Studying the Electrostatic Effects on the Dynamics of Charged Lunar Dust via Discrete Element Method

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STUDYING THE ELECTROSTATIC EFFECTS ON THE DYNAMICS OF CHARGED LUNAR DUST VIA DISCRETE ELEMENT METHOD

by

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ABSTRACT

Dust problems raise significant concerns in planetary surface exploration. The unusual behavior of the dust particles that surround the vehicle after engine cutoff has the potential to have more of an influence on surface systems than the high velocity lunar rocket plume ejecta in the landing process. A prevailing hypothesis attributes the levitation and transport of dust particles on the surface of airless bodies to the electrostatic effects and electric field. However, there is no accurate model considering the inter-particle electrostatic interactions, especially when the particles are charged by plume. This dissertation aims to understand the behavior of charged lunar regolith with a discrete element method (DEM) approach focusing on the inter-particle interactions and contact charge transfer. To accomplish this, the grain dynamics is coupled with mechanical and electrical particle interactions, and both short-range and long-range interactions between particles are incorporated. A tribo-charging model based on instantaneous collisions is adopted and validated by simulation and experimental data. Sensitivity analysis is conducted to quantify the effects of initial charge, tribo-charging, and E-field on transport of lunar dust. DEM simulations are then performed for a near realistic lunar environment that show the differences of position and velocity distributions between charged particles and uncharged particles. The results indicate that the charged dust particles have higher dispersion and wider distribution of velocity due to the electrostatic effects. This provides a possible explanation for the phenomena of the approximately 30 s dust lofting following Apollo Lunar Module landing. It is shown that tribo-charging has a more considerable effect on the dynamics of charged particles with a large amount of charge, while the change of E-field does not significantly affect the results. Furthermore, superquadrics and multi-sphere approximations are introduced as two approaches to aspherical geometry to accomplish high-fidelity simulation of lunar dust in the future.
ACKNOWLEDGMENTS

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# TABLE OF CONTENTS

LIST OF FIGURES ................................................................. vii

LIST OF TABLES ................................................................. ix

CHAPTER 1: INTRODUCTION .................................................. 1

Motivation ............................................................................. 1
Background ............................................................................. 2

CHAPTER 2: DISCRETE ELEMENT MODELING OF CHARGED LUNAR DUST DYNAMICS .................................................. 8

Discrete Element Method ....................................................... 8
Dynamics ................................................................................. 8
Integration Methods ................................................................. 11
Validation of Dynamics ............................................................. 13
Long-range Interactions: Coulomb Force ...................................... 16
Validation of Coulomb Force ..................................................... 17
Long-range Interactions: Gravitational Force ................................. 19
Validation of Gravitational Force ............................................... 20
Short-range Interactions: Contact Forces ...................................... 20
Short-range Interactions: Triboelectric Charging ............................. 23
Validation of Tribo-charging Model ............................................ 26
Aspheric Geometry Generation with Superquadrics Method ............. 32
Aspheric Geometry Generation with Multi-sphere Method ............... 35
Computational Cost Test ............................................................ 39
CHAPTER 3: INVESTIGATING ELECTROSTATIC EFFECTS ON CHARGED LUNAR DUST TRANSPORT ........................................ 41

Modifications to LIGGGHTS .................................................. 41

Sensitivity Analyses of Charged Lunar Dust Dispersion and Velocity .................................................. 43

Initial Charge ................................................................. 44

Tribo-charging ............................................................... 47

E-field ............................................................................ 53

A DEM Simulation for Charged Lunar Dust .................................................. 54

A DEM Simulation with Superquadric Particles .................................................. 59

CHAPTER 4: DISCUSSION, CONCLUSION, AND FUTURE WORK ........................................... 64

Discussion ................................................................. 64

Conclusion and Future Work .................................................. 67

LIST OF REFERENCES .......................................................... 70
# LIST OF FIGURES

1.1 Dust lofted into the region surrounding the Lunar Module after engine cutoff [49, 50]. ................................................................. 1

1.2 Schematic of the lunar surface electrostatic environment [66] ...................... 3

2.1 Model Structure ........................................................................ 8

2.2 2-Particle Case Trajectories ..................................................... 15

2.3 3-Particle Case Trajectories ..................................................... 16

2.4 Initial force (a) and time to first contact (b) as functions of varied Coulomb screening parameter, $\kappa$, during two particle electrostatic interactions ........ 18

2.5 Hertzian Contact Model [73] ..................................................... 21

2.6 Vibrating Box in LIGGGHTS ..................................................... 28

2.7 Comparison of Mean Charge Per Particle Measured in LIGGGHTS Simulation and in [32] ................................................................. 31

2.8 3 Simulations of Superquadrics with Different Shapes ......................... 34

2.9 DEM Simulation of Superquadrics in LIGGGHTS .............................. 35

2.10 Modeling of Golevka with Multi-sphere ........................................ 37

2.11 Modeling of HW1 with Multi-sphere ........................................... 38

3.1 DEM Work Flow ................................................................. 42

3.2 Sensitivity Analysis Simulation Setup ......................................... 45

3.3 Distribution of Charged Particles with/without Tribo-charging ............... 49

3.4 Dispersion of Charged Particles with/without Tribo-charging ................. 50

3.5 Distribution of Final Velocity of Charged Particles with/without Tribo-charging 51

3.6 Dispersion of Final Velocity of Charged Particles with/without Tribo-charging 52

3.7 Initial and Final Locations of Charged and Uncharged Particles ............... 55
<table>
<thead>
<tr>
<th>Section</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.8</td>
<td>Histograms of Final Positions with/without Initial Charge</td>
<td>57</td>
</tr>
<tr>
<td>3.9</td>
<td>Histograms of Final Velocities with/without Initial Charge</td>
<td>58</td>
</tr>
<tr>
<td>3.10</td>
<td>Initial and Final Locations of Charged and Uncharged Superquadric Particles</td>
<td>60</td>
</tr>
<tr>
<td>3.11</td>
<td>Histograms of Final Positions of Superquadric Particles with/without Initial Charge</td>
<td>61</td>
</tr>
<tr>
<td>3.12</td>
<td>Histograms of Final Velocities of Superquadric Particles with/without Initial Charge</td>
<td>62</td>
</tr>
</tbody>
</table>
LIST OF TABLES

2.1 Initial Conditions of 5 Simulation Trials ........................................... 14
2.2 Final Position Difference in MATLAB and LIGGGHTS .......................... 14
2.3 Initial force (no screening: \( \kappa = 0 \)) and time to first contact as functions of initial separation of two particles with 2.5 mm radii and \( \pm 10 \) nC initial charges 19
2.4 Initial force (no screening: \( \kappa = 0 \)) and time to first contact as functions of radii for two particles with 6 cm separation and \( \pm 10 \) nC initial charges .... 19
2.5 Initial force (no screening: \( \kappa = 0 \)) and time to first contact as functions of initial charges for two particles with 2.5 mm radii and 6 cm separation .... 20
2.6 Final charge as a function of coefficients of restitution and work functions of two particles with 6 mm separation, 2.5 mm radii, and \( \pm 10 \) nC initial charges . 27
2.7 Parameters Used in LIGGGHTS Simulation and in [32] ......................... 30
2.8 Parameters of 3 Superquadrics Simulations ........................................ 33
2.9 Force and Velocity of Two Particles with 6 cm Initial Separation ............ 33
2.10 Parameters of 2 Multi-sphere Simulations ........................................ 36
2.11 Run Time with Varying Conditions .................................................. 40
3.1 Particle Properties Used in Lunar Environment Simulation .................... 44
3.2 Standard Deviations of Final Position and Charge Transfer Varying Initial Charge ........................................................................................................ 46
3.3 Standard Deviations of Final Velocity Varying Initial Charge ................. 46
3.4 Standard Deviations of Final Position without Tribo-charging ............... 47
3.5 Standard Deviations of Final Velocity without Tribo-charging ............... 48
3.6 Standard Deviations of Final Position and Charge Transfer Varying E-field .. 54
3.7 Standard Deviations of Final Velocity Varying E-field .......................... 54
CHAPTER 1: INTRODUCTION

Motivation

Lunar dust is one of the principal issues in returning to the moon, which can cause serious problems for exploration activities including potential damage to spacesuits and equipment, reducing visibility on landings, and threatening astronaut health. In the “clearing” stage of Apollo landing, it took significantly longer than expected for a ballistic trajectory for visible dust surrounding the vehicle to dissipate after engine cutoff, as seen in Figure 1.1. This unusual dust behavior, which is best noted in the Apollo 14 landing video [43], has the potential to have more of an influence on surface systems than the high velocity lunar rocket plume ejecta in the landing process.

A prevailing hypothesis attributes this astronaut-witnessed unusual behavior to the accumulated charge on the particles [43, 75].

![Dust Lofting in Landing][49] ![Apollo 14 Lunar Module][50]

**Figure 1.1:** Dust lofted into the region surrounding the Lunar Module after engine cutoff [49, 50].

The goal of this dissertation is to understand the dynamics of lunar regolith with accumulated charge due to the plume and the interactions with the surrounding natural environment on the lunar surface. The outcome of the high-fidelity numerical modeling and simulation in this research
will advance our theoretical understanding of the physics behind these particulate lunar regolith interactions and the lunar dust environment.

The electrostatic dust charging and subsequent transport is a long-standing open question not only on the Moon but also on other airless bodies such as asteroids and comets, leading to potential risks to future surface exploration [75]. Thus, this dissertation will also benefit other space missions by providing a method to study the inter-particle interactions and electrostatic effects on charged dust particles.

Additionally, terrestrial industries such as mining, manufacturing, and pharmaceuticals, have investigated the electrostatic effects on dust particles and developed unique dust mitigation technologies. The electrostatic effects are a double-edged sword. The electrostatic charged powders have contributed to safety hazards during powder handling and processing in pharmaceuticals, especially on inhalation-powders [28, 78]. The electrostatic attraction can lead to inaccurate sampling in pharmaceuticals [57]. Electrostatic issues have also been noticed in Roll-to-Roll manufacturing operations and mining operations [60, 53]. Meanwhile, electrostatic effects have been employed to assess exposure to dust in primary health care [72], to remove dust on solar panels [52], and to do electrostatic powder coating in pharmaceuticals [56]. Increased understanding of the electrostatic effects on charged dust particles could lead to better control of processing and product performance. Studying the electrostatic effects on the dynamics of charged lunar dust leads to a greater understanding of dust-related standards and regulations as well as utilizing these potential solutions to lunar dust issues. This research could also assist in the development and manufacturing of dust-related products and delivery systems.

Background

The lunar surface is collisionally evolved as a result of meteoroid bombardment, thermal, and space weathering processes, which is not a static environment. The lunar regolith consists of
particles in a broad size distribution, including dust, which is usually defined as particles at the level of 100 µm and below [11]. Grains are loosed and ejected from the surface due to natural processes as well as from human activities such as lunar landers. Thus, lunar dust behavior must be adequately characterized and addressed for safe exploration and In-Situ Resource Utilization (ISRU) [68, 24].

In addition to the mechanical complexities of the lunar regolith, the plasma and electrical environment at the lunar surface contributes to the challenges to operating on the Moon. As a result of being immersed in the solar wind, the Moon develops surface charges, potential differences, and electric fields in the near-surface region, with strong variations over the course of the lunar day and night [11]. The charging currents on the lunar surface come from four main sources: photoemission of electrons, plasma electrons, plasma ions, and secondary electrons. The lunar dayside typically charges positive, while the nightside usually charges negative. However, there remain significant uncertainties in the charging processes and their variations [66]. Figure 1.2 shows the electrostatic environment in the solar wind on the lunar surface.

**Figure 1.2:** Schematic of the lunar surface electrostatic environment [66]

In this environment, dust particles accumulate charge and are strongly affected by electrostatic
forces that compete with the gravitational forces above the lunar surface, leading to unusual behavior including levitation and transport across the surface [11]. The levitation and transport of the fine components of regolith on the lunar surface has been linked to electrostatic effects and electric field, the same as on Martian and/or asteroid surfaces [11, 12, 27]. Additionally, grains in motion will be affected by mechanical and electrostatic forces resulting from effects such as tribo-charging.

A combination of experimental work and modeling is needed to build a full picture of regolith grain behavior in relevant environments, which is essential for continued lunar exploration. Experiments have been undertaken to understand grain charging with relevant materials. For instance, contact charging of lunar and Martian simulants is explored, providing useful information on relevant charging behaviors [64]. Tribochargeability of lunar dust simulants with various properties was studied experimentally [1, 18]. However, no theoretical models or simulations are produced from these work.

