Discrete Element Modelling of the dynamics of a Self-Rotating Object in dense Granular Media

Ping Liu, Xuan Zou, Jingyuan Zhou, Wenhui Tang and Xianwen Ran *
College of Liberal Arts and Sciences, National University of Defense Technology, Changsha 410073, China
*Corresponding author e-mail: ranxianwen@nudt.edu.cn

Abstract. Many reptiles can move significant distances through sand or many seeds drill out soil during germination by rotating their bodies. Inspired by the biological behaviour and challenged by the absence of physical mechanism for the locomotion in granular materials, we developed a numerical study of a self-excited spherical intruder in a granular bed under gravity, using discrete element method. In simulation, the intruder was rotated around x-axis with different friction coefficient µ and rotation angular velocity ω. We find that the space motion of intruder is sensitive to these two parameters. It moves farther in the Z+ direction with the increase of µ and ω, and there emerges opposite movement in the Y direction with the change of ω. We analysed the physical mechanisms governing these motions and proposed two qualitative theory: the tangential force raises with the increase of ω, which causes the intruder to lift faster; the competition mechanism between friction effect and squeezing effect leads to the motion differentiation of intruder in the Y direction. These results of this study pave the way for the design of an efficient bio-inspired robot moving within seabed or desert according to this mode of locomotion.

1. Introduction
Granular Materials (GMs) are defined as an ensemble of non-cohesive discrete macroscopic solid particles that interact through potential and dissipate energy on collisions [1]. GMs can behave like solids, liquids, and gases, depending on how we prepare and excite them [2]. There is a lack of well-developed theory to study the interaction between active objects and bed particles, but the response of dense GMs subject to the motion of an organism is important in many industrial and biological [3] settings. Therefore, probing the dynamics of GMs is of fundamental interest and also a challenging problem.

Recently, a number of researchers have studied the locomotion of self-vibrating sandfish in desert [4, 5]. They applied the resistive force theory (RFT) [6, 7] in fluid mechanics to model the sandfish swimming dynamics [8-10]. However, the rotation is also known as a common propulsion mechanism, but little effort has been made to investigate it. For example, the seeds of filaree (Pelargonium and Erodium cicutarium) can digging into cohesionless soils by helical rotation [11, 12], and many bacterial species (E.Coli) also propel themselves by rotating bundles of helical filaments [13, 14]. Thus, discovering the locomotion principle of self-rotating organisms in GMs is of great engineering significance, not least to the development of “diving” robots in sandy terrains.
In this paper, we carried out three-dimensional DEM simulations to imitate the locomotion of rotating spherical intruder, studying their trajectories with different friction $\mu$ and rotation velocity $\omega$. The rest of the paper is organized as follows: we describe the numerical simulation method in section 2; In section 3 we present the simulation system and all the simulation results including our analysis and discussion; we list our conclusions and suggestion for future work in Section 4.

2. Simulation method and parameter

We used open source software LIGGGHTS [15] to simulate the rotation process of SO in granular media. LIGGGHTS stands for LAMMPS Improved for General Granular Heat Transfer Simulations and implement massively parallel computing on distributed memory machines [16], which is based on Discrete Element Method (DEM). In DEM simulations, each particle is represented by a sphere, and contact interactions between particles are modelled with Hertz-Mindlin theory [17, 18]. The first step is detecting particle collision state between particles according to the initial position of particles.

The Contact state between two grains $(i, j)$ is shown in Figure 1. Here, $\vec{n}_i$ is a unit vector pointing from the mass center of particle $i$ to $j$.

$\vec{n}_{ij} = \frac{\vec{x}_i - \vec{x}_j}{|\vec{x}_i - \vec{x}_j|}$

where $x_i$ and $x_j$ are the positions of particle $i$ and particle $j$.

![Figure 1. The contact state of a pair of particles $(i, j)$](image)

The contact distance between the two particles is defined by

$d_{ij} = |\vec{x}_i - \vec{x}_j|$

Particle collisions can easily be detected by normal overlap $\delta_{n_{ij}}$, defined by

$\delta_{n_{ij}} = R_i + R_j - d_{ij}$

The relative velocity is expressed into normal and tangential components as given in equation (4) and (5) respectively,

$\vec{u}_{n_{ij}} = (\vec{u}_i - \vec{u}_j) \cdot \vec{n}_{ij} \cdot \vec{n}_{ij}$

