Numerical method for interaction between multi-particle and complex structures

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Abstract

We propose a numerical method for dealing with interactions between multiple particles and complex structures. In the method, the complex structures are represented on a grid by using the level set method. The interactions of particles and structures are calculated by a method based on the discrete element method. The method can treat the interaction between multi-particle and complex structures robustly.

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I. INTRODUCTION

Phenomena with particles and structures appear in the various research fields such as physics, engineerings and geophysics. However, numerical studies on the phenomena are difficult because interaction between complex structures and multi-particle must be taken into account. In the paper, we propose a numerical method to study these phenomena.

To simulate interaction among particles, the discrete element method (DEM) has been widely used [1–5]. In DEM, particles overlap during collision and the dynamics is defined though the force acting on the collision particles. DEM can deal with many-body colliding and sustained contact between particles. The present method is based on DEM. So far, to compute interaction among particles and structures, the structures are expressed by particles, linear elements in two dimension case and surface elements in the three dimensional case. In the paper, we propose a different approach based on the level set method [6–8].

In the present method, structures are represented by the zero level set (zero-contour) of the level set function. Although the level set method is an interface capturing method, it is convenient to compute the interaction among particles and structures. The important features of the level set method are that the unit normal for the interface and the distance from the interface are well defined. These characteristics play an important role in coupling DEM and the level set method.

The present method calculates beforehand the level set function for the structure on a grid. This means the distance from the structure and the normal vector for the structure are assigned on each grid point. Here, the normal vector is calculated as the gradient of the level set function. To compute collision between a structure and a particle, the distance between the particle and the structure, and the normal direction for the structure are required. This information can be obtained by interpolating the level set function at the center of the particle. If line elements or polygons are used to express the structure, complicated procedures are required such as computing smallest distances between the particle and elements. To calculate these, we must calculate distances between point (the particle center) and point (element vertex), and point and line (line element). In the three dimensional case, additionally, point-surface distance must be computed. However, in the present method these procedures are not required.

II. NUMERICAL METHOD

A. Particle-particle interaction (DEM)

Equations for translational and rotational motion for a spherical particle are

$$m\frac{d^2\mathbf{r}}{dt^2} = \mathbf{F}, \tag{1}$$

and

$$\mathbf{I}\frac{d\omega}{dt} = \mathbf{T}, \tag{2}$$

where $\mathbf{r}$ is the position of particle center, m the mass of particle, $\mathbf{F}$ the sum of all contact forces from other particles, ω the angular velocity, $\mathbf{T}$ the torque due to contact forces and $\mathbf{I}$ the moment of inertia.

Contact forces between spherical particles are modelled by a linear spring, a dashpot and a friction slider [1]. The normal interaction is expressed by a linear spring and a dashpot (Fig.1(a)), and the tangential interaction is expressed by a linear spring, a dashpot and a friction slider (Fig.1(b)).

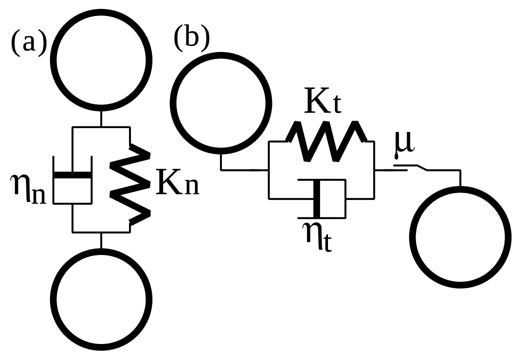

FIG. 1: Schematic figure of the discrete element method. K, η and ν refer to the linear spring, the dash pot and the slider, respectively

We consider two disks i and j of diameters d_i and d_j, with masses m_i and m_j, particle centers $\mathbf{r_i}$ and $\mathbf{r_j}$, velocities at mass center $\mathbf{c}_i$ and $\mathbf{c}_j$, and the angular velocities ω_i and ω_j. The contact forces are calculated in contact, namely,

$$\Delta \equiv \frac{d_i + d_j}{2} - |r_{i,j}| > 0, \tag{3}$$

where $\mathbf{r}_{i,j} \equiv \mathbf{r}_i - \mathbf{r}_j$ The normal component of the contact force $F_n^{i,j}$ due to the particle j acting on the particle i is

$$F_n^{i,j} = 2Mk_n\Delta - 2M\eta_n v_n, \tag{4}$$

with

$$v_n = (\mathbf{c}_i - \mathbf{c}_j) \cdot \mathbf{n}, \tag{5}$$

$$\mathbf{n} = \frac{\mathbf{r}_{i,j}}{|\mathbf{r}_{i,j}|}, \quad \mathbf{r}_{i,j} = \mathbf{r}_i - \mathbf{r}_j \tag{6}$$