Lunar dust in the terminator region and in the exosphere has been specifically investigated. The levitation and transport of lunar dust in the terminator region due to intense localized electric field, plasma environment, and surface charging, has been studied for a long time including the discussion of lunar "horizon glow" phenomenon caused by sunlit [15, 74, 51]. The LADEE Lunar Dust Experiment (LDEX) is an in-situ dust detector to directly detect dust particles at the orbital altitude covering an altitude range of 3 km to 250 km in order to characterize the variability of lunar dust in the lunar exosphere by mapping the size and density distribution of dust grains [26]. The data indicated that the closer to the lunar surface, the denser the cloud is, while a strong variability exists due to the highly fluctuating nature of the electric field polarization. A dynamic fountain model for lunar dust was developed to explain the high-altitude dust observations with the charged dust particles overcoming lunar gravity and any cohesive forces [67]. A reanalysis of the Apollo 15 observations was also conducted to retrieve exospheric dust concentration as a function
of altitude and distance from the terminator [20]. However, these research only considered the natural conditions, such as solar UV, X-rays, and local electric field, and did not focus on the charged particles near the surface.

A number of models studied dust charging behavior near the surface, especially to understand natural lofting processes. Starting from the electrostatic effects on dust grains, the electric field strength required for launching dust particles from the surface is evaluated, for which they must overcome the cohesive force between grains [22]. However, significant uncertainty exists in the method of launching small dust particles, and no particle-particle electrostatic interactions are taken into account. The electrostatic dust transport on other airless bodies, such as Asteroid Eros, has been simulated with 2-D and 3-D numerical models as well [12, 27]. The dynamics of charged dust above the surfaces of airless bodies is investigated across a wide range of dust grain size and of the surface gravity to identify the lofting heights using initial conditions from recent laboratory results. These initial conditions are derived from the experiment of simulant grains charging by UV light or electron beam, and the calculation of the charge and the trajectories are based on the UV and plasma environment without inter-particle interactions [79]. An electrostatic lofting model for lunar dust based on adhesion was proposed for accelerated separation process and ballistic projection process with lunar surface charging, but the interaction force between the lofted particles is also neglected [76].

The lunar dust transport resulting from plume impingement has been simulated considering plume-plume, plume-surface interactions, and particle-particle collisions [45]. However, the dynamics of charged dust particles after the plume effect, and the electrostatic interactions are not included.

So far, the research investigating the charged lunar dust focuses on the natural levitation and the conditions required for separating from the surface, while there is currently a gap in those studying the dynamics of dust particles charged by plume and subsequently in motion. No generalized
granular dynamics model has been built that also fully takes into account electrostatic interactions.

DEM techniques have been employed to simulate regolith behavior in relevant environments, including the lunar surface [19], the 3-D axisymmetric triaxial compression of lunar regolith simulant [23], and Martian rover interactions with martian regolith [30]. In another highly relevant study, DEM techniques were also applied to investigate the erosion flux of lunar soil resulting from rocket exhaust plume [7]. More broadly, DEMs have been widely used in molecular dynamics [3, 2, 4] and have been proven very useful in granular dynamics, such as for investigating rapid granular flow [8], with the advent of modern computational power monitoring each particle’s dynamics and allowing for more realistic force models [29]. DEM was adopted for the simulation of non-smooth granular dynamics at the scale of particle rearrangements [58], and was implemented to study the particle rearrangement during powder compaction [39]. In large-scale industrial problems, DEM was also involved to investigate the transient dynamics of fracturing solids [48].

Regarding the transport of dust particles, various approaches have been taken in other works. Fracture mechanics was employed to explain lofting particulate clouds of lunar dust in low ballistic trajectories rather than individual submicron dust particles in high trajectories [38]. An integrated hybrid model including a continuum–kinetic solver, a coupled two-phase flow model, and a model for inelastic grain–grain collisions, was adopted to simulate the lunar regolith when the exhaust plume impinges on the lunar surface [45]. A full-particle particle-in-cell (PIC) model is developed to obtain plasma sheath, surface charging, and the transition of surface E-field in dust particles levitation simulation [74].

In this dissertation, a discrete element method (DEM) approach is developed to explore charged particle behavior on the lunar surface, focusing on the inter-particle interactions of the macroscopic grains, especially when lofted by plume or other mechanical interactions.
DEM techniques are highly appropriate for simulating complex lunar regolith interactions and plume dynamics, but it is also essential to include electrostatic effects to accurately model particle trajectories. The public version of the open-source Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) Improved for General Granular and Granular Heat Transfer Simulations (LIGGGHTS\(^1\)) software package provides a DEM modeling framework for granular interactions [29, 13]. The electrostatic effects have been added to the well-used LIGGGHTS DEM code to model charged particles with inter-grain interactions in the lunar environment to explain the phenomenon of the ejecta that surround a vehicle after engine cutoff [54].

The dissertation is organized as follows. Chapter 2 introduces discrete element modeling and the validation of the models in LIGGGHTS. Chapter 3 discusses the investigation of electrostatic effects on charged lunar dust transport, including sensitivity analysis and DEM simulations of spherical and non-spherical particles in near realistic lunar environment. Chapter 4 presents the discussion of results and errors, concluding remarks, and the future work.

\(^1\)LIGGGHTS\(^®\) and CFDEM\(^®\) are registered trademarks and DCS Computing GmbH is the official producer of the LIGGGHTS\(^®\) and CFDEM\(^®\) coupling software

\(^2\)LIGGGHTS\(^®\)-PUBLIC is provided under the GNU General Public License v2.0
CHAPTER 2: DISCRETE ELEMENT MODELING OF CHARGED LUNAR DUST DYNAMICS

The structure of DEM simulation is shown in Figure 2.1. This chapter will introduce the long-range and short-range interactions while the fields have been built in LIGGHTS.

Figure 2.1: Model Structure

Discrete Element Method

Dynamics

The discrete element method (DEM) is a particle-based numerical model computing the individual behaviour of each particle where the interaction of the particles is monitored contact by contact and the motion of the particles modeled particle by particle [14]. DEM provides a high-fidelity...
solution for each particle dynamics; however, it is also known to be a computationally intensive method [36].

The charged particles dynamics is modeled as a multi-body dynamical system in DEM, generally described as in Equation 2.1.

\[
m\ddot{x} = \sum F \\
I\dot{\omega} + \omega \times (I\omega) = \sum M
\]  

(2.1)

Where \( m \) is the mass, \( x \) is the position vector, \( F \) is the force, \( I \) is the moment of inertia, \( \omega \) is the angle velocity about the principal axes, and \( M \) is the torque. \( \ddot{x} \) and \( \dot{\omega} \) are assumed constant over the time step \( \Delta t \). The system can also handle externally applied forces via \( F \). The equations of translational and rotational motion apply to point-like particles. Only translational motion is considered and no rotation is included for spherical particles in this dissertation. The resulting system of second order differential equations is solved numerically mostly via low-order finite difference methods [41].

For aspherical particles, accurate determination of orientation of a particle and then the determination of angular velocity is critical [55]. The finite rotation can be described by the quaternion, which is constructed from the unit axis of rotation \( e \) and the angle of rotation \( \alpha \) around this axis, as shown in Equation 2.2.

\[
q = (q_0, q_1, q_2, q_3)^T = \cos(\alpha/2) + e\sin(\alpha/2)
\]  

(2.2)

Orientation of a non-spherical particle is usually described as a rotation of the global observer-
fixed reference frame $\mathbf{e}$ to the local body-fixed reference frame $\mathbf{\hat{e}}$. $A$ is the rotation matrix between $\mathbf{e}$ and $\mathbf{\hat{e}}$.

$$A \mathbf{e} = \mathbf{\hat{e}}, \quad A^{-1} = A^T \quad (2.3)$$

$$A = \begin{bmatrix}
1 - 2(q_2^2 + q_3^2) & 2(q_1 q_2 - q_0 q_3) & 2(q_1 q_3 + q_0 q_2) \\
2(q_1 q_2 + q_0 q_3) & 1 - 2(q_1^2 + q_3^2) & 2(q_2 q_3 - q_0 q_1) \\
2(q_1 q_3 - q_0 q_2) & 2(q_2 q_3 + q_0 q_1) & 1 - 2(q_1^2 + q_2^2)
\end{bmatrix} \quad (2.4)$$

The orientation of a particle can be updated every time step using Equation 2.5 [55].

$$q_i = \frac{1}{2} q_i \circ \omega_t \quad (2.5)$$

$$q_{i0} = (-q_{i1} \omega_x - q_{i2} \omega_y - q_{i3} \omega_z) / 2$$

$$q_{i1} = (q_{i0} \omega_x + q_{i2} \omega_z - q_{i3} \omega_y) / 2$$

$$q_{i2} = (q_{i0} \omega_y + q_{i3} \omega_x - q_{i1} \omega_z) / 2$$

$$q_{i3} = (q_{i0} \omega_z + q_{i1} \omega_y - q_{i2} \omega_x) / 2$$

$$\omega_t = A_i^{-1} \Omega_i,$$

Where $\circ$ is quaternion multiplication, $\omega_t$ is the angular velocity in the local body-fixed reference frame, and $\Omega_i$ is the angular velocity in the global observer-fixed reference frame.
The rotational motion of a particle is updated by Equation 2.6 [55].

\[
\begin{align*}
\dot{\mathbf{L}}_i &= \mathbf{T}_i, \quad \mathbf{L}_i = \mathbf{I}_i \times \mathbf{\Omega}_i, \quad \mathbf{t}_i = \mathbf{A}_i^{-1} \mathbf{T}_i = \hat{\mathbf{I}}_i \dot{\mathbf{\Omega}}_i + \mathbf{\omega}_i \times \hat{\mathbf{I}}_i \mathbf{\omega}_i \\
t_{ix} &= \hat{I}_{ix} \omega_{ix} + (\hat{I}_{iz} - \hat{I}_{iy}) \omega_{iy} \omega_{iz} \\
t_{iy} &= \hat{I}_{iy} \omega_{iy} + (\hat{I}_{ix} - \hat{I}_{iz}) \omega_{iz} \omega_{ix} \\
t_{iz} &= \hat{I}_{iz} \omega_{iz} + (\hat{I}_{iy} - \hat{I}_{ix}) \omega_{ix} \omega_{iy}
\end{align*}
\]  

(2.6)

Where \( \mathbf{L}_i \) is the angular momentum of the particle, \( \mathbf{I}_i \) is the tensor of inertia, \( \mathbf{T}_i \) is the total torque acting on a particle with respect to the particle center in the global observer-fixed reference frame, \( \hat{\mathbf{I}}_i \) is the principal tensor of inertia, and \( \mathbf{t}_i \) is the total torque acting on a particle in the local body-fixed reference frame.

**Integration Methods**

The Velocity-Verlet method is the default integration option in LIGGGHTS to perform the numerical integration which is a widely used integration method of second order as initially proposed by Cundall [14] and summarized by Kruggel [31]. In this method, the vector of position and the vector of velocity are being tracked. Velocities in the upcoming time step \( t + \Delta t / 2 \) and positions at \( t + \Delta t / 2 \), as well as the angular velocities in the upcoming time step \( t + \Delta t / 2 \) and angle vectors at \( t + \Delta t / 2 \), are calculated as in Equation 2.7.
\[ \dot{x}_{t+\Delta t/2} = \dot{x}_{t-\Delta t/2} + \left[ \Sigma F_x/m_x \right]_t \Delta t \]
\[ x_{t+\Delta t} = x_t + \dot{x}_{t+\Delta t/2} \Delta t \]
\[ (\dot{\theta}_x)_{t+\Delta t/2} = (\dot{\theta}_x)_{t-\Delta t/2} + \left[ \Sigma M_x/I_x \right]_t \Delta t \]
(2.7)
\[ (\theta_x)_{t+\Delta t} = (\theta_x)_t + (\dot{\theta}_x)_{t+\Delta t/2} \Delta t \]

The Velocity-Verlet method is time reversible, easy to implement, and memory efficient [40]. The global error of Velocity-Verlet method is of order two, similar to the midpoint method, where the value at the midpoint between two time steps is used to update the value at next time step. Different from standard Runge-Kutta method, which is used in MATLAB ode45, Velocity-Verlet integrator is symplectic. However, in Velocity-Verlet method, it is assumed that acceleration only depends on position and does not depend on velocity.

Another available option in LIGGGHTS is rRESPA, reversible Reference System Propogator Algorithm, a variant of the numerical analytical propogator algorithm (NAPA). REPSA is a multi-timescale integrator in molecular dynamics for accelerating the integration of the equations of motion for systems with both short-range and long-range forces. It was first invented for treating the problem of high frequency oscillators coupled to low frequency oscillators [70].

The gist of this method is to update the forces at different time steps, where the short-range force is computed after each time step and the long-range force is computed every \( n \) time steps. The total force \( F(x) \) can be decomposed into short-range forces \( F_s(x) \) and long-range forces \( F_l(x) \) as shown
in Equations 2.8 [71].

\[
\begin{align*}
F(x) &= F_s(x) + F_l(x) \\
F_s(x) &= S(x)F(x) \\
F_l(x) &= [1 - S(x)]F(x)
\end{align*}
\]  

(2.8)

\(S(x)\) is a switching function that switches from 1 to 0 so that \(F_s(x)\) and \(F_l(x)\) can be updated separately. This strategy could reduce the number of forces updated at each time step and thereby reduce the computing time. rRESPA is the reversible algorithm derived from RESPA [71]. In LIGGGHTS, there are \(N\) hierarchical levels for rRESPA algorithm, where level 1 is the innermost loop (shortest timestep) and level \(N\) is the outermost loop (largest timestep), so that forces can be updated with different time step sizes.

