Euler-Lagrangian dynamics to the physical interpretation with granular constraints for MD simulations

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In this article, Euler-Lagrangian dynamics explain that the two particle interaction has non-conservative forces about the frame of the center of mass. This interpretation clarifies the underlying interaction and the system descriptions become advantages for MD simulations.

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A Molecular Dynamics (MD) Simulation is based on Newton’s second law on time evolution within the framework of classical mechanics. The motion of granular dynamics can be described by Euler-Lagrangian dynamics. From a comprehensive point of view, the Euler-Lagrangian dynamics is presented to clearly and easily identify the pair interaction and contacting time among the individual particles. The kinetic energy and the potential energy are used to obtain the Lagrangian of the particle with the generalized coordinate and its associated granular interaction term. In this work, the system of N particles was the only constraint used to move the particles through the external gravitational force and the energy dissipated in friction.

For a granular system of N particles moving in three dimensional space with constraints, D’Alembert’s principle requires knowledge of the constraint forces, (typically and static), kinetic frictional force and particle sliding. What was needed was a description of the system that makes compromises when dealing with the constraint relations. D’Alembert’s principle provides such a description for systems involving holonomic or nonholonomic constraints in allowing virtual displacements, \( \delta r_i = \sum_a \delta r_{q_a} \delta q_a \) in contrast with a real displacement \( \delta r_i \). There are two types of constraints. The first one is holonomic constraints which can be solved for using kinematics; here there is no work \( (F_i^{(c)} \cdot \delta r_i = 0) \) because virtual displacements \( \delta r_i \) are orthogonal to the corresponding constraint forces \( F_i^{(c)} \). The second is nonholonomic constraints which must be solved for using dynamics; here consequently we have a work term \( (F_i^{(c)} \times \delta r_i \neq 0) \).

As a consequence of these constraint relations, this problem is solved by choosing Lagrange’s equation. The Euler–Lagrange equations, \( L(q_a, \dot{q}_a) \) in the generalized coordinates, \( q_a \) for a discrete system is

\[
\frac{d}{dt} \frac{\partial L}{\partial \dot{q}_a} - \frac{\partial L}{\partial q_a} = Q_a
\]  

(1)

Here \( L \equiv T - V - U \) is the Lagrangian of the system.

The generalized constraint forces, \( Q_a \) are derived from D’Alembert’s principle for the virtual work for applied forces. Two nonconservative components are associated with respect to \( \dot{q}_a \) and \( q_a \). The generalized constraint forces on the right-hand side are given by

\[
Q_a \equiv F_i^{(c)} \cdot \frac{\partial r_{ij}}{\partial q_a} = F_i^{(f)} \cdot \frac{\partial r_{ij}}{\partial q_a} - \frac{\partial F}{\partial \dot{q}_a} \tag{2}
\]

where \( F_i^{(f)} \) is only for the friction force and \( F \) is known as Rayleigh’s dissipation function \( F = \frac{1}{2} \sum_{a,b} c_{ij} \dot{q}_a \dot{q}_b \) (if \( c_{ij} = c_{ji} \), the symmetric tensor).

The Lagrange equation with Rayleigh’s dissipation function and contact friction becomes

\[
\frac{d}{dt} \frac{\partial L}{\partial \dot{q}_a} - \frac{\partial L}{\partial q_a} + \frac{\partial F}{\partial \dot{q}_a} = Q_a^{(f)} \tag{3}
\]

where \( Q_a^{(f)} = F_i^{(f)} \cdot \frac{\partial r_{ij}}{\partial q_a} \). The generalized constraint force is presented by a frictional force.

In the case in which particles were assumed to be the spherical rigid bodies located in the gravitational field, the generalized coordinates were decoupled into the center of mass coordinates (the axes of the inertial coordinate system) and the Euler angles (\( \theta, \phi, \psi \)). Since the spherical rigid body is symmetrical for the Euler angles, the moment of inertia for an ideal homogeneous sphere of radius \( R \) is \( I = \frac{2}{5} mR^2 \) is about the principal axis of the center of mass. From the relations above we can compute one term relating the kinetic energy \( T \) of the translational motion and the spin rotation itself about the center of mass. Another term relating the potential energy of the gravity potential \( V \) and a pairwise interaction potential \( U(r_{ij}) \), is given where the distance between the centers of the two particles is \( r_{ij} = |r_i - r_j| \) with respect to a fixed frame and \( r_i, r_j \) is the relative position vector of the center of mass \( m_i, m_j \).