where M is the reduced mass ($M = m_i m_j/(m_i + m_j)$), k_n the spring constant, η_n the normal damping coefficient and v_n the normal component of the relative velocity, $\mathbf{n}$ the unit normal. The tangential component of the contact force $F_s^{i,j}$ is

$$F_s^{i,j} = min(|h_s^{i,j}|, \mu|F_n^{i,j}|)sgn(h_s^{i,j}), \tag{7}$$

with

$$h_s^{i,j} = -2Mk_s u_s - 2M\eta_s v_s, \tag{8}$$

$$u_s = \int_{t_0}^{t} v_s dt, \tag{9}$$

$$v_s = (\mathbf{c}_i - \mathbf{c}_j) \cdot \mathbf{s} + (\frac{d_i}{2}\omega_i + \frac{d_j}{2}\omega_j), \tag{10}$$

where μ is the Coulomb friction coefficient for slider, k_s the tangential spring constant, u_s the tangential displacement, t_0 the time at the impact, η_s the tangential damping parameter, v_s the tangential velocity, $\mathbf{s}$ the unit tangential vector. $\mathbf{F}_i$ and $\mathbf{T}_i$ are calculated as follows

$$\mathbf{F}_i = \Sigma_j (F_n^{i,j} + F_s^{i,j}), \tag{11}$$

$$\mathbf{T}_i = \frac{d_i}{2}\Sigma_j (\mathbf{n} \times F_s^{i,j}). \tag{12}$$

B. Structure-particle interaction (level set method)

The interfaces of the structures are expressed by the level set method. The level set method is an interface-capturing method and has been applied to various problems with interfaces [6–8]. This method expresses the surface of an $N-1$ dimension as a zero level (or contour) of an N-dimensional level set function ψ. The signed distance function

$$\begin{aligned} \psi = 0 &\ \text{ at the interface} \\ |\nabla\psi| = 1 &\ \text{ for the whole region} \end{aligned} \tag{13}$$

is used as the level set function as shown in Fig. 2. In the paper, the level set method is used on a regular Cartesian fixed grid. Although the Cartesian fixed grid is used, the level set formulation can express subgrid information and complex geometries as shown in Fig. 2 and Fig. 3. An advantage of the level set method is that the unit normal is always well

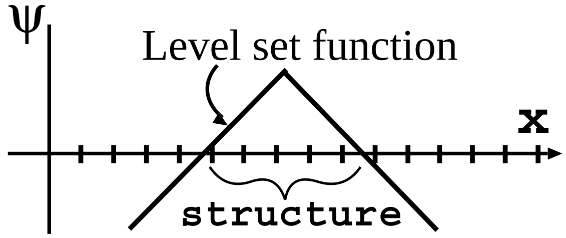

FIG. 2: Schematic figure of a level set function in the one dimensional case.

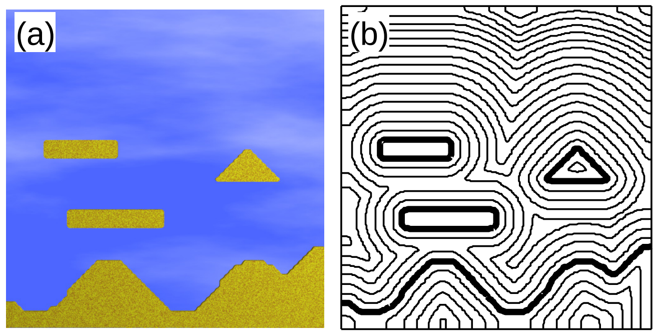

FIG. 3: An example of a level set function in the two dimensional case. (a) shows the shape of structures. (b) shows the contour lines of the level set function for the structure. The thick and thin lines represent the zero level set and the contour lines of the level set function. A 70×70 Cartesian grid is used.

defined from the level set function

$$\mathbf{n}_{ls} = \frac{\nabla \psi}{|\nabla \psi|}. \tag{14}$$

The unit normal is useful for computing interaction between particles and structures by using the distance function.

