A Note on Discrete Element Method (DEM)

Tianju Xue

December 8, 2022

1 Governing equations

The equations of motion for a single 3D rigid object can be written as the following ODEs:

$$\frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}t} = \boldsymbol{v}, \tag{1a}$$

$$\frac{\mathrm{d}\boldsymbol{q}}{\mathrm{d}t} = \frac{1}{2}\boldsymbol{\omega} \otimes \boldsymbol{q}, \tag{1b}$$

$$\frac{\mathrm{d}\boldsymbol{v}}{\mathrm{d}t} = \frac{1}{m}\boldsymbol{f}, \tag{1c}$$

$$\frac{\mathrm{d}\boldsymbol{\omega}}{\mathrm{d}t} = \boldsymbol{I}^{-1}(\boldsymbol{\tau} - \boldsymbol{\omega} \times (\boldsymbol{I}\boldsymbol{\omega})), \tag{1d}$$

where $\boldsymbol{x} \in \mathbb{R}^3$ is the Cartesian position of the centroid, $\boldsymbol{q} \in \mathbb{R}^4$ is the quaternion that describes the rotational position of the object, $\boldsymbol{v} \in \mathbb{R}^3$ is the velocity of the centroid, $\boldsymbol{\omega} \in \mathbb{R}^3$ is the angular velocity of the object, $\boldsymbol{f} \in \mathbb{R}^3$ is the net force on the object, $\boldsymbol{\tau} \in \mathbb{R}^3$ is the net torque, m is the mass, and $\boldsymbol{I} \in \mathbb{R}^{3\times 3}$ is the inertia tensor with respect to the centroid. Here, Eq. 1a is obvious, Eq. 1b is the quaternion description of rotational kinetics [1, 2], Eq. 1c is Newton's law, and Eq. 1d is Euler's equation for rigid body dynamics [3]. These are the standard equations for rigid body dynamics. One can also consult any typical DEM literature for details, like [4].

The equations for a single object cannot stand alone to be solved, because for example $\boldsymbol{f}$ may depend on the position of another object. For a systematic treatment, let us assume we have n objects. Denote $\boldsymbol{u} \in \mathbb{R}^{13\times n}$ to be the state variable such that

$$\boldsymbol{u} = \begin{bmatrix} \boldsymbol{x}^1 & \boldsymbol{x}^2 & & \boldsymbol{x}^n \\ \boldsymbol{q}^1 & \boldsymbol{q}^2 & \dots & \boldsymbol{q}^n \\ \boldsymbol{v}^1 & \boldsymbol{v}^2 & & \boldsymbol{v}^n \\ \boldsymbol{\omega}^1 & \boldsymbol{\omega}^2 & & \boldsymbol{\omega}^n \end{bmatrix}, \tag{2}$$

where the i^{th} column of $\boldsymbol{u}$ is the state vector for the i^{th} object. Therefore the system of ODEs for all objects can be abstracted as

$$\frac{\mathrm{d}\boldsymbol{u}}{\mathrm{d}t} = \boldsymbol{r}(\boldsymbol{u}), \tag{3}$$

where $\boldsymbol{r} : \mathbb{R}^{13\times n} \to \mathbb{R}^{13\times n}$ is the right hand side function.

2 Shape representation

The formulation above does not consider the shape of the object as a variable. Let's add the dependency now. There are various ways to parametrize an irregular 3D object, such as level-set method [5], parametric surface [6], overlapping rigid cluster method [7], point cloud based method [4], and polyhedron method [8]. It is also promising to use a neural network for shape representation [9], whose application in DEM can be interesting to explore.

Denote the parameters controlling object shape to be $\boldsymbol{p} \in \mathbb{R}^m$. We can now write $\boldsymbol{u} = \boldsymbol{u}(t, \boldsymbol{p})$, and $\boldsymbol{r} = \boldsymbol{r}(\boldsymbol{u}, \boldsymbol{p})$. For a process from initial time t_0 to final time t_f, if we are given the shape parameter $\boldsymbol{p}$ and the initial conditions for $\boldsymbol{u}$, we should be able to solve for $\boldsymbol{u}(t, \boldsymbol{p}) \in \mathcal{U}$.

3 Contact modeling

In Eq. 1, the only term that is not obvious is the force $\boldsymbol{f}$. Typically, we need to have a robust mechanism to detect and evaluate the contact forces contained in $\boldsymbol{f}$. Up to now, we have generally followed the treatment in [5]. Other approaches might also apply, such as in [4]. We will see.

References

[1] https://www.ashwinnarayan.com/post/how-to-integrate-quaternions/.

[2] https://www.euclideanspace.com/physics/kinematics/angularvelocity/QuaternionDifferentiation2.pdf.

[3] https://en.wikipedia.org/wiki/Euler%27s_equations_(rigid_body_dynamics).

[4] L. Zhan, C. Peng, B. Zhang, and W. Wu, "A surface mesh represented discrete element method (smr-dem) for particles of arbitrary shape," *Powder Technology*, vol. 377, pp. 760–779, 2021.

[5] R. Kawamoto, E. Andò, G. Viggiani, and J. E. Andrade, "Level set discrete element method for three-dimensional computations with triaxial case study," *Journal of the Mechanics and Physics of Solids*, vol. 91, pp. 1–13, 2016.

[6] J. E. Andrade, K.-W. Lim, C. F. Avila, and I. Vlahinić, "Granular element method for computational particle mechanics," *Computer Methods in Applied Mechanics and Engineering*, vol. 241, pp. 262–274, 2012.

[7] A. K. Ashmawy, V. V. Hoang, B. Sukumaran, *et al.*, "Evaluating the influence of particle shape on liquefaction behavior using discrete element modeling," in *The Thirteenth International Offshore and Polar Engineering Conference*, International Society of Offshore and Polar Engineers, 2003.

[8] B. Nassauer, T. Liedke, and M. Kuna, "Polyhedral particles for the discrete element method," *Granular matter*, vol. 15, no. 1, pp. 85–93, 2013.

[9] J. J. Park, P. Florence, J. Straub, R. Newcombe, and S. Lovegrove, "Deepsdf: Learning continuous signed distance functions for shape representation," in *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pp. 165–174, 2019.