rotation matrix A_{ij} can be expressed as

$$A_{ij} = \left(1 - 2\boldsymbol{e}^2\right)\delta_{ij} + 2e_ie_j - 2e_0\epsilon_{ijk}e_k. \tag{3.32}$$

Then the rotated vector $\boldsymbol{p}'$ is given by

$$\begin{aligned} \boldsymbol{p}' &= A\boldsymbol{p} \\ &= \left(1-2\boldsymbol{e}^2\right)\boldsymbol{p} + 2\left(\boldsymbol{p}\cdot\boldsymbol{e}\right)\boldsymbol{e} - 2e_0\left(\boldsymbol{p}\times\boldsymbol{e}\right). \end{aligned} \tag{3.33}$$

Note that $A^{-1}_{ij} = A_{ji}$ since A is an unitary matrix. Thus, the inverse transformation is given by

$$\begin{aligned} \boldsymbol{p} &= A^{-1}\boldsymbol{p}' \\ &= \left(1-2\boldsymbol{e}^2\right)\boldsymbol{p}' + 2\left(\boldsymbol{p}'\cdot\boldsymbol{e}\right)\boldsymbol{e} + 2e_0\left(\boldsymbol{p}'\times\boldsymbol{e}\right). \end{aligned} \tag{3.34}$$

Each particle has its own Eulerian parameters and we can trace their temporal evolution, using the angular velocity of each particle in every time step as follows:

At the beginning, Eulerian parameters of an particle are assumed to be

$$e_0^0 = 1, \quad \boldsymbol{e}^0 = 0. \tag{3.35}$$

We consider the Eulerian parameters and the angular velocity of the particle at time t_n as $e_0^n, \boldsymbol{e}^n$ and $\boldsymbol{\omega}$, respectively. Then, using the following variables

$$\varDelta\theta = \omega\varDelta t \tag{3.36}$$

$$\varDelta e_0 = \cos\frac{\varDelta\theta}{2} \tag{3.37}$$

$$\varDelta\boldsymbol{e} = \hat{\boldsymbol{\omega}}\sin\frac{\varDelta\theta}{2}, \tag{3.38}$$

the Eulerian parameters at time $t_{n+1} = t_n + \varDelta t$ are given by

$$e_0^{n+1} = e_0^n\varDelta e_0 - \boldsymbol{e}^n\cdot\varDelta\boldsymbol{e} \tag{3.39}$$

$$\boldsymbol{e}^{n+1} = e_0^n\varDelta\boldsymbol{e} + \boldsymbol{e}^n\varDelta e_0 - \boldsymbol{e}^n\times\varDelta\boldsymbol{e}\,. \tag{3.40}$$

Note: Taking the limitation $\varDelta t \to 0$, we can obtain

$$\dot{e_0} = -\frac{1}{2}\boldsymbol{e}\cdot\boldsymbol{\omega} \tag{3.41}$$

$$\dot{\boldsymbol{e}} = \frac{1}{2}\left(e_0\boldsymbol{\omega} - \boldsymbol{e}\times\boldsymbol{\omega}\right). \tag{3.42}$$

3.9 Tracing $\boldsymbol{n}_1$ and $\boldsymbol{n}_2$

By using Eulerian parameters of particle 1 at time t, $e_0(t)$ and $\boldsymbol{e}(t)$, $\boldsymbol{n}_1(t)$ (and $\boldsymbol{n}_2(t)$) at time t can be obtained as follows.

Considering that particle 1 and 2 contact at time $t = t_0$, $\boldsymbol{n}_1$ and $\boldsymbol{n}_2$ at this time are given by

$$\boldsymbol{n}_1(t_0) = -\boldsymbol{n}_2(t_0) = \frac{\boldsymbol{x}_2(t_0) - \boldsymbol{x}_1(t_0)}{|\boldsymbol{x}_2(t_0) - \boldsymbol{x}_1(t_0)|}. \tag{3.43}$$

Next, by using rotation matrix at time t_0, $A(t = t_0)$, which is a function of $e_0(t_0)$ and $\boldsymbol{e}(t_0)$ as shown in Eq. (3.32), $\boldsymbol{n}_1(0)$ is calculated,

$$\boldsymbol{n}_1(0) = A^{-1}(t_0)\boldsymbol{n}_1(t_0). \tag{3.44}$$

Then, by using rotation matrix at time t, $A(t)$, which is a function of $e_0(t)$ and $\boldsymbol{e}(t)$, $\boldsymbol{n}_1(t)$ is calculated,

$$\boldsymbol{n}_1(t) = A(t)\boldsymbol{n}_1(0). \tag{3.45}$$

4 Treatment of energy dissipation and displacement correction in inelastic regime

In this section I describe the calculation processes of energy dissipation and displacement correction for each degree of freedom in inelastic regime.