In this dissertation, Velocity-Verlet integrator is adopted since most of the functions in LIGGGHTS support it and it works well with simulation of hard particles. There are numerous challenges to incorporate realistic interactions between complex, realistic particles. Currently, grains are modeled to behave as if the entirety of the charge acts at the center of mass, such as conductors with spherical symmetry and insulators with homogeneously distributed charge.

**Validation of Dynamics**

Simulations are first conducted to validate the dynamics model with only Coulomb force in LIGGGHTS. The validation of other long-range and short-range interactions in LIGGGHTS will be introduced later in the dissertation. In these simulations, two or three particles with assigned initial velocities are run in both LIGGGHTS and MATLAB\(^1\), and the trajectories in LIGGGHTS and MATLAB are then compared. The time step size is 1 \(\mu\)s and the simulations are run for 0.2 s. The simulations in LIGGGHTS and MATLAB have the same initial conditions. For two-particle cases, the

\(^1\)MATLAB\(^®\) is a registered trademark of The MathWorks, Inc.
Table 2.1: Initial Conditions of 5 Simulation Trials

<table>
<thead>
<tr>
<th>Case</th>
<th>No. of Particles</th>
<th>Initial Velocity Relation</th>
<th>Initial velocity-1 (m/s)</th>
<th>Initial velocity-2 (m/s)</th>
<th>Initial velocity-3 (m/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2</td>
<td>zero</td>
<td>(0,0,0)</td>
<td>(0,0,0)</td>
<td>NA.</td>
</tr>
<tr>
<td>2</td>
<td>2</td>
<td>perpendicular</td>
<td>(0,0.2,0)</td>
<td>(0.2,0,0.2)</td>
<td>NA.</td>
</tr>
<tr>
<td>3</td>
<td>2</td>
<td>parallel</td>
<td>(0.2,0,0)</td>
<td>(0.4,0,0)</td>
<td>NA.</td>
</tr>
<tr>
<td>4</td>
<td>3</td>
<td>zero</td>
<td>(0,0,0)</td>
<td>(0,0,0)</td>
<td>(0,0,0)</td>
</tr>
<tr>
<td>5</td>
<td>3</td>
<td>perpendicular</td>
<td>(0,0.2,0)</td>
<td>(0.2,0,0.2)</td>
<td>(0,0,0.1)</td>
</tr>
</tbody>
</table>

Table 2.2: Final Position Difference in MATLAB and LIGGGHTS

<table>
<thead>
<tr>
<th>Case</th>
<th>Final Position Difference-1 (norm, meter)</th>
<th>Final Position Difference-2 (norm, meter)</th>
<th>Final Position Difference-3 (norm, meter)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$8.1234 \times 10^{-5}$</td>
<td>$8.1232 \times 10^{-5}$</td>
<td>NA.</td>
</tr>
<tr>
<td>2</td>
<td>$1.4808 \times 10^{-6}$</td>
<td>$1.1439 \times 10^{-6}$</td>
<td>NA.</td>
</tr>
<tr>
<td>3</td>
<td>$2.3807 \times 10^{-6}$</td>
<td>$2.5334 \times 10^{-6}$</td>
<td>NA.</td>
</tr>
<tr>
<td>4</td>
<td>$1.7350 \times 10^{-6}$</td>
<td>$2.2260 \times 10^{-6}$</td>
<td>$1.4028 \times 10^{-6}$</td>
</tr>
<tr>
<td>5</td>
<td>$9.4860 \times 10^{-7}$</td>
<td>$2.2614 \times 10^{-6}$</td>
<td>$1.5929 \times 10^{-6}$</td>
</tr>
</tbody>
</table>

particles are initially located at (0, 0, 0) m and (0.04, 0.04, 0.04) m, and assigned the initial charge of $\pm 10 \text{nC}$, respectively. For three-particle cases, the particles are initially located at (0, 0, 0) m, (0.02, 0.02, 0.02) m, and (0, 0.04, 0) m, and assigned the initial charge of $10 \text{nC}$, $-10 \text{nC}$, and $10 \text{nC}$, respectively. The following 5 cases with different sets of initial velocity, as shown in Table 2.1, are implemented.

The sets of particles start from the same initial positions in MATLAB and LIGGGHTS, respectively. The trajectories for each case from MATLAB and LIGGGHTS are plotted on the same plot, respectively. It is not hard to confirm that they match each other from the plots in Figure 2.2 and Figure 2.3. The differences in final position are recorded in Table 2.2.
Figure 2.2: 2-Particle Case Trajectories
Long-range Interactions: Coulomb Force

Electrostatic interactions between charged particles can be modeled using a basic Coulomb force, which will be repulsive or attractive based on the sign of the charge. When the particles are in a natural plasma environment, or when there are additional interactions due to the charged particles themselves, there can be an additional “screening” of these forces, typically represented by a factor related to Debye length, which is a scale of how far a charge carrier’s electrostatic effect persists [25]. Based on the local charge concentration, a target charged particle will experience a screened
Coulomb force due to the presence of other charged particles in close vicinity because in reality the long-range electrostatic effects are suppressed by the flow of particles and the effective Coulomb interaction between particles is reduced to a finite range [25, 46].

The coulomb force, $F_c$ is implemented between a pair of two particles $i$ and $j$ as in Equation 2.9.

$$F_{c,ij} = \frac{q_i q_j}{4 \pi \varepsilon_0 \varepsilon_r} \left( \frac{\kappa}{r_{ij}} + \frac{1}{r_{ij}^2} \right) e^{-\kappa r_{ij}} \hat{r}_{ij} \quad r_{ij} < r_c$$

(2.9)

where $q_i$ and $q_j$ are the charges of the two interacting particles, $r_{ij}$ is the separation between their centers of mass, $\kappa$ is the inverse of the Debye length, $\varepsilon_0$ is the permittivity of free space, and $\varepsilon_r$ is the relative permittivity of the space between the particles. To improve the computation time of the simulation, the force is assumed to be negligible if the particles are separated by a distance equal to or larger than a cut-off distance, $r_c$. While the particles have a physical size in the model, the charge is treated as if it were homogeneously distributed around the particle center of mass.

Particle and plasma characteristics $\varepsilon_r$ and $\kappa$ are user-specified constants, while the charges on the particles, $q$, are defined via initial conditions and then allowed to vary in the simulation. The special case where $\kappa$ is zero represents a completely Coulombic interaction with no screening. Use of the $\kappa$ values allows refinement for more realistic interaction values. To simplify the problem in this dissertation, $\kappa$ is set to zero and $\varepsilon_r$ is set to 1.

Validation of Coulomb Force$^2$

Initial simulations with two charged particles are conducted to evaluate the performance of the Coulomb force in LIGGGHHTS. In the benchmark case, the particles are assigned the initial charges of $\pm 10 \text{nC}$ and initially separated by 6 cm. The value of the screening parameter, $\kappa$ is varied. As

$^2$Part of this section has been published in the conference proceedings of Earth and Space 2021 [54]
shown in Figure 2.4, when the $\kappa$ term increases, the distance at which the electrostatic effects act decreases, which leads to longer times until particles contact, and the overall electrostatic force decreases. When $\kappa > 150$, the screened electrostatic force is too small to move the two particles to contact in the same simulation time. The first contact is detected at the time step where the separation between the two particles drops below the sum of their radii. A more precise contact time is then determined via interpolation between the time steps before and after the collision.

\begin{figure}[h!]
\centering
\subfloat[Initial Force vs. $\kappa$]{{
\includegraphics[width=0.4\textwidth]{initial_force.png}
}} \hspace{0.5cm}
\subfloat[Time to Contact vs. $\kappa$]{{
\includegraphics[width=0.4\textwidth]{time_to_contact.png}
}}
\caption{Initial force (a) and time to first contact (b) as functions of varied Coulomb screening parameter, $\kappa$, during two particle electrostatic interactions}
\end{figure}

Tables 2.3, 2.4, and 2.5 show the resulting initial forces and time to first contact from varying initial separation, particle radii, and initial charges, respectively. A larger initial separation distance leads to smaller initial force between particles and longer time to contact with each other. The size of particle does not affect the initial electrostatic force as it is assumed that the charge is at the center of the particle. However, a smaller size particle with less mass needs shorter time to first contact with the larger acceleration. Larger initial charges, or precisely speaking larger product of the two initial charges, lead to larger initial electrostatic force and shorter time to first contact.
Table 2.3: Initial force (no screening: $\kappa = 0$) and time to first contact as functions of initial separation of two particles with 2.5 mm radii and ±10 nC initial charges

<table>
<thead>
<tr>
<th>Separation (m)</th>
<th>Force (N) @ 1 ms</th>
<th>Contact Time (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.04</td>
<td>$5.618212 \times 10^{-4}$</td>
<td>0.083165</td>
</tr>
<tr>
<td>0.06</td>
<td>$2.496682 \times 10^{-4}$</td>
<td>0.154154</td>
</tr>
<tr>
<td>0.08</td>
<td>$1.404343 \times 10^{-4}$</td>
<td>0.238213</td>
</tr>
</tbody>
</table>

Table 2.4: Initial force (no screening: $\kappa = 0$) and time to first contact as functions of radii for two particles with 6 cm separation and ±10 nC initial charges

<table>
<thead>
<tr>
<th>Radius (mm)</th>
<th>Force (N) @ 1 ms</th>
<th>Contact Time (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Particle 1</td>
<td>Particle 2</td>
<td></td>
</tr>
<tr>
<td>1.0</td>
<td>1.0</td>
<td>$2.498537 \times 10^{-4}$</td>
</tr>
<tr>
<td>2.5</td>
<td>2.5</td>
<td>$2.496682 \times 10^{-4}$</td>
</tr>
<tr>
<td>5.0</td>
<td>5.0</td>
<td>$2.496571 \times 10^{-4}$</td>
</tr>
<tr>
<td>1.0</td>
<td>5.0</td>
<td>$2.497554 \times 10^{-4}$</td>
</tr>
</tbody>
</table>

Long-range Interactions: Gravitational Force

It is also important for physical systems considering long-range forces to include inter-particle gravitational attraction, although it is small in magnitude. LIGGGHTS does include a background gravitational field, but it omits the gravitational force between particles $i$ and $j$ as given by

$$\vec{F}_{g,ij} = G \frac{m_im_j}{r^2} \hat{r}_{ij} \quad r < r_c$$

where $G$ is the universal gravitational constant, $m_i$ and $m_j$ are the masses of the two particles, $r$ is the separation between their centers of mass, and $r_c$ is the cut-off distance at which to assume negligible interaction for numerical simplicity.
Table 2.5: Initial force (no screening: $\kappa = 0$) and time to first contact as functions of initial charges for two particles with 2.5 mm radii and 6 cm separation

<table>
<thead>
<tr>
<th>Initial Charge (nC)</th>
<th>Force (N) @ 1 ms</th>
<th>Contact Time (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>+5</td>
<td>$6.241468 \times 10^{-5}$</td>
<td>0.308285</td>
</tr>
<tr>
<td>-5</td>
<td>$2.496682 \times 10^{-4}$</td>
<td>0.154154</td>
</tr>
<tr>
<td>+10</td>
<td>$5.617892 \times 10^{-4}$</td>
<td>0.102937</td>
</tr>
<tr>
<td>-10</td>
<td>$1.872488 \times 10^{-4}$</td>
<td>0.178024</td>
</tr>
</tbody>
</table>

Validation of Gravitational Force

The inter-particle gravitational force is relatively small in current simulations compared to the electrostatic force which is the main focus of this dissertation. In a simulation of two particles with density of 2500 kg/m$^3$, radii of 2.5 mm, initial charges of $\pm 10$ nC, and initially separated by 6 cm, the gravitational force between the two particles is $4.963644 \times 10^{-16}$ N, compared to the Coulomb force of $2.496682 \times 10^{-4}$ N with the same initial conditions. Even when the initial distance is as close as 0.6 cm, the gravitational force is $4.963644 \times 10^{-14}$ N, still relatively small compared to the Coulomb force of $2.629448 \times 10^{-2}$ N at the same time. As a result, it is usually ignored in simulations. When applied to small particles affected by being in the vicinity of a much larger particle, the gravitational force will have a more pronounced effect on the motion of the particles.

Short-range Interactions: Contact Forces

When charged or uncharged particles come into contact they will experience a charge transfer that is based on variables including contact type, contact area, material properties, and particle charge state. Interactions may include brief contacts (bouncing), sticking, rolling, or contacts of multiple particles, with the area of contact, length of time in contact, and number of contacts potentially

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3Part of this section has been published in the conference proceedings of Earth and Space 2021 [54]
influencing the distribution of charge. In order to study these effects, conduction and tribo-charging are integrated with LIGGGHTS built-in Hertz contact model to produce a new contact model that accounts for electrostatics. The dissertation will only focus on the inter-particle triboelectric charging process considering the insulated properties of the lunar dust.