$\vec{u}_{t_{ij}} = (\vec{u}_i - \vec{u}_j) - \vec{u}_{n_{ij}}$

where $R_i$ and $R_j$ are the radii of particle $i$ and particle $j$. Two particles are independent of each other when $\delta_{n_{ij}} \leq 0$ and there is no contact force. However, when $\delta_{n_{ij}} > 0$, the two particles collide against each other and the contact force are calculated by Hertz-Mindlin model, which are given by...
The normal force $F_{nij}$ and tangential force $F_{tij}$ are both functions of overlap $\delta_{ij}$ and relative velocity $\bar{u}_{ij}$ with stiffness $k_{ij}$ and damping coefficient $\gamma_{ij}$. The two coefficient in these equations are function of material parameters: Young’s Modulus $E$, Poisson Ratio $\nu$, Restitution Coefficient $e$, and Friction Coefficient $\mu$ (the specific values are shown in Table 1.). It should be noted that the friction coefficient of intruder is not written in the Table 1, because we monitored the friction between the intruder and bed particles with the range of $0.4 \sim 0.6$ in our subsequent simulations.

### Table 1. Material Parameters

| Parameters | Young’s Modulus | Poisson Ratio | Restitution Coefficient | Friction Coefficient | Radius | Density |
|------------|-----------------|---------------|-------------------------|----------------------|--------|---------|
| Intruder   | $10^7$ Pa       | 0.25          | 0.5                     | unfixed              | 0.06 m | 2500 kg/m$^3$ |
| Bedparticels | $10^7$ Pa       | 0.25          | 0.9                     | 0.45                 | 0.01 m | 2500 kg/m$^3$ |

These forces are then used to predict the particles future location and velocity for next time-step. The process above is repeated for every particle in the system for each time step till the required number of time-steps.

### 3. Simulation results and analyse

#### 3.1. Simulation system

To perform numerical simulations of an organism moving in a granular medium, we have created a container with a large spherical particle (represents the intruder) immersed in the middle of bed medium. The simulation container is a 3D box of $0.5 \times 1.0 \times 1.3$ m in the x, y, z directions with periodic boundary conditions along x and y directions. The particles are treated as infinite array of images of itself and they moving out at one end of boundary re-enters at the opposite boundary, creating a periodic movement of them. At the beginning of the simulations, bed particles are created at the top of the box, as shown in Figure 2(a), and are then poured into the box until the surface reaches $z=0.6$ m (see Figure 2(b)). A large spherical intruder is generated at the top of the box and is then inserted to the position of $(x,y,z) = (0,0,0)$, as shown in Figure 2 (c). The system is relaxed for more than two hours to reach equilibrium, which is used for the following simulations.

![Figure 2. The generation process of the simulation system](image)
3.2. Simulation results and analysis
Starting from the equilibrated initial state (Figure 2(c)), we performed a series of simulations and each one ran \(5 \times 10^6\) steps with the time-step of \(10^{-5}\) seconds. For testing the effect of angular velocity \(\omega\) and friction coefficient \(\mu\) on the locomotion of the intruder, we forced the intruder to rotate about x-axis with different \(\omega\) and \(\mu\). We set the value of rotation angular velocity to be \(\omega = 10 \times 2^i\) rad/s, \(i = 0,1,2,...,6\). Most notably, the positive value of \(\omega\) indicates that the intruder rotates anti-clockwise around x-axis. Next, we will introduce the trajectories of the intruder in the x, y, z directions and analyze their physical principles behind that movements.

3.2.1. The motion of the intruder in the Z direction. The friction coefficient \(\mu\) between the intruder and bed particles varies from 0.4 to 0.65. The observations from the Figure 3 are summarized as follows.

1. When \(\mu = 0.4\), the intruder all keeps steady in its original position with the change of rotation angular velocity \(\omega\).
2. When \(\mu > 0.4\), the intruder moves in Z+ direction, i.e. it rises, and the rising rate grows with the increase of \(\omega\) for a fixed friction coefficient \(\mu\).
3. The higher the friction coefficient \(\mu\), the higher the rising, under the condition of a fixed rotating velocity \(\omega\).

We analyze the physical principles behind these observations. When our intruder rotates, the main interaction force between the intruder and the surrounding bed particles is tangential friction. Equation (7) has given the tangential force between any two particles. Here, we regard \(i\) and \(j\) as our target intruder and one bed particle respectively. Supposing that the translational motion of grain pair \((i,j)\) and the rotation motion of bed particle \(j\) are both very small, and \(\delta_{ij} \ll R_j\), then we get the tangential slip velocity,

\[
\tilde{u}_{ij} = \tilde{u}_{ij} + (\hat{x}_i - \hat{x}_j) \times \tilde{\omega}_{ij} = R_i (\tilde{n}_{ij} \times \tilde{\omega}_i) 
\]