4.1 Normal direction

There are two processes of energy dissipation for normal direction: one is at the moment of contact of particles and the other is at the moment of separation.

4.1.1 At the moment of contact

As described in the previous section 3.4, particle contact begins at $\delta = 0$, at which the potential in the normal direction is negative,

$$U_n(\delta = 0) = -\frac{8}{15}4^{\frac{1}{3}}F_c\delta_c \simeq -0.847F_c\delta_c. \tag{4.1}$$

We assume that this energy difference from 0 is dissipated at the beginning of contact. By that assumption, particle velocities are continuous at the moment of contact. There can be another assumption that the particles are accelerated abruptly at the moment of contact, transforming the energy difference into kinetic energy of the particles. We take the former assumption because we think velocity continuity is preferable. In addition, considering physically, some amount of energy should be lost by sound wave excited by the particle contact. According to the analysis by Chokshi et al. (1993), this energy loss by sound wave reaches $0.4F_c\delta_c$. Therefore, the energy loss at the moment of contact assumed in our calculation is reasonable.

4.1.2 At the moment of separation

As described in the previous section 2, particles are kept in contact even if $\delta < 0$ and cannot be separated till $\delta = -\delta_c$. Taking a look carefully at Fig. 2, U_n is positive at the moment of separation,

$$U_n(\delta = -\delta_c) = \frac{4}{45}F_c\delta_c \simeq 0.09F_c\delta_c. \tag{4.2}$$

It is considered that this energy is stored in the form of elastic energy and is released by the separation. We assume, therefore, that this amount of energy is dissipated at the particle separation.

Note that these are energy dissipated not per a particle, but per *a pair of contact particles*.

4.2 Sliding and rolling

When the displacements for sliding and rolling become greater than critical values, inelastic deformation is considered to occur. To treat this inelastic behavior, the following processes are carried out:

1. At the beginning of calculation, we set up the critical values of displacements.
2. When the displacements exceed the critical values, the displacements are reduced to the critical values.
3. Potentials, forces and torques are calculated with the reduced displacements. Amount of energy dissipated can be also calculated.
4. We need to correct a contact point vector $\boldsymbol{n}_1(t)$ because the sliding and rolling displacements in the next following steps are calculated by using $\boldsymbol{n}_1(t)$. In other words, the correction of displacements are recorded in the contact point vector. Actually, $\boldsymbol{n}_1(t)$ is calculated through $\boldsymbol{n}_1(0)$ (see Eq. (3.45)), thus we need to correct $\boldsymbol{n}_1(0)$.

In the following sections, details of above processes for each degree of freedom are described.

4.2.1 Sliding motion

- Critical displacement for sliding

  According to Dominik and Tielens (1996), when the particles are sliding each other over the elastic limit, the frictional force is given by

$$F_{fric} = \frac{Ga_0^2}{2\pi}, \tag{4.3}$$

  where we assume $a = a_0$ and ignore the difference among materials for simplicity[3]. Considering that the inelastic sliding occurs when the elastic force given by Eq. (3.23) reaches to F_{fric}, we obtain the critical displacement ζ_{crit}:

$$8a_0G^*\zeta_{crit} = \frac{Ga_0^2}{2\pi} \quad \Longleftrightarrow \quad \zeta_{crit} = \frac{2-\nu}{16\pi}a_0. \tag{4.4}$$

  (In the above equation, we have simplified the elastic force.)

  Therefore, the critical value of displacement for sliding motion, ζ_{crit} is given by the material properties.

- Displacement correction and energy dissipation

  When $|\boldsymbol{\zeta}| > \zeta_{crit}$, $\boldsymbol{\zeta}$ is corrected to $\boldsymbol{\zeta}'$:

$$\boldsymbol{\zeta}' = \zeta_{crit}\frac{\boldsymbol{\zeta}}{|\boldsymbol{\zeta}|}. \tag{4.5}$$

[3] Dominik and Tielens (1996) derived a general formula of F_{fric}:

$$F_{\mathrm{fric}} = \frac{Ga^2}{2\pi} + \begin{cases} 0 & (\text{for silicate, graphite,etc...}) \\ \frac{1}{3}F_n - \frac{\pi a^2}{3}p_{\mathrm{crit}} & (\text{for ice, metal}) \end{cases}$$

$$\textit{where,}\quad p_{crit} = \frac{2.67}{\pi}\frac{b^3}{\sigma^3}G - \frac{24.72}{\pi}\frac{b^4}{\sigma^5}\gamma,$$

where b is the interatomic distance in the material and $2^{\frac{1}{6}}\sigma$ is the equilibrium distance in the pair-potential model. For details, see Dominik and Tielens (1996).