The particle-particle contact forces govern how particles resist interpenetration and rebound off each other in collisions. The Hertzian model is a contact model with high fidelity in LIGGGHTS, which treats the particles as an elastic material with a defined Young’s modulus and Poisson ratio [34]. Figure 2.5 shows the particle to particle contact and particle to wall interaction in Hertzian contact model.

![Hertzian Contact Model](image)

**Figure 2.5:** Hertzian Contact Model [73]

Given Young’s moduli $Y_i, Y_j$, Poisson ratio $\nu_i, \nu_j$, and coefficient of restitution $e$, Equation 2.10 is used to calculate the contact force between two granular spherical particles in this Hertzian model [21], when the distance $r$ between two particles of radii $R_i$ and $R_j$ is less than their contact distance.
\( d = Ri + Rj \). There is no force between the particles when \( r > d \).

\[
F = (k_n \delta n_{ij} - \gamma_n v_{ni,ij}) + (k_t \delta t_{ij} - \gamma_t v_{ti,ij})
\] (2.10)

The first term of the RHS of Equation (2.10) is the normal force between the two particles including a spring force and a damping force, while the second term is the tangential force including a shear force and a damping force. The limit of maximum Hertzian tangential force is governed by \( F_t \leq \mu F_n \), where \( F_t \) is the tangential force, \( F_n \) is the normal force, and \( \mu \) is the coefficient of static friction.

The coefficients in Equation 2.10 are calculated from the material properties as:

\[
\begin{align*}
k_n &= \frac{4}{3} Y^* \sqrt{R^*} \delta_n, \\
k_t &= 8G^* \sqrt{R^*} \delta_n, \\
\gamma_n &= -2\sqrt{\frac{5}{6}} \beta \sqrt{S_n m^*} \geq 0 \\
\gamma_t &= -2\sqrt{\frac{5}{6}} \beta \sqrt{S_t m^*} \geq 0 \\
S_n &= 2Y^* \sqrt{R^*} \delta_n, \\
S_t &= 8G^* \sqrt{R^*} \delta_n \\
\beta &= \frac{\ln(e)}{\sqrt{\ln^2(e) + \pi^2}} \\
1 - \nu^2 &= \frac{Y_1}{Y_1} + \frac{1 - \nu_2^2}{Y_2} \\
\frac{1}{Y^*} &= \frac{1}{2(2 - \nu_1)(1 + \nu_1)} + \frac{2(2 - \nu_2)(1 + \nu_2)}{Y_2} \\
\frac{1}{G^*} &= \frac{1}{Y_1} + \frac{1}{Y_2} \\
\frac{1}{R^*} &= \frac{1}{R_1} + \frac{1}{R_2}, \\
m^* &= \frac{1}{m_1} + \frac{1}{m_2}
\end{align*}
\] (2.11)

Where \( \delta n_{ij} \) is normal overlap distance of the i-th and j-th particles, \( \delta t_{ij} \) is tangential overlap distance, \( v_{ni,ij} \) is normal component of the relative velocity, \( v_{ti,ij} \) is tangential component of the relative velocity, \( k_n \) is elastic constant for normal contact, \( k_t \) is elastic constant for tangential contact, \( \gamma_n \) is...
viscoelastic damping constant for normal contact, $\gamma$ is viscoelastic damping constant for tangential contact, and $R^*$ is effective radius.

Short-range Interactions: Triboelectric Charging

In electrostatics, triboelectric charging is important as well as challenging with no exact model existing so far. Tribo-charging is a type of contact electrification that mostly takes place between different materials but can also happen between particles in same material with different sizes [10]. The charge amount could depend on material, size, surface roughness, temperature, and other properties.

Using the model in [25] the trajectories of triboelectrically charged particles with electrostatic forces were modelled in a commercial DEM software. The model was developed depending on a key parameter $\alpha$, which is the time constant of the charge generation. $\alpha$ was used as the main driver for the charge transfer process and determined by the experimental results, while it was specific to the materials used in those simulation and experiment. A tribo-charging model depending on contact area and work function difference in introduced in [46] to predict tribocharging in Hopper-chute flow with DEM-based simulation and experiment, where the charge transfer via tribo-charging only counts once per collision at the maximum impact time step and does not take the electric field into account. The model in [32] also depends on contact area and work function difference, but it includes the total electric field and is evaluated at each time step. In addition, the experiment of granular insulating material particles was conducted to validate the DEM numerical simulation model using in-house code [32]. It is worthwhile to mention that the latest tribo-charging model developed from the model in [46] also includes electric field [47].

It is assumed as above that the net charge on any particle is distributed homogeneously at each time step. In the model from [46], the charge transferred via triboelectric charging is a function of the work function difference between the contacting particles, the contact area, and the cut-off
distance for charge transfer. The charge transferred by triboelectric charging, $\Delta q$, is calculated as in Equation 2.12.

$$
\Delta q_{ij} = \frac{\varepsilon_0 A_{ij,\text{max}}}{z q_e} (\phi_i - \phi_j)
$$

(2.12)

where $\Delta q$ is the charge transferred between the particle $i$ and the particle $j$ during a single collision, $\varepsilon_0$ is the permittivity of free space, $A$ is the contact area, $z$ is the cut-off distance for charge transfer, $q_e$ is the charge of an electron, $\phi$ is the work function of the particle, which is the minimum energy required to extract an electron from the surface of a solid, and $q$ is the charge on the particle. In order to determine the contact area, $A$, at that time step, the Hertzian contact model described above is used, and the overlap distance in the normal direction between the two particles at the current time step, $\delta n_{ij}$, is compared with the same variable at the previous two time steps. When this distance is maximized, the contact area is the greatest, representing the moment of maximum impact.

According to the model in [32], the charge transferred by triboelectric charging, $\Delta q$, is calculated as in Equation 2.13.

$$
\Delta q_{ij,n} = \frac{\varepsilon_0 \Delta A_{ij,n}}{z q_e} \left( \phi_i - \phi_j - E_{ij,n} z q_e \frac{d_{ij}}{||d_{ij}||} \right)
$$

(2.13)

where $\Delta q$ is the charge transferred between the particle $i$ and the particle $j$ during time step $n$ to time step $n + 1$, $\varepsilon_0$ is the permittivity of free space, $\Delta A$ is the contact surface (as defined in Equation 2.14) variation between particles $i$ and $j$ during time step $n$ to time step $n + 1$, $z$ is the cut-off distance for charge transfer, $q_e$ is the charge of an electron, $\phi$ is the work function of the particle, $E_{ij,n}$ is the electric field located at the point of impact between the two particles at time
step \(n\), \(\mathbf{d}_{ij}\) is the position vector between the two particles, and \(q\) is the charge on the particle.

\[
A_{ij,n} = \pi R^* \delta n_{ij}, \quad R^* = \frac{R_i R_j}{R_i + R_j}
\]

Where \(R^*\) is the effective radius and \(\delta n_{ij}\) is the normal overlap between the particle \(i\) and the particle \(j\).

The charge transferred is only taken into account when \(\Delta A\) is positive.

The electric field at the center of a particle is derived by the Coulomb’s law and the principle of superposition [32],

\[
\mathbf{E}_i = \mathbf{E}_{\text{ext}} + \frac{1}{4\pi \varepsilon_0} \sum_{k=1}^{N} q_k \frac{\mathbf{d}_{ik}}{||\mathbf{d}_{ik}||^3}
\]

where \(\mathbf{E}_{\text{ext}}\) represents an external electric field which should be added in virtue of the principle of superposition to the electric field induced by each discrete charge \(q_k\), and \(N\) is the total number of particles in the domain. The electric field \(\mathbf{E}_{ij}\) is computed at the contact point between the colliding particles \(i\) and \(j\), which is linearly interpolated from the values of \(\mathbf{E}_i\) and \(\mathbf{E}_j\) located at each particle center.

The second term of the RHS of Equation 2.15 represents the total E-field induced by each discrete charged particle to include the influence of other charged particles nearby and is evaluated in the tribo-charging model during contact as indicated.

Although the model in Equation 2.12 [46] is good for computational efficiency as the charge transfer is evaluated less frequently, the varying electric field it does not include could be critical in the lunar dust environment. Thus, to improve the simulation accuracy, the model in Equation 2.13 [32]
is adopted where the electric field at the point of contact between the two particles are incorporated and the charge transfer is evaluated at each time step. Meanwhile, the experimental results from the same paper are used to validate the simulation results conducted in LIGGGHTS.

**Validation of Tribo-charging Model**

For validation, the tribo-charging model in Equation 2.12 with the Hertzian contact model in Equation 2.10 is first implemented with two particles to validate the functions of work function and tribo-charging added to LIGGGHTS.

The tribo-charging model in Equation 2.13 is then combined with the Hertzian contact model in Equation 2.10 to quantify the charge transfer between particles for high accuracy. Simulations with the new combined model are validated against numerical and experimental results from [32].

The simulations of two charged particles are conducted with varied parameters to demonstrate the charge transfer process based on the tribo-charging model in Equation 2.12. The cut-off distance of charge transfer is set to 250 nm as in [46]. Each pair of particles is given initial charges of $\pm 10 \text{nC}$ and different combinations of work functions in eight trials as shown in Table 2.6. They begin 0.06 m away from each other and are attracted toward the center. When the two particles have the same work function 3 eV, no charge transfer via tribo-charging occurs since the charge transferred depends on the difference between work functions. As a result, they keep their initial charges. When the two particles are assigned different work functions, charge transfer occurs. In the trial where they have work functions 10 eV and 3 eV, respectively, the largest amount of electrons flow from one particle with lower work function to the other one with higher work function since this is the combination with the biggest difference between two work functions among the four trials for each coefficient of restitution.

When the coefficient of restitution is set to the smallest allowable value of approximately 0.05,

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4Part of this section has been published in the conference proceedings of Earth and Space 2021 [54]
Table 2.6: Final charge as a function of coefficients of restitution and work functions of two particles with 6 mm separation, 2.5 mm radii, and ±10 nC initial charges

<table>
<thead>
<tr>
<th>Coefficient of Restitution</th>
<th>Work Function (eV)</th>
<th>Charge (nC)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Particle 1</td>
<td>Particle 2</td>
</tr>
<tr>
<td>0.05</td>
<td>3</td>
<td>3</td>
</tr>
<tr>
<td>0.05</td>
<td>4</td>
<td>3</td>
</tr>
<tr>
<td>0.05</td>
<td>7</td>
<td>3</td>
</tr>
<tr>
<td>0.05</td>
<td>10</td>
<td>3</td>
</tr>
<tr>
<td>0.90</td>
<td>3</td>
<td>3</td>
</tr>
<tr>
<td>0.90</td>
<td>4</td>
<td>3</td>
</tr>
<tr>
<td>0.90</td>
<td>7</td>
<td>3</td>
</tr>
<tr>
<td>0.90</td>
<td>10</td>
<td>3</td>
</tr>
</tbody>
</table>

particles remain together after the collision and the charge transfer only occurs once. When the coefficient of restitution is set to 0.90, particles bounce back after the first contact and then several bounces happen between them. Each collision has the charge transfer occurred once. As a result, the pair of particles with higher coefficient of restitution has more charges transferred via tribo-charging in the same simulation time.

To validate the tribo-charging model in Equation 2.13, a simulation of a vibrating box containing 20 g of Polyamide (PA) and 20 g of Polycarbonate (PC) is implemented in LIGGGHTS to reproduce the results of the simulation and the experiment in [32]. The results from LIGGGHTS simulation is then validated with both numerical and experimental results published in [32]. In this simulation, the neutral mixture is introduced in the vibrating box connected to the ground and vertically vibrated with an amplitude of 1 mm at a frequency of 50 Hz during 90 s before separated in a free-fall electrostatic separator and measured in a Faraday cage.

A vibrating box is set up in LIGGGHTS as shown in Figure 2.6. The particle-wall interactions are included and the wall is treated as if it is grounded.

In this numerical experiment, the vibrating box contains particles made of 2 materials, Polyamide
Figure 2.6: Vibrating Box in LIGGGHTS

(PA) and Polycarbonate (PC), with work functions of 3.9 eV and 4.2 eV, respectively [32]. The system is simulated for 90 s real world time with a time step size of 1 µs as 0.1 to 10 µs is suggested in [32] for the integration of the second Newton’s law. The cut-off distance of tribo-charging is set to 500 nm. The charge limits for PA and PC have been set to 70 pC per particle and $-190$ pC per particle, respectively, since PA tends to charge positively and PC tends to charge negatively in this experiment due to their work function difference [32]. The cut-off distance for electrostatic force is set to 2 cm. An external E-field of 100 000 V/m is also added to the charge transfer model in virtue of the principle of superposition to the electric field due to charged particles nearby.

The computation time for a 90 s simulation can be quite problematic, especially for "hard" particles with high Young’s Modulus and high coefficient of restitution, since it would be difficult to track the short contacts during one time step. To overcome that limitation, it is a common practice to adopt a lower Young’s Modulus based on the previous investigations of Young’s Modulus [37, 8]. In addition, some parameters including coefficient of restitution and coefficient of friction are not
specified [32]. Different from the spherical particles used in LIGGGHTS simulation, cylindrical particles are used in [32]. The height of the cylinder is mentioned in their preliminary work [33]. In this LIGGGHTS simulation, the densities are kept the same as in the reference, but the difference in shape leads to different mass per particle and per surface area.