The distance between particles \( i \) and \( j \) about a fixed point \( O \), the relative position about the normal and tangential direction, is independent. Above all, the relative
The relative tangential displacement is

\[ \delta r_{ij} = (\hat{r}_{ij} \cdot \delta r_{ij}) \hat{r}_{ij} + \delta r_{ij} \times (\hat{r}_{ij} \times \hat{r}_{ij}) - \int_{t_c}^{t} \omega_{ij} \times \hat{r}_{ij} d\tau \]  

Here the center of angular velocity is \( \omega_{ij} \equiv (R_i \omega_i + R_j \omega_j) / (R_i + R_j) \), with angular velocities \( \omega_i \) and \( \omega_j \) in a rotating coordinate frame with each particle at the center of mass of the system during contact time \( t_c \).

The relative normal displacement is

\[ \delta r_{ij} = (\hat{r}_{ij} \cdot \delta r_{ij}) \hat{r}_{ij} \]  

and the relative tangential displacement is

\[ \delta r_{ij} = (\hat{r}_{ij} \cdot \delta r_{ij}) \hat{r}_{ij} - \int_{t_c}^{t} \omega_{ij} \times \hat{r}_{ij} d\tau \]  

A comparison with the above gives the relative velocity as

\[
\frac{d\hat{r}_{ij}}{dt} = \hat{r}_{ij} - \omega_{ij} \times r_{ij} = (\hat{r}_{ij} \cdot v_{ij}) \hat{r}_{ij} + \hat{r}_{ij} \times (v_{ij} \times \hat{r}_{ij}) - \omega_{ij} \times r_{ij}
\]

where \( \hat{r}_{ij} = r_{ij}/r_{ij} \) and \( r_{ij} = r_i - r_j \), the relative velocity in term of \( j \).

The relative velocity \( \hat{r}_{ij} = v_{ij} = v_i - v_j \) has the components of the relative normal displacement

\[ v_{ij} = (\hat{r}_{ij} \cdot v_{ij}) \hat{r}_{ij} \]  

and the relative tangential velocity is given by

\[ v_{ij} = \hat{r}_{ij} \times (v_{ij} \times \hat{r}_{ij}) - \omega_{ij} \times r_{ij} \]  

When granular particles have pairwise collisions, they collide instantly and have an infinitesimally small time for the Hertz’s potential. This impulse imparts interactions between each particle. Figure shows analytic geometry, before instantaneous deformation, at which point the bodies touch at an adjacent point. The curvatures of the two bodies are represented with radii of curvature \( R_i \) and \( R_j \). At the contact area, the bodies are compressed with smooth curvature. The shape of the particle is changed by the curvature due to the elastic restoration force. Previously, Hertz’s theory had been used with a quadratic equation. However, contact pressure provides displacement under the surface. This contact pressure is distributed throughout the curvature. The pressure distribution function acts at each contact radius \( a \). The distribution of normal stress in the contact area as a function of distance was also reported [2]. The granular particles behave like hard sphere which contact one another with a deformable contact force. The forces between the two particles can be approximated well by Hertz theory of elasticity. The granular interaction potential is a power law from Hertz theory. Hertz contact is presented to determine each granular surface interaction for granular flows. The generalized expression for the normal contact force acting on a granular body, in which the governing equation is either loaded in tension or in compression, is obtained from the stress and strain relation of the material. The Hertz potential is derived from the results of stress-strain analysis that are attributed to granular flow sensitivity. Granular particle interactions have a virtual depth in the relation with a remarkable normal contact of relative deformation in terms of a tangential contact by a friction on a contact surface. A substantial solution to the problem of a normal contact has been known as Hertz’s theory.

We are led to the relations of the overlap displacement as defined by \( \delta r_{ij} \) where the normal displacement \( \delta r_{ij} \equiv R_i + R_j - |r_i - r_j| \) is the depth of indentation or normal overlap for the contact between the two bodies of radii \( R_1 \) and \( R_2 \). When \( \delta r_{ij} > 0 \), a contact force is generated that otherwise would have zero potential. The noncohesive granular interaction is described by Hertz-Mindlin potential between particles,

\[
U(r_{ij}) = \frac{2}{5} k \delta r_{ij}^{5/2}
\]

FIG. 1: Schematic of the vector analysis contacting on particle acting \( j \rightarrow i \).
where \( k_n = \frac{4}{3} E^* \sqrt{R^*} \) is the stiffness of the pairwise interaction proposed in Hertz theory (Hertz 1895) and the tangential term \( k_t = 8G^* \sqrt{R^*} \) is the tangential force (Mindlin 1949) with the effective Radius \( R^* = R_i R_j / (R_i + R_j) \) and the effective Young’s modulus \( E^* = \left( \frac{1-v_i^2}{E_i} + \frac{1-v_j^2}{E_j} \right)^{-1} \), \( E \) the Young’s modulus and the effective Shear modulus is \( G^* = \left( \frac{2(2-v_i)(1+v_i)}{E_i} + \frac{2(2-v_j)(1+v_j)}{E_j} \right)^{-1} \). Poisson’s ratio is \( \nu \) for the contacting particle \( i \) and \( j \) respectively [1, 2, 3, 4].