To construct the level set function for structures, we can use methods found in [7, 9–11] such as the Fast Marching method for solving the Eikonal equation

$$|\nabla \psi| = 1. \tag{15}$$

The interaction between the structures expressed by the level set function and particles are computed based on DEM. To compute the interaction, information about the distance from the interface and the normal direction to the interface are needed. In the level set formulation, this information is well defined. Therefore, DEM is slightly modified by using the level set function ψ and the $\mathbf{n}_{ls}$ of (14). The procedures of DEM are replaced as follows:

$$(3) \Rightarrow \quad \Delta \equiv \frac{d_i}{2} - |\psi| > 0, \tag{16}$$

$$(4) \Rightarrow \quad F_n^{i,ls} = k_n\Delta - \eta_n v_n, \tag{17}$$

$$(5) \Rightarrow \quad v_n = \mathbf{c}_i \cdot \mathbf{n}_{ls}, \tag{18}$$

$$(6) \Rightarrow \quad \mathbf{n}_{ls} = \mp\frac{\nabla\psi}{|\nabla\psi|}, \tag{19}$$

$$(7) \Rightarrow \quad F_s^{i,ls} = min(|h_s^{i,ls}|, \mu|F_n^{i,ls}|)sgn(h_s^{i,ls}), \tag{20}$$

$$(8) \Rightarrow \quad h_s^{i,ls} = -k_s u_s - \eta_s v_s, \tag{21}$$

$$(9) \Rightarrow \quad u_s = \int_{t_0}^{t} v_s dt, \tag{22}$$

$$(10) \Rightarrow \quad v_s = \mathbf{c}_i \cdot \mathbf{s}_{ls} + \frac{d_i}{2}\omega_i, \tag{23}$$

here ψ_i is ψ at the position of particle center. ψ_i is estimated by using an interpolation. A linear interpolation is used in this paper. In (19), "+" sign is used for $\psi_{structure} > 0$ and "−" sign is used for $\psi_{structure} < 0$

III. VALIDATION

To certify the present method, we carried out a simple test problem. Fig. 4 shows the configuration. The slope is represented by the level set function on a Cartesian fixed grid

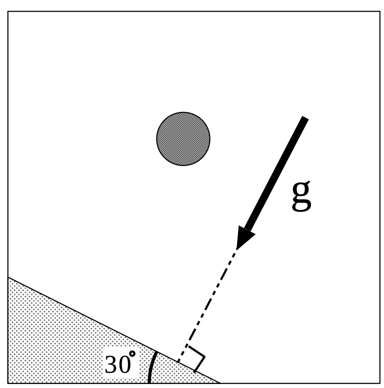

FIG. 4: Schematic figure of a test problem.

of 50×50. The direction of gravity is perpendicular to the slope. In this test problem, damping and rotation of the particle are not taken into account. In this configuration, if the particle is released with the velocity$= 0$ from height h for the slope, the particle must return to the same position at $t = 2\sqrt{2h/g}$. The numerical result compared with the exact solution is shown in Fig. 5. Table I displays the errors at $t = 2, 4, 6, 8$[s]. Error$_1$ and error$_2$ are defined as error$_1$=|(numerical result)-(exact solution)| and error$_2$=error$_1/h$.

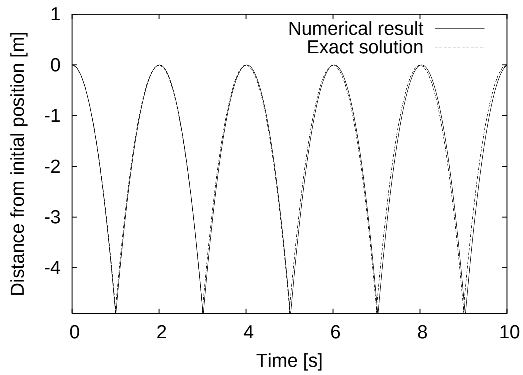

FIG. 5: Time evolution of the height of particle from the slope. The solid line and the dotted line represent the numerical result and exact solution, respectively. Five cycles are plotted. $k_n = 5\times 10^7$ is used.

TABLE I: Error of our algorithm.

Time(s)	$Error_1$	$Error_2$
2	2.98×10^{-4}	6.08×10^{-5}
4	1.25×10^{-3}	2.55×10^{-4}
6	2.87×10^{-3}	5.86×10^{-4}
8	5.14×10^{-3}	1.05×10^{-3}
10	8.08×10^{-3}	1.65×10^{-3}

IV. NUMERICAL RESULTS

We carried out numerical simulations in which the particles interact with structures in the gravity field. As a set of parameters, we use $k_n = 5 \times 10^7$, $\eta_n = 2\sqrt{k_n}$, $k_s = 0.2k_n$, $\eta_s = \eta_n$ and $\mu = 0.5$. A 70×70 grid is used for the level set function. Fig. 6 shows the numerical results when 5 particles interact with structures. A simulation with 65 particles is also performed, as shown in Fig. 7. The results show that the method is robust.

V. SUMMARY

We have proposed a numerical method based on the level set method and DEM. The validity of the method has been shown by the test problem. The method can deal with interaction between multiple particles and complex structures robustly.