However, theoretically, changing Young’s Modulus has direct influence on the contact dynamics and results in different contact forces as stated by Equation 2.11. According to Equation 2.13 and Equation 2.14, increasing radius and contact area also affects the amount of charge transferred via tribo-charging. Larger surface area generally contributes to more charge transfer. Additionally, varying the coefficient of restitution and the coefficient of friction can change the number of collisions and the contact time. As a result, the charge transfer is affected.

Thus, two simulations (Sim 1 and Sim 2) with different parameters including Young’s Modulus, coefficient of restitution, coefficient of friction and surface area within reasonable ranges are implemented to reduce the potential errors. Parameters used in LIGGGHTS simulations and in [32] including Young’s Modulus, radius, shape, etc. are summarized in Table 2.7. In Sim 1, "softer" particles with lower Young’s Modulus, low coefficient of restitution, and relatively low coefficient of friction are adopted. The radius of the spherical PA and PC particles are the same as the radius of cylindrical PA and PC particles in [32]. The same total mass is used in Sim 1 as in [32]. In Sim 2, realistic Young’s Modulus is adopted together with higher coefficient of restitution and coefficient of friction. To get the same surface area as the cylinder used in [32], the radius of PA and PC particles are increased from 1 mm and 1.25 mm to 1.41 mm and 1.63 mm, respectively. The numbers of PA and PC particles in Sim 2 are the same as in [32].

The outcome of the two LIGGGHTS simulations are plotted along with the simulation and experimental results in [32] shown in Figure 2.7. However, the unit for the average charge per particle on the plot in [32] was corrected from nC to pC. Considering the text and the results from the preliminary work [33], the unit used for the charge is pC instead of nC, which is the same as shown
Table 2.7: Parameters Used in LIGGGHTS Simulation and in [32]

<table>
<thead>
<tr>
<th>Properties</th>
<th>Sim 1</th>
<th>Sim 2</th>
<th>Used in [32]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Young’s Modulus (GPa)</td>
<td>PA=0.25, PC=0.25, Al=0.25</td>
<td>PA=2.5, PC=2.3, Al=2.5</td>
<td>PA=2.5, PC=2.3, Al=69</td>
</tr>
<tr>
<td>Coefficient of Restitution</td>
<td>PA=0.7, PC=0.65, Al=0.1, PA&amp;PC=0.5</td>
<td>PA=0.7, PC=0.65, Al=0.1, PA&amp;PC=0.9</td>
<td>Not mentioned, 0.5 - 0.9</td>
</tr>
<tr>
<td>Coefficient of Friction</td>
<td>PA=0.1, PC=0.31, Al=1.05, PA&amp;PC=0.21, PA&amp;Al=0.21, PC&amp;Al=0.21</td>
<td>PA=0.1, PC=0.31, Al=1.05, PA&amp;PC=0.9, PA&amp;Al=0.9, PC&amp;Al=0.9</td>
<td>Not mentioned</td>
</tr>
<tr>
<td>No. of Particles</td>
<td>n1=4225, n2=2038</td>
<td>n1=1877, n2=1133</td>
<td>n1=1877, n2=1133</td>
</tr>
<tr>
<td>Shape</td>
<td>Sphere</td>
<td>Sphere</td>
<td>Cylinder</td>
</tr>
<tr>
<td>Dimension (mm)</td>
<td>r1=1, r2=1.25</td>
<td>r1=1.41, r2=1.63</td>
<td>r1=1, r2=1.25, h=3</td>
</tr>
</tbody>
</table>

In the 90s simulation, the particles experience a significant amount of collisions. Charge transfer by tribo-charging happens during those contacts until the charge amount on individual particle reaches the charge limit. PC has a higher work function than PA which means it is more difficult to remove an electron from PC than from PA. As a result, PA charges positively and PC charges negatively eventually.

From the comparison, it is not hard to notice that the results from the LIGGGHTS simulations match well with the results reported in [32]. There are some discrepancies in the first 15 seconds, but when it comes closer to the end, the LIGGGHTS simulations match better to both numerical and experimental results presented in [32]. The discrepancies may result from the differences in the properties, such as shape and mass per particle, but they are within a reasonable range. This comparison validates the tribo-charging model in LIGGGHTS. The video of the simulation in LIGGGHTS named TribochargingValidation.mp4 can be found in the supplemental files.
Figure 2.7: Comparison of Mean Charge Per Particle Measured in LIGGGHTS Simulation and in [32]
Aspheric Geometry Generation with Superquadrics Method

The spherical particles are first used in the modeling and simulation in order to simplify the problem. However, the lunar dust particles are highly angular so that the specific surface area for lunar soil is nearly 8 times a sample of spheres with the same size distribution [11]. The angular nature and complex shapes not only affect the bulk mechanics of the material, but also affect the electric charge transfer by increasing surface area according to Equation 2.13.

Superquadrics is one of the two widely used approaches to represent the real complex-shaped particles with discrete element modeling [61, 16]. The superquadrics is an extension of spheres and ellipsoids, and has a good trade-off between model complexity and shape flexibility [55]. This method was first introduced by Barr [6]. The governing equation of superquadrics is as follow,

\[
f(x, y, z) = \left( \frac{x}{a} \right)^{n_1} + \left( \frac{y}{b} \right)^{n_2} + \left( \frac{z}{c} \right)^{n_1} - 1 = 0
\] (2.16)

where \(a, b, c\) are the half-lengths of the particles along its principal axes, and \(n_1\) and \(n_2\) are blockiness parameters controlling the level of edge sharpness.

The shape of superquadrics is controlled by changing the 5 shape parameters \((a, b, c, n_1, n_2)\) in Formula 2.16. When \(n_1 = n_2 = 2\), the superquadrics gives an ellipsoid. Cylinder is obtained when \(n_1 = 2\) while \(n_2 >> 2\). A box-like shape is obtained when \(n_1 >> 2\) and \(n_2 >> 2\) [55].

However, the disadvantage of the superquadric method is that this method is not applicable if the aspheric particle shape is far from ellipsoidal, cylinder-like, or box-like. In addition, the contact detection of superquadric approach could be complicated and computationally expensive.

Three simulations of superquadrics with different shapes are implemented in LIGGGHTS to evaluate the performance of the Coulomb force on non-spherical particle with parameters listed in Table
Table 2.8: Parameters of 3 Superquadrics Simulations

<table>
<thead>
<tr>
<th>Case</th>
<th>Shape</th>
<th>Density (kg/m³)</th>
<th>a (m)</th>
<th>b (m)</th>
<th>c (m)</th>
<th>n₁</th>
<th>n₂</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Cylinder</td>
<td>2500</td>
<td>0.004</td>
<td>0.004</td>
<td>0.008</td>
<td>10</td>
<td>2</td>
</tr>
<tr>
<td>2</td>
<td>Box</td>
<td>2500</td>
<td>0.004</td>
<td>0.004</td>
<td>0.008</td>
<td>10</td>
<td>10</td>
</tr>
<tr>
<td>3</td>
<td>Irregular</td>
<td>2500</td>
<td>0.004</td>
<td>0.004</td>
<td>0.008</td>
<td>3</td>
<td>2</td>
</tr>
</tbody>
</table>

Table 2.9: Force and Velocity of Two Particles with 6 cm Initial Separation

<table>
<thead>
<tr>
<th>Initial Charge (nC)</th>
<th>Mass (kg)</th>
<th>Force (N) @ 1 ms</th>
<th>Velocity (m/s) @ 1 ms</th>
</tr>
</thead>
<tbody>
<tr>
<td>+10 -10</td>
<td>1.956919 × 10⁻³</td>
<td>2.496551 × 10⁻⁴</td>
<td>1.274478 × 10⁻⁴</td>
</tr>
<tr>
<td>+10 -10</td>
<td>2.456075 × 10⁻³</td>
<td>2.496551 × 10⁻⁴</td>
<td>1.015461 × 10⁻⁴</td>
</tr>
<tr>
<td>+10 -10</td>
<td>1.620827 × 10⁻³</td>
<td>2.496555 × 10⁻⁴</td>
<td>1.538752 × 10⁻⁴</td>
</tr>
</tbody>
</table>

2.8. In each simulation, the two particles are assigned the initial charges of ±10 nC and initially separated by 6 cm. They start to move from rest and stop after particles contact. The screenshots of LIGGGHTS simulations are shown in Figure 2.8, and the results of force and velocity are recorded in Table 2.9.

Compared the results to the simulation of spherical particles in Table 2.3, the electrostatic forces for these two superquadrics are the same as the forces for spherical particles since the charge can only be assigned at the center of the particle so far. These results validate the Coulomb force on superquadric particles in LIGGGHTS when the charge is at the center of the particle.

In addition to the translational motion, rotational motion is included in simulation of superquadrics, as shown in Figure 2.9. The video of the simulation in LIGGGHTS showing irregular superquadrics with rotation named SuperquadricsSample.mp4 can be found in the supplemental files.
Figure 2.8: 3 Simulations of Superquadrics with Different Shapes
Multi-sphere is another popular approach to represent the real complex-shaped particles with discrete element modeling in addition to superquadrics [61, 16]. The multi-sphere method has been specifically adopted to yield fast numerical approximation of electrostatic forces across charged...
Table 2.10: Parameters of 2 Multi-sphere Simulations

<table>
<thead>
<tr>
<th>Case</th>
<th>Shape</th>
<th>Density (kg/m³)</th>
<th>No. of Spheres</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Golevka</td>
<td>2500</td>
<td>79</td>
</tr>
<tr>
<td>2</td>
<td>HW1</td>
<td>2500</td>
<td>64</td>
</tr>
</tbody>
</table>

bodies with orientation-dependent forces or torques on generic geometries, which has been extended from rigid body to flexible shapes [65, 42].

This section briefly introduces the generation of aspherical geometry with multi-sphere to accomplish high-fidelity simulation in the future.

In multi-sphere method, a set of prime spheres are allowed to overlap and be glued together to approximate a particle with complex shape. Theoretically, any shape can be represented by multi-sphere method [55]. However, high accuracy shape approximation requires a large number of prime spheres which could be significantly computationally expensive.

The CLUMP code provides a unified framework, where a particle morphology can be approximated using different multi-sphere generation approaches [5]. The inputs are 3-D files of the shape and the outputs are stored in formats, such as txt, used by some of the most popular DEM codes including LIGGGHTS. The code is user-friendly and the run time is quite reasonable.

Two cases of multi-sphere simulation using CLUMP are run under lunar gravity for testing. The shapes are from Asteroid Golevka and Asteroid HW1 [62, 63]. The parameters used in the simulations are listed in Table 2.10. The original shapes, approximations from CLUMP, and the screenshots in LIGGGHTS simulation are shown in Figure 2.10 and 2.11.

From the diagrams, the original shapes can be identified. Since less than 100 spheres are used for each shape, the simulation is fast and easy to run. If more prime spheres are adopted, a smoother surface and a model closer to original shape could be obtained while the computation time would
Figure 2.10: Modeling of Golevka with Multi-sphere
Figure 2.11: Modeling of HW1 with Multi-sphere
be much longer. More multi-sphere generation approaches need to be investigated, such as the method based on a modified greedy heuristic algorithm [35], the Ferrellec and McDowell method used in CLUMP [17], and the new Euclidean distance transform approach proposed in CLUMP [5]. For the next step, the particle contact model and tribo-charging model need to be updated to accommodate aspherical particles. The charge will be assigned to individual prime spheres instead of at the center of the combined particle to represent the non-uniform charge distribution on angular particles.

Computational Cost Test

The setting of the DEM simulations has been chosen balancing the performance and computational cost. A test of run time was conducted prior to the tribo-charging validation and sensitivity analysis to decide the simulation settings. All the test simulations are run with the same types of particles in the same box region for 15000 steps. The inter-particle interactions are applied. The number of particles, the time step size, the number of cores used in computing, and the cut-off distance of Coulombic interaction are varied. For each case, only one attribute is varying. Four cores are used for all the cases except the cases varying the number of cores. 6263 particles are simulated for all the cases except the cases varying the number of particles. The time step size of 1 µs is used for all the cases except the cases varying the time step size. The cut-off distance of Coulombic interaction is set to 0.1 m for all the cases except the cases varying the cut-off distance. The computational cost of each case is recorded in Table 2.11.