The amount of energy dissipated, $\Delta E_{dis,s}$, is calculated as

$$\Delta E_{dis,s} = k_s \boldsymbol{\zeta}' \cdot (\boldsymbol{\zeta} - \boldsymbol{\zeta}') = k_s \zeta_{crit} (|\boldsymbol{\zeta}| - \zeta_{crit}) . \tag{4.6}$$

Note that $\Delta E_{dis,s}$ is counted for a pair of contact particles.

- Correction of contact point vector

The displacement excess is given by

$$\Delta \boldsymbol{\zeta} = \boldsymbol{\zeta} - \boldsymbol{\zeta}' . \tag{4.7}$$

It seems that a contact point vector of particle 1, $\boldsymbol{n}_1(t)$, is corrected such as[4]

$$\boldsymbol{n}_1'(t) = \boldsymbol{n}_1(t) - \frac{1}{2}\frac{\Delta \boldsymbol{\zeta}}{r_1} . \tag{4.8}$$

$\boldsymbol{n}_1$ must be, however, a unit vector and thus be normalized. Therefore, we need to consider the normalization and add some correction to the above equation. Here, let l be the size of the apparent correction,

$$l = \left| \frac{1}{2}\frac{\Delta \boldsymbol{\zeta}}{r_1} \right| , \tag{4.9}$$

and l' be the true size of the correction. By using l and l', the corrected point vector (before normalized) is given by

$$\boldsymbol{n}_1'(t) = \boldsymbol{n}_1(t) - \frac{1}{2}\frac{\Delta \boldsymbol{\zeta}}{r_1}\frac{l'}{l} . \tag{4.10}$$

l' is calculated as follows:

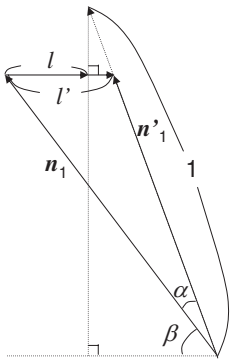

Figure 4:

As delineated in Fig. 4, we consider two equations for giving l'

$$\begin{cases} \cos\beta - \cos(\beta + \alpha) = l \\ \cos\beta - \sqrt{l'^2 - 2l'\cos\beta + 1}\cos(\beta + \alpha) = l', \end{cases} \tag{4.11}$$

where

$$\cos\beta = \frac{\boldsymbol{n}_1(t) \cdot \Delta \boldsymbol{\zeta}}{|\Delta \boldsymbol{\zeta}|} , \tag{4.12}$$

[4]Divided by r_1 because $\boldsymbol{n}_1$ is a unit vector. The factor $\frac{1}{2}$ reflects that the displacement excess is equally divided into two contact particles.

and α is an angle between $\boldsymbol{n}_1$ and $\boldsymbol{n}_1'$ as shown in Fig. 4. Solving these equations (unknown quantities are l' and α), we obtain

$$l' = \cos\beta - \frac{(\cos\beta - l)\sin\beta}{\sqrt{1-(\cos\beta - l)^2}} \tag{4.13}$$

$\boldsymbol{n}_1'(0)$ is calculated by operating the rotation matrix $A^{-1}(t)$

$$\boldsymbol{n}_1'(0) = A^{-1}(t)\left(\boldsymbol{n}_1(t) - \frac{1}{2}\frac{\Delta\boldsymbol{\zeta}}{r_1}\frac{l'}{l}\right) = \boldsymbol{n}_1(0) - \frac{1}{2r_1}\frac{l'}{l}A^{-1}\Delta\boldsymbol{\zeta} \tag{4.14}$$

Normalizing $\boldsymbol{n}_1'(0)$, we obtain a new corrected $\boldsymbol{n}_1(0)$ such as

$$\boldsymbol{n}_1^c(0) = \frac{\boldsymbol{n}_1'(0)}{\left|\boldsymbol{n}_1'(0)\right|} \tag{4.15}$$

4.2.2 Rolling motion

- Critical displacement for rolling

  According to the idea by Dominik and Tielens (1995), the critical value of rolling displacement, ξ_{crit}, should be 2 Å for particles with any size and material. In contrast, an experiment by Heim et al. (1999) suggests that $\xi_{crit} \sim 32$ Å for 1.8 μm SiO_2 particles.

  The appropriate value of ξ_{crit} is not clear so far. Therefore, ξ_{crit} is treated as a parameter in our calculation.

- Displacement correction, energy dissipation and correction of contact point vector

  (Same as in the case of sliding motion.)