In the case of \(k_{ij} |\delta_{ij}| \lesssim \mu_{ij} |\tilde{F}_{ij}|\),

![Figure 3. The movement of intruder in the Z direction at different \(\mu\) and \(\omega\)](image)
\[
\vec{F}_{ij} = k_{ij} \vec{\delta}_{ij} - \gamma_{ij} \vec{u}_{ij}
\]

\[
= (k_{ij} \, dt - \gamma_{ij}) \vec{n}_{ij} - k_{ij} \, dt (\vec{u}_{ij} \cdot \vec{n}_{ij}) \vec{n}_{ij}
\]

\[
= R_i (k_{ij} \, dt - \gamma_{ij}) (\vec{n}_{ij} \times \vec{\omega}_{i}) - k_{ij} R_i dt (\vec{n}_{ij} \times \vec{\omega}_{i}) \vec{n}_{ij}
\]

\[
= R_i (k_{ij} \, dt - \gamma_{ij}) (\vec{n}_{ij} \times \vec{\omega}_{i})
\]

Due to \( \vec{n}_{ij} \perp \vec{\omega}_{i} \), then \( \vec{F}_{ij} = R_i (k_{ij} \, dt - \gamma_{ij}) |\vec{\omega}_{i}| \). Supposed that both \( k_{ij} \) and \( \gamma_{ij} \) are constants, then \( \vec{F}_{ij} = k \vec{\omega} \). It can be seen that the tangential force is proportional to the rotation angular velocity. Therefore, the intruder will rise and its rising rate increases with the rotating angular velocity \( \omega \).

In other cases, when \( k_{ij} |\vec{\delta}_{ij}| > \mu |\vec{F}_{ij}| \), according equation (7), the tangential force is given by,

\[
F_{ij} = \mu |\vec{F}_{ij}| \frac{|\vec{\delta}_{ij}|}{|\vec{\delta}_{ij}|} \quad k_{ij} |\vec{\delta}_{ij}| > \mu |\vec{F}_{ij}|
\]

There is significant positive correlation between the lifting force and \( \mu \). Consequently, the intruder rises higher with a larger friction coefficient.

### 3.2.2. The motion of the intruder in the X direction.

The movements of intruder in X direction at different \( \mu \) and \( \omega \) are very small and irregular, which does not exceed the radius of the intruder.

![Figure 4.](image)

The random motion of the intruder is caused by the imbalance of forces. There are two reasons resulting in the force imbalance. One is the effect of gravity, the other is the effect of rotation. When intruder rotating on the x-axis, the gravity doesn’t affect the movement of intruder in the X direction, and the effect of the x-rotation on the intruder is symmetrical in the Y direction. Therefore, the intruder moves random and tiny.

### 3.2.3. The motion in the Y direction.

The motion of intruder in Y direction appears obvious differentiation at different \( \omega \). Specifically, there is a critical rotation angular velocity \( \omega_c \approx 80 \text{ rad/s} \).

When \( \omega < \omega_c \), the intruder moves in Y+ direction and it moves faster with the increase of \( \omega \); when \( \omega \geq \omega_c \), the intruder moves in Y- direction, and the larger the \( \omega \) is, the farther the intruder moves in the Y- direction. It should be noted that the intruder moves further in the Y- direction with a larger \( \mu \).
When the intruder rotates around x-axis, it is subjected to extrusion and friction at the same time. The extrusion action refers to that: the bed particles above the intruder will flow along the rotation direction affected by the rotation of intruder and the gravity themselves, which makes the bed particles above easier to accumulate on the Y-side of the intruder, as shown in Figure 6(a). Therefore, the intruder will be pushed to Y+ direction under the extrusion action. In addition, the friction action means that: the intruder will be moved in the direction of larger friction force when the force experienced is unbalanced. Obviously, the normal pressure on lower surface of intruder is larger than that on the upper surface (i.e. \( N_1 > N_2 \)), under the effect of gravity. Therefore, the friction force on the lower surface exceeds that on the upper surface (i.e. \( f_1 > f_2 \)), and then the resultant force in the Y direction points to Y- direction. The intruder will move in the Y-direction under the action of friction, see Figure 6(b).

There is a competition between the action of extrusion and friction. When \( \omega \) is small, the squeezing effect is greater than the friction effect, so the intruder moves to Y+ direction; When \( \omega \) becomes larger, the friction effect is greater than the squeezing effect, so the intruder moves to Y- direction. All in all, under the joint influence of extrusion and friction, the movement of the intruder in the Y direction emerges differentiation with the variety of \( \omega \).