According to the test results, the time step size itself does not affect the run time significantly, but obviously, the smaller the time step size is, the more steps are needed to simulate particle behavior for a fixed timespan. Additionally, a smaller time step size could improve the simulation accuracy and avoid losing track of small particles. The number of particles has a relationship close to linear with the run time. Longer run time is needed to simulate more particles. The cut-off distances of forces and interactions also affect the run time. The interactions between two particles will only be
Table 2.11: Run Time with Varying Conditions

<table>
<thead>
<tr>
<th>No. of Particles</th>
<th>Run Time (s)</th>
<th>Time Step Size (µs)</th>
<th>Run Time (s)</th>
<th>No. of Cores</th>
<th>Run Time (s)</th>
<th>Cut-off (m)</th>
<th>Run Time (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>3000</td>
<td>271.034</td>
<td>1</td>
<td>1130.06</td>
<td>1</td>
<td>2883.47</td>
<td>0.006</td>
<td>35.0610</td>
</tr>
<tr>
<td>6263</td>
<td>1130.06</td>
<td>10</td>
<td>1150.63</td>
<td>4</td>
<td>1130.06</td>
<td>0.01</td>
<td>86.9012</td>
</tr>
<tr>
<td>10000</td>
<td>2955.94</td>
<td>25</td>
<td>1150.56</td>
<td>6</td>
<td>1340.66</td>
<td>0.02</td>
<td>289.766</td>
</tr>
</tbody>
</table>

The test results indicate that run with multiple cores is apparently faster than run with only one core. However, the simulation using six cores is slightly slower than the one using four cores. Thus, four cores are used in most of the simulations in this dissertation.
CHAPTER 3: INVESTIGATING ELECTROSTATIC EFFECTS ON CHARGED LUNAR DUST TRANSPORT

 Modifications to LIGGGHTS

Typically, DEM simulations focus on mechanical interactions, and neglect long-range inter-particle interactions as well as electrostatic effects.

LIGGGHTS provides a DEM modeling framework for granular interactions written in parallel C++ code [29, 13]. LIGGGHTS uses a standard second order Velocity-Verlet integration algorithm as the default integrator, solving the equations of motion and rRESPA multi-timestep integrator as another option [71]. LIGGGHTS iterates through each particle in the simulation to determine its interactions during each time step. Because the included background fields are constant, these forces may be calculated without considering the other particles in the simulations. Computing forces between particles requires iterating through all pairs of particles and is computationally intensive. If a contact is detected between two particles, the specified contact model is applied to the pair to determine the contact force. The contributions from field forces, long-range forces, and short-range forces are summed to achieve a net force on each particle from which integration can be performed to determine the motion of the system. There is no provision for inter-particle electrostatic forces and charge transfer in the public LIGGGHTS distribution.

LIGGGHTS is often implemented to solve industrial manufacturing problem, such as in application for charging system of ironmaking blast furnace [77], in analysis of the compaction of a cohesive material [59], and in simulation of magnetorheological fluids [34].

In this dissertation, the module of short-range forces is enhanced to start the exploration of charge transfer, and more importantly, long-range electrostatic and gravitational forces that are essential to exploring the behavior of charged dust grains are implemented. Both standard and screened
Coulomb potentials are integrated into the LIGGGHTS framework to provide a basis for long-range electrostatic interactions. A gravitational potential is incorporated to enable inter-grain gravitational interactions, but the inter-particle gravitational force is relatively small compared to the electrostatic force which is the main focus of the present research, and can be neglected in current simulation. The properties such as work function and electrical conductivity are incorporated to the library of available material characteristics to investigate the charge transfer between grains.

A basic flowchart of the DEM work flow in this research is shown in Figure 3.1, where \( p \) represents particle position, \( v \) represents velocity, and \( q \) represents the charge on the particle.

![Figure 3.1: DEM Work Flow](image-url)
Due to the complex shape of the lunar regolith grains, studies begin with spherical grains and proceed to non-spherical grains. The module of electrostatic interactions has already been ported from LAMMPS to LIGGGHTS [54]. The coul/cut pair style and the coul/debye pair style in LAMMPS compute the standard Coulombic interaction and the screened Coulombic interaction for molecular systems, respectively. Since the Coulombic interactions for granular systems have the same form as the Coulombic interactions for molecular systems, the code of these two pair styles has been integrated into the LIGGGHTS source code so that the inter-particle electrostatic interactions can be implemented in LIGGGHTS. Conduction and triboelectric charging were also added to the contact model in LIGGGHTS [54].

Sensitivity Analyses of Charged Lunar Dust Dispersion and Velocity

A sensitivity analysis is conducted to quantify the effects of initial charge, tribo-charging, and E-field on dispersion and velocity of lunar dust. The chemical composition of lunar dust varies across the lunar surface. One of the most widely distributed lunar soil simulant is JSC-1 [64, 11]. Defined as an industry standard simulant for education and research, JSC-1 is a low-titanium mare-like soil with a high percentage of glass comparable to Apollo 14 lunar sample 14163 [11].

In this simulation, two types of particles based on JSC-1 and lunar samples are used consisting of 50% of each type. The properties of particles are summarized in Table 3.1 [11, 44, 9]. According to Equation 2.13, work function is the driving factor of tribo-charging; however, it is difficult to be measured accurately. Thus, an estimation of work function is adopted where the two types of particles have work function of 5 eV and 5.3 eV, respectively [69].

Figure 3.2 introduces the setup of the simulation for sensitivity analysis, where 100 particles will fall for 1 s under lunar gravity in each run. The particles start from rest on a fictitious floor with the dimensions of 1 mm by 1 mm at the height of $h_0 = 0$ m. The particles are then released at the start of the simulation.
Table 3.1: Particle Properties Used in Lunar Environment Simulation

<table>
<thead>
<tr>
<th>Properties</th>
<th>P1</th>
<th>P2</th>
<th>P1&amp;P2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Young’s Modulus (MPa)</td>
<td>65</td>
<td>65</td>
<td></td>
</tr>
<tr>
<td>Poisson’s Ratio</td>
<td>0.33</td>
<td>0.33</td>
<td>0.33</td>
</tr>
<tr>
<td>Density (kg/m³)</td>
<td>1500</td>
<td>1500</td>
<td>1500</td>
</tr>
<tr>
<td>Work Function (eV)</td>
<td>5.0</td>
<td>5.3</td>
<td></td>
</tr>
<tr>
<td>Radius (µm)</td>
<td>50</td>
<td>50</td>
<td></td>
</tr>
<tr>
<td>Percentage by Number (%)</td>
<td>0.5</td>
<td>0.5</td>
<td>0.5</td>
</tr>
<tr>
<td>Coefficient of Restitution</td>
<td>0.45</td>
<td>0.45</td>
<td>0.45</td>
</tr>
<tr>
<td>Coefficient of Friction</td>
<td>0.84</td>
<td>0.84</td>
<td>0.84</td>
</tr>
</tbody>
</table>

Lunar gravity \(1.62 \text{ m/s}^{-2}\) is applied downward in z direction as in Figure 3.2. Each simulation is run for 1 s with a time step size of 1 µs. Figure 3.2b illustrates the particles in motion, where the color scale represents the amount of charge on each particle.

*Initial Charge*

According to the experiment in [64], a JSC-1 particle with a radius of 50 µm can get a charge on the order of 0.016 pC - 0.16 pC from contact charging. Thus, in order to conduct sensitivity analysis of initial charge, the initial charge is randomly assigned in uniform distributions around these values. For each case, the seed used for random number generator is the same to keep the simulation reproducible and the results comparable.

A case with no charge, no initial velocity, and no E-field is first run as a baseline in Case 1. Tribo-charging is included in all 9 cases except the baseline case. In all cases, no external E-field is applied and all particles start from rest. For each simulation, the average position is recorded with the standard deviations of the final X, Y, Z positions to represent the dispersion of the particles. The average velocity in three directions with the standard deviations of final velocity is also recorded to
Figure 3.2: Sensitivity Analysis Simulation Setup

investigate the motion of particles. The average percentage of difference between final charge and initial charge on each particle due to tribo-charging is recorded as well. The standard deviations of final position and the percentage of difference of 10 cases with varying initial charge are summarized in Table 3.2, and the standard deviations of final velocity in X, Y, Z directions are shown in
**Table 3.2:** Standard Deviations of Final Position and Charge Transfer Varying Initial Charge

<table>
<thead>
<tr>
<th>Case</th>
<th>Range of Initial Charge (pC)</th>
<th>STD of Final X (mm)</th>
<th>STD of Final Y (mm)</th>
<th>STD of Final Z (mm)</th>
<th>Average Percent of Charge Change (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>0.31412</td>
<td>0.31587</td>
<td>0.13255</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>[-6.4E-5, 6.4E-5]</td>
<td>0.31308</td>
<td>0.31009</td>
<td>0.12648</td>
<td>2.4010</td>
</tr>
<tr>
<td>3</td>
<td>[-6.4E-4, 6.4E-4]</td>
<td>0.31803</td>
<td>0.31296</td>
<td>0.13221</td>
<td>0.31812</td>
</tr>
<tr>
<td>4</td>
<td>[-6.4E-3, 6.4E-3]</td>
<td>0.5513</td>
<td>0.65907</td>
<td>0.42561</td>
<td>0.42848</td>
</tr>
<tr>
<td>5</td>
<td>[-3.2E-2, 3.2E-2]</td>
<td>1.7903</td>
<td>2.8532</td>
<td>1.9231</td>
<td>0.44867</td>
</tr>
<tr>
<td>6</td>
<td>[-6.4E-2, 6.4E-2]</td>
<td>3.5222</td>
<td>5.6161</td>
<td>3.7637</td>
<td>0.54407</td>
</tr>
<tr>
<td>7</td>
<td>[-3.2E-1, 3.2E-1]</td>
<td>15.890</td>
<td>24.765</td>
<td>11.654</td>
<td>0.36502</td>
</tr>
<tr>
<td>8</td>
<td>[-6.4E-1, 6.4E-1]</td>
<td>31.295</td>
<td>46.350</td>
<td>17.079</td>
<td>0.29656</td>
</tr>
<tr>
<td>9</td>
<td>[-3.2, 3.2]</td>
<td>146.48</td>
<td>231.96</td>
<td>65.922</td>
<td>5.8586</td>
</tr>
<tr>
<td>10</td>
<td>[-6.4, 6.4]</td>
<td>293.03</td>
<td>489.85</td>
<td>212.78</td>
<td>27.250</td>
</tr>
</tbody>
</table>

**Table 3.3:** Standard Deviations of Final Velocity Varying Initial Charge

<table>
<thead>
<tr>
<th>Case</th>
<th>Range of Initial Charge (pC)</th>
<th>STD of Final Velocity in X (mm/s)</th>
<th>STD of Final Velocity in Y (mm/s)</th>
<th>STD of Final Velocity in Z (mm/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>0.062013</td>
<td>0.059019</td>
<td>0.11282</td>
</tr>
<tr>
<td>2</td>
<td>[-6.4E-5, 6.4E-5]</td>
<td>0.059961</td>
<td>0.054621</td>
<td>0.10763</td>
</tr>
<tr>
<td>3</td>
<td>[-6.4E-4, 6.4E-4]</td>
<td>0.075525</td>
<td>0.086496</td>
<td>0.11706</td>
</tr>
<tr>
<td>4</td>
<td>[-6.4E-3, 6.4E-3]</td>
<td>0.41691</td>
<td>0.58915</td>
<td>0.45469</td>
</tr>
<tr>
<td>5</td>
<td>[-3.2E-2, 3.2E-2]</td>
<td>1.8952</td>
<td>2.8704</td>
<td>2.0224</td>
</tr>
<tr>
<td>6</td>
<td>[-6.4E-2, 6.4E-2]</td>
<td>3.7168</td>
<td>5.6748</td>
<td>3.9105</td>
</tr>
<tr>
<td>7</td>
<td>[-3.2E-1, 3.2E-1]</td>
<td>16.291</td>
<td>25.744</td>
<td>13.055</td>
</tr>
<tr>
<td>8</td>
<td>[-6.4E-1, 6.4E-1]</td>
<td>33.535</td>
<td>47.082</td>
<td>18.317</td>
</tr>
<tr>
<td>9</td>
<td>[-3.2, 3.2]</td>
<td>153.00</td>
<td>236.56</td>
<td>73.821</td>
</tr>
<tr>
<td>10</td>
<td>[-6.4, 6.4]</td>
<td>299.31</td>
<td>492.21</td>
<td>245.07</td>
</tr>
</tbody>
</table>

Table 3.3.
Table 3.4: Standard Deviations of Final Position without Tribo-charging

<table>
<thead>
<tr>
<th>Case</th>
<th>STD of X (mm)</th>
<th>Difference to Tribo-charging Cases (%)</th>
<th>STD of Y (mm)</th>
<th>Difference to Tribo-charging Cases (%)</th>
<th>STD of Z (mm)</th>
<th>Difference to Tribo-charging Cases (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.31412</td>
<td>0</td>
<td>0.31587</td>
<td>0</td>
<td>0.13255</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>0.31416</td>
<td>0.34589</td>
<td>0.31575</td>
<td>1.8233</td>
<td>0.13260</td>
<td>4.8448</td>
</tr>
<tr>
<td>3</td>
<td>0.31902</td>
<td>0.31040</td>
<td>0.31895</td>
<td>1.9128</td>
<td>0.13652</td>
<td>3.2589</td>
</tr>
<tr>
<td>4</td>
<td>0.56291</td>
<td>2.1102</td>
<td>0.69387</td>
<td>5.2790</td>
<td>0.42487</td>
<td>-0.1728</td>
</tr>
<tr>
<td>5</td>
<td>2.0713</td>
<td>15.695</td>
<td>3.0028</td>
<td>5.2417</td>
<td>1.8028</td>
<td>-6.2569</td>
</tr>
<tr>
<td>6</td>
<td>4.0412</td>
<td>14.736</td>
<td>5.9498</td>
<td>5.9404</td>
<td>3.6174</td>
<td>-3.8872</td>
</tr>
<tr>
<td>7</td>
<td>17.949</td>
<td>12.958</td>
<td>29.031</td>
<td>17.224</td>
<td>10.973</td>
<td>-5.8499</td>
</tr>
<tr>
<td>8</td>
<td>35.291</td>
<td>12.769</td>
<td>55.490</td>
<td>19.720</td>
<td>18.606</td>
<td>8.9404</td>
</tr>
<tr>
<td>9</td>
<td>173.92</td>
<td>18.732</td>
<td>268.51</td>
<td>15.756</td>
<td>96.558</td>
<td>46.475</td>
</tr>
<tr>
<td>10</td>
<td>369.40</td>
<td>26.064</td>
<td>550.84</td>
<td>12.450</td>
<td>169.02</td>
<td>-20.567</td>
</tr>
</tbody>
</table>

Tribo-charging

To evaluate the effect of tribo-charging on the dispersion of final position and distribution of final velocity of charged particles, Case 1 to 10 are re-run without tribo-charging.