Comparisons of this with the Lagrangian obtained previously can be expressed by the gravitational potential

\[
V(r_i) = m_i \mathbf{r}_i \cdot \mathbf{g}
\]  

(11)

where \( \mathbf{g} \) is the gravitational acceleration vector.

The pair dissipative function can be derived from Rayleigh’s dissipation function

\[
\mathcal{F} = \frac{1}{2} \gamma m^* \delta \mathbf{r}_{ij}^2
\]  

(12)

where \( \gamma \) is a dissipative constant or viscous damping coefficient given a coefficient of normal restitution \( e \) for a contacting time with normal and tangential contact.

When the particle \( i \) is moving to another particle \( j \) at contacting time, it follows that the force of constraint exerted by kinetic friction (\( \mu_k \), the kinetic coefficient of friction) of each particle has done real work after the collision. Thus the virtual displacement, \( \delta \mathbf{r} \), is tangent to the other particle and orthogonal to the constraint force. If both particles are at a rest state (\( \mu_s \leq \mu_k \)), the sphere at contact experiences the only force on the pebble from the static friction (\( \mu_s \), the static coefficient of friction) which is perpendicular to the curved part of particle. The normal and tangential direction is independent, and then each term must be separate. The motion of the \( i \)th particle is given by a contact force and a damping force during collisions. If the tangential force is generated, the generalized constraint force is

\[
Q_{ij}^{(t)} = -\text{sign}(\delta \mathbf{r}_{ij \perp}) \min(\mu_i |\mathbf{F}_{ij\|}|, |\mathbf{v}_{ij\perp}|) \mathbf{F}_{ij\perp}
\]

Thus, the Lagrange’s equation of the net binary system can be expressed in term of \( r_{ij} \)

\[
L = \frac{1}{2} m^* |\delta \mathbf{r}_{ij}|^2 - U(r_{ij})
\]  

(13)

where \( m^* = m_i m_j / (m_i + m_j) \) is the reduced mass of the system.

As a consequence of the decoupling, the Lagrange equations of motion separate into two equations, one for the center of mass coordinates and another for the Euler angles. Each set can be analyzed independently to apply this prescription to a two body problem for a virtual displacement. The present simulations use a normal and tangential contact model comprised of the following:

\[
|\delta \mathbf{r}_{ij}|^2 = |\delta \mathbf{r}_{ij\|}|^2 + \left( 1 + \frac{1}{\zeta} \right) |\delta \mathbf{r}_{ij\perp}|^2
\]  

(14)

where \( \zeta = \left( \frac{1}{m_i \omega_i} + \frac{1}{m_j \omega_j} \right)^{-1} \) from the particle moment of
inertia $\tilde{I}_i = I_i/m_i R_i^2$ and $\tilde{I}_j = I_j/m_j R_j^2$ about the torque acting on two particle.

Finally, we can implement Euler-Lagrangian dynamics to find out the governing equation and contact time used to simulate the MD method. Although the theoretical approach is Hertz’s contact to the Lagrangian solution, problems arise including general friction through contacting area where $F_{ji} = -F_{ji}$, Newton 3rd law and the tangential component $F_{ij\perp}$ and $\delta r_{ij\perp}$ which can be described to meet the requirement of Coulomb yield criterion if $|F_{ij\perp}| < \mu_s F_{ij\parallel}$. Until the particles are separated, the potential calculation is performed for the interaction only once on each pair of particles. The equations of motion follow directly from the Lagrangian formulation described above.

The normal component of the contact force can be written as

$$F_{ij\parallel} = k_n \delta r_{ij\parallel}^3/2 - \gamma_n m^* v_{ij\parallel}$$

(15)

The shear component of the contact force can be written as

$$F_{ij\perp} = -k_t \sqrt{\delta r_{ij\perp}} - \gamma_t m^* v_{ij\perp}$$

(16)

The equation of motion will be expressed in normal and tangential directions on contact condition, $|F_{ij\perp}| > \mu_s F_{ij\parallel}$, $F_{ij\perp} = -\mu_s F_{ij\parallel}$, $F_{ij\perp} = -\gamma_t m^* v_{ij\perp}$ which generates the rolling friction from the center of particle $j$ to the center of particle $i$. This component in the direction of motion is attributed by performance of the Hertz-Mindlin theory to improve the terms of the tangential force. The simulation will demonstrate the essential results of the contact deformable interaction. Twobody forces are represented by the potential, which is enough to permit the surface effects. The governing equation, constructed from two-body functions, is applied to the many body system problem with a contact dynamic using a MD simulation (or DEM).

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