4. Conclusion
Inspired by the biological experiments of *Escherichia coli* propelling themselves forward by rotating helix in a viscous fluid, we used LIGGGHTS to simulate the performance of a spherical intruder rotating around x-axis. We employed our simulations to test the effects of friction coefficient \( \mu \) and rotation angular velocity \( \omega \) on the 3-dimensional (3D) space motion of intruder. Our findings showed that the intruder will rise in the Z direction and rise faster with the increase of \( \mu \) and \( \omega \), which was due to the tangential force is proportional to both the angular velocity and the friction coefficient. Moreover, we discovered that the intruder will move to Y+ direction with \( \omega < \omega_c \), and move to Y- direction with \( \omega \geq \omega_c \). We also studied the mechanism of this differentiation in the Y direction, learning that the
extrusion action competes with friction action, and the separatist movement in the Y direction is caused by the combined influence of extrusion and friction. Our simulation predicts reasonably well the locomotion of a self-rotating object within granular medium. The results of this study have the potential to develop a bio-inspired robot that can rapidly rise to the sand surface to a significant. Furthermore, our work provides a feasible scheme for robot moving forwards or backwards within granular medium.

In the future, we will explore the effect of density and size of the intruder on its 3D movement. We also plan to measure the resistance of the GMs near the intruder to verify our conjecture that the rotation loosens the sand surrounding the intruder's body and leading to vertical burrowing.

Acknowledgments
This work was financially supported by National Natural Science Foundation of China (Grant No. 11002162) and General Scientific Research Projects of NUDT (Grant No. ZK16-03-01). The authors are grateful to the Sunway-TaihuLight supercomputer Center for the technical support given.

References
[1] H. M. Jaeger, S. R. Nagel, R. P. Behringer. Granular solids, liquids, and gases [J]. Rev. Mod. Phys., 1996, 68(4) 1259-1273.
[2] R. M. Nedderman. Statics and Kinematics of Granular Materials [M]. Cambridge University Press, 1992.
[3] R. D. Maladen, Y. Ding, P. B. Umbanhowar, A. Kamor, D. I. Goldman. Mechanical models of sandfish locomotion reveal principles of high performance subsurface sand-swimming [J]. J. R. Soc. Interface., 2011, 8(62): 1332-1345.
[4] R. D. Maladen, Y. Ding, C. Li, et al. Undulatory Swimming in Sand: Subsurface Locomotion of the Sandfish Lizard [J]. Science, 2009, 325(5938): 314-8.
[5] W. Wu, C. Lutz, S. Mersch, et al. Characterization of the microscopic tribological properties of sandfish (Scincus scincus) scales by atomic force microscopy [J]. Beilstein J. Nanotechnol., 2018, 9:2618-2627.
[6] J. Gray, G. J. Hancock. The Propulsion of Sea-Urchin Spermatozoa [J]. J.exp.biol., 1955, 32(4):620 – 622.
[7] T. J. Ui, R. P. Husse, R. P. Roger. Stokes drag on a cylinder in axial motion [J]. Phys. Fluids, 1998, 27(4):787-795.
[8] C. Li, P. B. Umbanhowar, H. Komsuoglu, D. E. Koditschek, D. I. Goldman. Sensistive dependence of motion of a legged robot on granular media. P. Natl. Acad. Sci. USA., 2011, 30(7) 739-805.
[9] B. Percier B, S. Manneville, J. N. Mcelwaine, et al. Lift and drag forces on an inclined plow moving over a granular surface [J]. Phys. Rev. E., 2011, 84(5):051302.
[10] Y. Ding, N. Gravish, D. I. Goldman. Drag induced lift in granular media [J]. Phys. Rev. Lett., 2011, 106(2):028001.
[11] D. Evangelista , S. Hotton, J. Dumais. The mechanics of explosive dispersal and self-burial in the seeds of the filaree, Erodium cicutarium (Geraniaceae) [J]. J. Exp. Biol., 2011, 214(4):521-529.
[12] W. Jung, S. M. Choi, W. Kim, et al. Reduction of granular drag inspired by self-burrowing rotary seeds [J]. Phys. Fluids., 2017, 29(4):041702.
[13] R. Vogel, H. Stark. Force-extension curves of bacterial flagella [J]. Eur. Phys. J. E., 2010, 33(3):259-271.
[14] T. B. Darbois, A. Ibarra, F. Melo. Helical Locomotion in a Granular Medium [J]. Phys. Rev. Lett., 2017, 119(6):068003.1-068003.5.
[15] C. Kloss, C. Goniva, A. Hager, et al. Models, algorithms and validation for opensource DEM and CFD-DEM [J]. Prog. Comput. Fluid. Dy., 2012, 12(2-3):págs. 140-152.
[16] M. Vangoe, C. Feilmayr, S. Pirker, et al. Data-assisted CFD modeling of transient blast furnace tapping with a dynamic deadman [J]. Appl. Math. Model., 2019, 73(SEP.):210-227.
[17] Kloss, Christoph. LIGGGHTS-Open Source Discrete Element Simulations of Granular Materials Based on Lammps [M]. Supplemental Proceedings, 2011, 2, 781-788.

[18] P. A. Cundall, O. D. L. Strack. A discrete numerical model for granular assemblies [J]. Géotechnique, 2008, 30(3):331-336.