Table 3.4 summarizes the comparison of the standard deviations of the final position between the cases without tribo-charging and the cases with tribo-charging. A positive value represents the standard deviation for the case without tribo-charging is larger than the one for the case with tribo-charging, and vice versa. The comparison of the standard deviations of the final velocity in three directions between the cases without tribo-charging and the cases with tribo-charging is recorded in Table 3.5. similarly, a positive value represents the standard deviation of velocity for the case without tribo-charging is larger than the one for the case with tribo-charging, and vice versa.

The average positions of particles in X, Y, Z directions with error bars are plotted on semi-log scale as shown in Figure 3.3, while the standard deviations of final X, Y, Z positions with and without tribo-charging are plotted on log-log scale versus the initial charge in Figure 3.4. The average velocities of particles in X, Y, Z directions with error bars are plotted on semi-log scale in
Table 3.5: Standard Deviations of Final Velocity without Tribo-charging

<table>
<thead>
<tr>
<th>Case</th>
<th>STD of Final Velocity in X (mm/s)</th>
<th>Difference to Tribo-charging Cases (%)</th>
<th>STD of Final Velocity in Y (mm/s)</th>
<th>Difference to Tribo-charging Cases (%)</th>
<th>STD of Final Velocity in Z (mm/s)</th>
<th>Difference to Tribo-charging Cases (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.062013</td>
<td>0</td>
<td>0.059019</td>
<td>0</td>
<td>0.11282</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>0.061991</td>
<td>3.3862</td>
<td>0.058857</td>
<td>7.7555</td>
<td>0.12091</td>
<td>3.2871</td>
</tr>
<tr>
<td>3</td>
<td>0.078378</td>
<td>3.7771</td>
<td>0.090024</td>
<td>4.0786</td>
<td>0.45537</td>
<td>0.15003</td>
</tr>
<tr>
<td>4</td>
<td>0.41792</td>
<td>0.24220</td>
<td>0.60890</td>
<td>3.3524</td>
<td>1.8998</td>
<td>-6.0628</td>
</tr>
<tr>
<td>5</td>
<td>2.0896</td>
<td>10.254</td>
<td>3.0344</td>
<td>5.7136</td>
<td>3.8510</td>
<td>-1.5212</td>
</tr>
<tr>
<td>8</td>
<td>36.767</td>
<td>9.6395</td>
<td>56.247</td>
<td>19.465</td>
<td>106.88</td>
<td>44.789</td>
</tr>
<tr>
<td>9</td>
<td>181.46</td>
<td>18.604</td>
<td>273.70</td>
<td>15.702</td>
<td>175.69</td>
<td>-28.313</td>
</tr>
<tr>
<td>10</td>
<td>376.06</td>
<td>25.642</td>
<td>558.94</td>
<td>13.556</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Figure 3.5, while the standard deviations of final velocity in X, Y, Z directions with and without tribo-charging are shown in Figure 3.6 on log-log scale.

When the initial charge is very small in the first few cases, the standard deviations of final positions vary a little. Starting from [-6.4E-4,6.4E-4] pC, the standard deviations are almost in linear relationship with the initial charge range on log-log scale for all 3 components according to Figure 3.4. Thus, more charge leads to higher dispersion of dust particles at the final moment. When the initial charge is relatively small, tribo-charging does not play a big role in the 1 s numerical experiment. However, the average percentage of charge change per particle increases as more tribo-charging happens when initial charge increases. With the increase of the initial charge, tribo-charging becomes more and more important and can contribute up to 27% of the final charge as in Case 10. Meanwhile, the difference of standard deviations of final position between cases with and without tribo-charging becomes larger with increased initial charge. The difference can be as large as 46% for Z direction and 26% for X and Y directions as shown in Table 3.4.
Figure 3.3: Distribution of Charged Particles with/without Tribo-charging
Figure 3.4: Dispersion of Charged Particles with/without Tribo-charging
Figure 3.5: Distribution of Final Velocity of Charged Particles with/without Tribo-charging
Figure 3.6: Dispersion of Final Velocity of Charged Particles with/without Tribo-charging
The standard deviations of final velocity have similar trends with the standard deviations of final position that are approximately in linear relationship with the initial charge range on log-log scale according to Figure 3.5. The increase of initial charge does not have a significant impact on the velocity in Z direction because of the lunar gravity in Z direction. The difference of standard deviations of final velocity between cases with and without tribo-charging can be as large as 44% for Z direction and 25% for X and Y directions as shown in Table 3.5.

Thus, more charge leads to higher dispersion and wider distribution of final velocity of dust particles.

**E-field**

According to the estimation of the electric field on the lunar surface [66, 11], a range of 1 V/m to 10 V/m is reasonable, although it could be as high as 1000 V/cm over the major portion of the sunlit area in the terminator region [11, 15]. The lunar surface on the dayside typically charges positive while on the nightside the surface usually charges negative [66]. Thus, varying external E-field in Z direction is applied to conduct the sensitivity analysis. The standard deviations and percentage of charge difference of 9 cases are recorded in Table 3.6, while the standard deviations of final velocity in X, Y, Z directions are recorded in Table 3.7. The initial charge is randomly assigned in uniform distribution of $-0.064 \text{ pC} - 0.064 \text{ pC}$ for all cases from Case 11 to 18. Case 6 from Table 3.2 and Table 3.3 is the starting point with the same initial charge as Case 11 to 18.

According to Table 3.6 and Table 3.7, E-field shows less impact while the inter-particle electrostatic effects are dominant.

The video of the simulation for sensitivity analysis named SA100.mp4 can be found in the supplemental files.
### Table 3.6: Standard Deviations of Final Position and Charge Transfer Varying E-field

<table>
<thead>
<tr>
<th>Case</th>
<th>E-field (V/m)</th>
<th>STD of Final X (mm)</th>
<th>STD of Final Y (mm)</th>
<th>STD of Final Z (mm)</th>
<th>Average Percent of Charge Change (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>6</td>
<td>0</td>
<td>3.5222</td>
<td>5.6161</td>
<td>3.7637</td>
<td>0.54407</td>
</tr>
<tr>
<td>11</td>
<td>4</td>
<td>4.0186</td>
<td>6.1608</td>
<td>3.4054</td>
<td>0.58652</td>
</tr>
<tr>
<td>12</td>
<td>-4</td>
<td>3.7559</td>
<td>6.3157</td>
<td>3.6140</td>
<td>0.54264</td>
</tr>
<tr>
<td>13</td>
<td>10</td>
<td>3.6670</td>
<td>6.2727</td>
<td>3.5960</td>
<td>0.53621</td>
</tr>
<tr>
<td>14</td>
<td>-10</td>
<td>3.7741</td>
<td>5.8906</td>
<td>3.9304</td>
<td>0.51379</td>
</tr>
<tr>
<td>15</td>
<td>50</td>
<td>3.7823</td>
<td>6.3405</td>
<td>3.7041</td>
<td>0.41598</td>
</tr>
<tr>
<td>16</td>
<td>-50</td>
<td>3.8946</td>
<td>5.5813</td>
<td>3.8550</td>
<td>0.58022</td>
</tr>
<tr>
<td>17</td>
<td>100</td>
<td>3.8351</td>
<td>6.2850</td>
<td>3.6382</td>
<td>0.58337</td>
</tr>
<tr>
<td>18</td>
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<td>3.5144</td>
<td>6.0565</td>
<td>3.1784</td>
<td>0.54282</td>
</tr>
</tbody>
</table>

### Table 3.7: Standard Deviations of Final Velocity Varying E-field

<table>
<thead>
<tr>
<th>Case</th>
<th>E-field (V/m)</th>
<th>STD of Final Velocity in X (mm/s)</th>
<th>STD of Final Velocity in Y (mm/s)</th>
<th>STD of Final Velocity in Z (mm/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>6</td>
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<td>3.7168</td>
<td>5.6748</td>
<td>3.9105</td>
</tr>
<tr>
<td>11</td>
<td>4</td>
<td>4.0674</td>
<td>6.2355</td>
<td>3.5878</td>
</tr>
<tr>
<td>12</td>
<td>-4</td>
<td>3.8573</td>
<td>6.4037</td>
<td>3.7293</td>
</tr>
<tr>
<td>13</td>
<td>10</td>
<td>3.7897</td>
<td>6.3287</td>
<td>3.8685</td>
</tr>
<tr>
<td>14</td>
<td>-10</td>
<td>3.7605</td>
<td>5.9912</td>
<td>4.1722</td>
</tr>
<tr>
<td>15</td>
<td>50</td>
<td>3.8627</td>
<td>6.3755</td>
<td>3.8617</td>
</tr>
<tr>
<td>16</td>
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<td>3.9111</td>
<td>5.6259</td>
<td>4.0962</td>
</tr>
<tr>
<td>17</td>
<td>100</td>
<td>3.8340</td>
<td>6.3155</td>
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</tr>
<tr>
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<td>3.5355</td>
<td>6.1053</td>
<td>3.5239</td>
</tr>
</tbody>
</table>

A DEM Simulation for Charged Lunar Dust

In this section, a scenario is present where all the aforementioned forces are combined to produce a near realistic simulation in the lunar environment. In the sensitivity analysis, the effects of initial charge, tribo-charging, and E-field are isolated. The DEM simulation in this section is conducted under the influence of all of them with more particles for a longer simulation time.
In this simulation, 500 particles are simulated. The properties of the particles are the same as in Table 3.1. The contact model in Equation 2.11 combined with Coulomb force in Equation 2.9 and the triboelectric charge transfer model in Equation 2.13 is applied in the simulation of lunar dust particle transport. The values of initial charge and E-field are picked based on the sensitivity analysis. Lunar gravity $1.62 \text{ ms}^{-2}$ is applied downward in $z$ direction while a E-field of $4 \text{ V/m}$ is applied in the opposite direction. In this case, the initial charge is assigned randomly in the uniform distribution of $-0.64 \text{ pC} - 0.64 \text{ pC}$ as in Case 8. The simulation starts at the height of $h_0 = 0 \text{ m}$ where all the particles lying or piling up on a floor with the dimensions of $2 \text{ mm} \times 2 \text{ mm}$. After being released from rest, the particles are falling instantly. The simulation runs for $2 \text{ s}$ real time with a time step size of $1 \mu\text{s}$.

The 3-D plot of the initial and final locations of particles with initial charge and of particles without charge is shown in Figure 3.7.

![Figure 3.7: Initial and Final Locations of Charged and Uncharged Particles](image)

The histograms of final X, Y, Z positions of the case initially charged compared to the case without
initial charge are shown in Figure 3.8 and the histograms of final velocity in X, Y, Z directions are shown in Figure 3.9.

The 3-D plot directly shows the comparison of charged particles and uncharged particles. For the uncharged case, the initial and final locations are seen as two dots (in blue and black, respectively) on the plot since all the particles are close to each other. For the case with assigned initial charge, the initial locations are shown in blue which are at the same location as the uncharged case, while the red dots represent the final locations of the spread out particles. According to the plot, the particles with initial charge shown in red are hovering around the group of particles without initial charge shown in black (where the purple arrow is pointing to) at the final moment.

As shown in Figure 3.8c, charged particles have higher dispersion of final Z position than uncharged particles, the same as in the histograms of final X, Y positions shown in Figure 3.8a and Figure 3.8b, respectively. Without initial charge, the final X positions stay within a range of $-1.7940 \text{ mm}$ to $2.2162 \text{ mm}$, the final Y positions stay within a range of $-3.0819 \text{ mm}$ to $2.3926 \text{ mm}$, and the final Z positions stay within a range of $-3241.4 \text{ mm}$ to $-3237.7 \text{ mm}$. When initially charged, the final X positions are in a range of $-386.93 \text{ mm}$ to $670.68 \text{ mm}$, the final Y positions are in a range of $-448.59 \text{ mm}$ to $543.06 \text{ mm}$, and the final Z positions are in a range of $-3625.0 \text{ mm}$ to $-3143.6 \text{ mm}$. The particles are more widely distributed with initial charge. This result is consistent with the 3-D plot.