  When $|\boldsymbol{\xi}| > \xi_{crit}$, $\boldsymbol{\xi}$ is corrected to $\boldsymbol{\xi}'$:

$$\boldsymbol{\xi}' = \xi_{crit}\frac{\boldsymbol{\xi}}{|\boldsymbol{\xi}|}. \tag{4.16}$$

  The amount of energy dissipated, $\Delta E_{dis,r}$, is calculated as

$$\Delta E_{dis,r} = k_r\boldsymbol{\xi}'\cdot(\boldsymbol{\xi} - \boldsymbol{\xi}') = k_r\xi_{crit}\left(|\boldsymbol{\xi}| - \xi_{crit}\right). \tag{4.17}$$

  Note that $\Delta E_{dis,r}$ is counted for a pair of contact particles.

  The corrected point vector (before normalized) at $t = 0$ is given by

$$\boldsymbol{n}_1'(0) = A^{-1}(t)\left(\boldsymbol{n}_1(t) - \frac{1}{2}\frac{\Delta\boldsymbol{\xi}}{r_1}\frac{l'}{l}\right) = \boldsymbol{n}_1(0) - \frac{1}{2r_1}\frac{l'}{l}A^{-1}\Delta\boldsymbol{\xi} \tag{4.18}$$

  and the new corrected $\boldsymbol{n}_1(0)$ is given by

$$\boldsymbol{n}_1^c(0) = \frac{\boldsymbol{n}_1'(0)}{\left|\boldsymbol{n}_1'(0)\right|} \tag{4.19}$$

4.3 Twisting motion

- Critical angle for twisting

  According to Dominik and Tielens (1996), when the particles are twisting each other over the elastic limit, the resistant torque for twisting is given by

$$M_{t,fric} = \frac{Ga_0^3}{3\pi}, \tag{4.20}$$

  where we assume $a = a_0$ and ignore the difference among materials for simplicity[5]. Considering that the inelastic twisting occurs when the torque due to elastic twisting given by Eq. (3.28) reaches to $M_{t,fric}$, we obtain the critical angle for twisting, ϕ_{crit}:

$$\frac{16}{3}Ga_0^3\phi_{crit} = \frac{Ga_0^3}{3\pi} \quad \Longleftrightarrow \quad \phi_{crit} = \frac{1}{16\pi} \simeq 0.02 \simeq 1.1^\circ. \tag{4.21}$$

- Displacement correction and energy dissipation

  When $|\boldsymbol{\phi}| > \phi_{crit}$, $\boldsymbol{\phi}$ is corrected to $\boldsymbol{\phi}'$:

$$\boldsymbol{\phi}' = \phi_{crit}\frac{\boldsymbol{\phi}}{|\boldsymbol{\phi}|}. \tag{4.22}$$

  The amount of energy dissipated, $\Delta E_{dis,t}$, is calculated as

$$\Delta E_{dis,t} = k_t\boldsymbol{\phi}' \cdot (\boldsymbol{\phi} - \boldsymbol{\phi}') = k_t\phi_{crit}\left(|\boldsymbol{\phi}| - \phi_{crit}\right). \tag{4.23}$$

  Note that $\Delta E_{dis,t}$ is counted for a pair of contact particles.

References

Chokshi, A., Tielens, A. G. G. M. and Hollenbach, D., 1993, Astrophys. J. 407, 806.
Dominik, C. and Tielens, A. G. G. M., 1995, Phil. Mag. A 72, 783.
Dominik, C. and Tielens, A. G. G. M., 1996, Phil. Mag. A 73, 1279.
Johnson, K. L., 1985, Contact mechanics, Cambridge Univ. Press.
Johnson, K. L., Kendall, K. and Roberts, A. D., 1971, Proc. R. Soc. Lond. A. 324, 301.

[5] Dominik and Tielens (1996) derived a general formula of $M_{t,fric}$:

$$M_{t,fric} = \frac{Ga^3}{3\pi} + \begin{cases} 0 & \text{(for silicate, graphite,etc...)} \\ \frac{1}{3}F_c a_0\left(\frac{3}{4}\hat{a}^4 - \hat{a}^{\frac{5}{2}}\right) - \frac{2}{9}\pi a^3 p_{\rm crit} & \text{(for ice, metal)} \end{cases}$$

$$where, \quad p_{crit} = \frac{2.67}{\pi}\frac{b^3}{\sigma^3}G - \frac{24.72}{\pi}\frac{b^4}{\sigma^5}\gamma,$$

where $\hat{a} = a/a_0$, b is the interatomic distance in the material and $2^{\frac{1}{6}}\sigma$ is the equilibrium distance in the pair-potential model. For details, see Dominik and Tielens (1996).