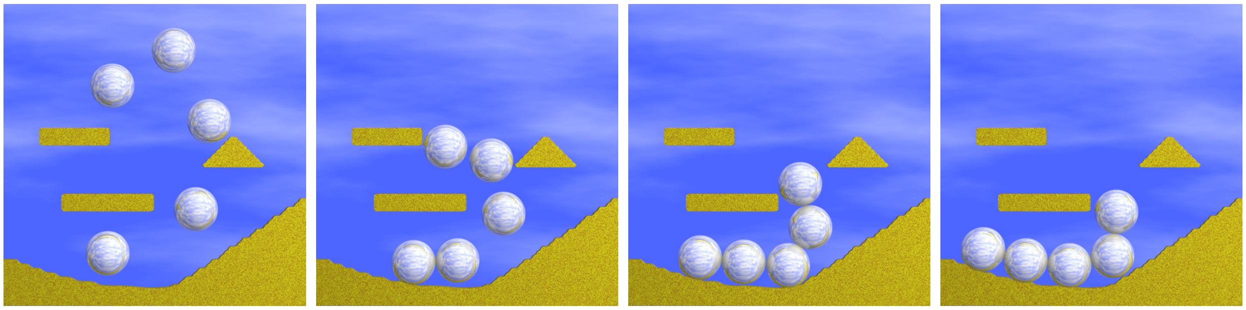

FIG. 6: Snapshots of interaction between 5 particles and the structures at $t = 0, 1, 2, 3$ [s]. The movie is available from [13].

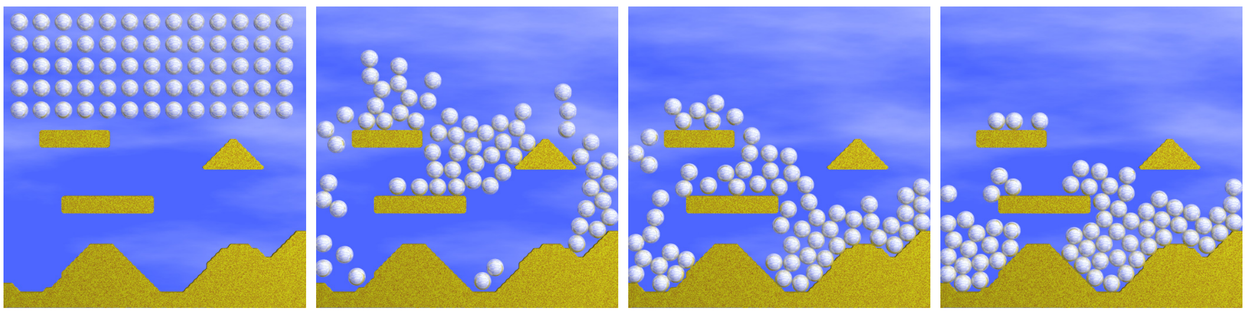

FIG. 7: Snapshots of interaction between 65 particles and the structures at $t = 0, 1, 2, 3$ [s]. The movie is available from [13].

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[1] P.A. Cundall O.D.L. Strack, A discrete numerical model for granular assemblies, Geotechnique, **29** 47 (1979).

[2] C.S. Campbell, Rapid granular flow, Annual Review of Fluid Mechanics, **2** (1990).

[3] G. Mustoe (ed.), Engineering Computation **9** Special Issue (1992).

[4] K. Yamane, M. Nakagawa, S.A. Altobelli, T. Tanaka, Y. Tsuji, Steady particulate flows in a horizontal rotating cylinder , Pysics of Fluid **10** 1419 (1998).

[5] N. Mitarai and H. Nakanishi, Hard Sphere Limit of Soft Sphere Model for Granular Materials: Stiffness Dependence of Steady Granular Flow Phys. Rev. E **67** 021301 (2003)

[6] S. Osher and J.A. Sethian, Front propagating with curvature-dependent speed: Algorithms based on Hamilton-Jacobi formulation, J. Comput. Phys. **79**, 12 (1988).

[7] J.A. Sethian, Level Set Methods and Fast Marching Methods, Cambridge University Press (1999).

[8] S. Osher and R. Fedkiw, Level Set Methods and Dynamics Implicit Surface, Applied Mathematical Sciences 153, Springer (2003).

[9] D. Adalsteinsson and J.A. Sethian, The Fast Construction of Extension Velocities in Level Set Methods, J. Comput. Phys. **148**, 2 (1999).

[10] K. Yokoi, Numerical method for complex moving boundary problems in a Cartesian fixed grid, Phys. Rev. E **65** 055701(R) (2002).

[11] Y.R. Tsai, Rapid and accurate computation of the distance function using grids, J. Comput. Phys. **178** 175 (2001).

[12] M. Sussman, P. Smereka and S. Osher, J. Comput. Phys. **114**, 146 (1994).

[13] http://www.kensuke.biz.