According to Figure 3.9, charged particles have wider distribution of final velocity in X, Y, Z directions than uncharged particles. Without initial charge, the final velocities in X direction stay within a range of $-0.42201 \text{ mm/s}$ to $0.63312 \text{ mm/s}$, the final velocities in Y direction stay within a range of $-1.0659 \text{ mm/s}$ to $0.72132 \text{ mm/s}$, and the final velocities in Z direction stay within a range of $-3240.7 \text{ mm/s}$ to $-3238.9 \text{ mm/s}$. When initially charged, the final velocities in X direction are in a range of $-193.39 \text{ mm/s}$ to $335.21 \text{ mm/s}$, the final velocities in Y direction are in a range of $-224.21 \text{ mm/s}$ to $271.32 \text{ mm/s}$, and the final velocities in Z direction are in a range of
Figure 3.8: Histograms of Final Positions with/without Initial Charge
Figure 3.9: Histograms of Final Velocities with/without Initial Charge
−3435.3 mm/s to −3191.9 mm/s. The charged particles can gain high velocity compared to the uncharged particles.

The electrostatic effects apparently affect the distributions of final position and final velocity of charged dust particles. The video of the first 1 s simulation in LIGGGHTS named DEM500.mp4 can be found in the supplemental files.

A DEM Simulation with Superquadric Particles

After the DEM simulation of spherical particles is successfully implemented, a DEM simulation of non-spherical particles is conducted in LIGGGHTS with inter-particle electrostatic interactions. The default contact model for superquadrics in LIGGGHTS is combined with Coulomb force in Equation 2.9, while charge transfer is not included in the simulation of superquadrics.

In this simulation, 500 superquadric particles are simulated in a near realistic lunar environment. The properties of the particles are the same as in Table 3.1 except the dimensions. The irregular shaped particles have the dimensions of a = 50 µm, b = 50 µm, c = 50 µm, n1 = 3, n2 = 2, so that they are on the same scale as the spherical particles. The assigned initial charge and E-field are the same as applied in the simulation of 500 spherical particles, and lunar gravity 1.62 ms$^{-2}$ is applied downward in z direction. The simulation starts at the height of $h_0 = 0$ m where all the particles lying or piling up on a floor with the dimensions of 20 mm by 20 mm. After being released from rest, the particles fall instantly. The simulation runs for 2 s real time with a time step size of 1 µs.

The 3-D plot of the initial and final locations of particles with initial charge and of particles without charge is shown in Figure 3.10.

The histograms of final X, Y, Z positions of the case initially charged compared to the case without initial charge are shown in Figure 3.11 and the histograms of final velocity in X, Y, Z directions are shown in Figure 3.12.
From the 3-D plot, the initial and final locations are seen as two horizontal planes (in blue and black, respectively) for the uncharged case. All the particles start from rest and stay close to each other in a free fall under lunar gravity. For the case with assigned initial charge, the initial locations are shown in blue which are at the same location as the uncharged case, while the red dots represent the final locations of the spread out charged particles. According to the plot, the particles with initial charge shown in red are hovering around the group of particles without initial charge shown in black at the final moment.

Compared to the uncharged case where most of the particles stopped at the same height, the charged particles may stop at different heights after the fall. The uncharged particles have almost the same distributions of final X and Y positions as the distributions of initial X and Y positions. However, as shown in Figure 3.11, charged particles have much higher dispersion of final X, Y, Z positions than uncharged particles. Without initial charge, the final X positions stay within a range of $-9.8572$ mm to $9.9101$ mm, the final Y positions stay within a range of $-9.7809$ mm to

**Figure 3.10:** Initial and Final Locations of Charged and Uncharged Superquadric Particles
(a) Histogram of Final X Position

(b) Histogram of Final Y Position

(c) Histogram of Final Z Position

**Figure 3.11:** Histograms of Final Positions of Superquadric Particles with/without Initial Charge
Figure 3.12: Histograms of Final Velocities of Superquadric Particles with/without Initial Charge
9.8536 mm, and the final Z positions stay within a range of \(-3240.0\) mm to \(-3239.9\) mm. When initially charged, the final X positions are in a range of \(-149.12\) mm to \(178.68\) mm, the final Y positions are in a range of \(-163.08\) mm to \(134.35\) mm, and the final Z positions are in a range of \(-3296.8\) mm to \(-3152.5\) mm. This result is consistent with the 3-D plot.

According to Figure 3.12, charged particles have wider distribution of final velocity in X, Y, Z directions than uncharged particles. Without initial charge, the final velocities in X direction and in Y direction stay as 0, and the final velocities in Z direction are \(-3240.0\) mm/s. When initially charged, the final velocities in X direction are in a range of \(-78.145\) mm/s to \(85.770\) mm/s, the final velocities in Y direction are in a range of \(-78.848\) mm/s to \(67.294\) mm/s, and the final velocities in Z direction are in a range of \(-3302.0\) mm/s to \(-3195.3\) mm/s. The particles can gain high velocity with initial charge.

The electrostatic effects apparently affect the distributions of final position and final velocity of charged superquadric dust particles. The results of position and velocity with superquadric particles are similar to the results with spherical particles. The video of the simulation with 500 superquadric particles in LIGGGHTS named Superquadrics500.mp4 can be found in the supplemental files.

To accomplish high-fidelity simulation in the future, the particle contact model with tribo-charging needs to be updated to accommodate aspherical particles. The approximations of particles with non-uniform charge distributions will be investigated.
CHAPTER 4: DISCUSSION, CONCLUSION, AND FUTURE WORK

Discussion

The simulations show that the dust particles have higher dispersion and wider distribution of final velocity when they are charged due to electrostatic effects. According to the sensitivity analysis, the standard deviations of final position increase with increasing initial charge. The standard deviations are almost in linear relationship with the range of initial charge on log-log scale for all X, Y, Z components except when the initial charge is very small. More charge also leads to wider distribution of final velocity of dust particles. The standard deviations of final velocity in all three directions are approximately in linear relationship with the initial charge range on log-log scale and are increasing with the increased initial charge. The dust particles can spread out widely and gain high velocity when they are charged. Although the average position and velocity do not significantly change with varying initial charge, the standard deviations vary significantly. When the range of initial charge increases from 0 to [-6.4, 6.4] pC with tribo-charging turned on, the standard deviation of X position can increase from 0.31412 mm to 293.03 mm, the standard deviation of Y position can increase from 0.31587 mm to 489.85 mm, and the standard deviation of Z position can increase from 0.13255 mm to 212.78 mm. The standard deviation of velocity in X direction increases from 0.062013 mm/s to 299.31 mm/s, the standard deviation of velocity in Y direction increases from 0.059019 mm/s to 492.21 mm/s, and the standard deviation of velocity in Z direction increases from 0.11282 mm/s to 245.07 mm/s. For the cases without tribo-charging, the standard deviation of X position increases from 0.314 12 mm to 369.40 mm, the standard deviation of Y position increases from 0.31575 mm to 550.84 mm, and the standard deviation of Z position increases from 0.13255 mm to 169.02 mm. With the increase of initial charge, the standard deviation of velocity in X direction can increase from 0.061 991 mm/s to 376.06 mm/s, the standard deviation of velocity in Y direction increases from 0.058 857 mm/s to 558.94 mm/s, and the
standard deviation of velocity in Z direction increases from 0.11282 mm/s to 175.69 mm/s. It is worth noting that the X and Y components are in uniform distributions of a 1 mm range initially and almost all the particles start at the same height, thus the standard deviations of final position are considerable which can be up to 550 mm for one direction with an increase of three orders of magnitude, according to Table 3.4. The velocity in Z direction does not significantly change due to the lunar gravity in Z direction. Although all the particles start from rest, the standard deviations of final velocity can be as high as 558 mm/s in one direction with an increase of two orders of magnitude, according to Table 3.5.

Meanwhile, the impact of tribo-charging increases with more initial charge. With the increase of initial charge, tribo-charging can contribute up to 27% of the final charge and the difference of standard deviations of final position between cases with and without tribo-charging can be as large as 46% for Z direction and 26% for X and Y directions. The difference of standard deviations of final velocity between cases with and without tribo-charging can be as large as 44% for Z direction and 25% for X and Y directions. However, the results indicate that the E-field does not play a significant role in particles dispersion and in final velocity distribution while the inter-particle electrostatic effect is dominant. There is not too much change in the standard deviations of final position and of final velocity with varying E-field. When the E-field varies from $-100$ V/m to 100 V/m, the standard deviation of X position stays within a range from 3.5144 mm to 4.0186 mm, the standard deviation of Y position stays within a range from 5.5813 mm to 6.3405 mm, and the standard deviation of Z position stays within a range from 3.1784 mm to 3.9304 mm, according to Table 3.6. Similarly, the standard deviation of velocity in X direction is within a range from 3.5355 mm/s to 4.0674 mm/s, the standard deviation of velocity in Y direction is within a range from 5.6259 mm/s to 6.4037 mm/s, and the standard deviation of velocity in Z direction is within a range from 3.5239 mm/s to 4.1722 mm/s, according to Table 3.7.

In the DEM simulation of 500 spherical particles for 2 s, the 3-D plot and histograms, as shown
in Figure 3.7, 3.8, and 3.9, indicate that the charged particles are hovering around the uncharged particles while the uncharged particles stay close to each other falling under lunar gravity. Dust particles spread out and are moving at different speeds after they are initially charged. The charged particles have wider distributions of final position and of final velocity compared to the uncharged particles that have almost same distributions as they had initially.

A DEM simulation of 500 non-spherical particles was conducted later. Superquadrics are used to model the angular complex-shaped lunar regolith. Rotation has been considered in the simulation although no rotation of spherical particles is included. The results are similar to the results of the simulation with spherical particles since the charge is still assigned at the center of the particle. The contact model and charge transfer model need to be modified to satisfy the requirements of simulating irregular-shaped particles with non-uniform charge distribution on individual particle, and the rotation could have an influence on the results. Multi-sphere method is another approach to model complex-shaped lunar regolith that the charge could be assigned at different parts of a combined particle in the future work.

In the sensitivity analysis and the DEM simulations in the lunar environment, the range of initial charge is relatively small and derived from a contact charging only experiment [64]. In the real world, dust particles could get much more charge in the plasma environment due to rocket plume when perturbed by lunar landers. In addition, the particles in the simulation started from rest while the charged particles may have initial velocity due to the impingement of rocket exhaust on the lunar surface. Spherical particles are first used in the simulation to simplify the problem, while most of the real lunar regolith is highly angular for which the specific surface area is nearly 8 times a sample of spheres with the same size distribution [11]. The increased surface area with complex shapes could lead to more charge on the individual particles. As a result, electrostatic effects and tribo-charging could have a more significant effect on real lunar dust. The density used in the simulation is the bulk density of lunar regolith taking into account the porosity [11]. The
individual particle density should be higher than the bulk density, which leads to more mass of each particle in reality. Finally, the simulations are only run for 1 s or 2 s. The effect could be more noticeable in a longer time.

In this dissertation, a discrete element method (DEM) approach incorporating inter-particle interactions and charge transfer is developed and successfully implemented to model and simulate the electrostatic effects on the dynamics of lunar dust particles when they are charged by plume or other mechanical interactions. According to the sensitivity analysis and DEM simulations, charged particles can be hovering around uncharged particles and moving at various speeds, while uncharged particles stay close after falling under lunar gravity. The particles can spread out and gain high velocity when they are charged due to the electrostatic effects. With increase of initial charge, the charged particles have wider distributions of final position and of final velocity, and tribo-charging becomes more and more important for dust particle transport. When varying E-field, the distributions of final position and of final velocity do not change significantly.

A large-scale simulation with high-performance computing could be the next step to better investigate the dispersion and velocity of a large number of charged dust particles for a longer time, for which more computational power is required. However, for longer time simulations, the accumulated errors from computation should be considered, especially with particles on the micrometer scale.

Conclusion and Future Work

With limited knowledge of the real lunar environment, this work aims to advance our understanding of the electrostatic effects on the dynamics of charged dust particles in the lunar environment. The outcome of this research contributes to a comprehensive picture of the electrostatic granular mechanics required for the safety and success of future lunar landing missions, and also prepares the future space missions for the dust problems. A DEM approach is developed to investigate the
dynamics of charged dust particles on the lunar surface, focusing on their inter-particle interactions and contact charge transfer. This model of dust particle dynamics includes both short-range and long-range interactions between spherical particles. A tribo-charging model based on instantaneous collisions between particles is adopted and validated by comparing the simulation results to existing simulation and experimental data. Improvements have been made to LIGGGHTS to support the modified Hertz contact model incorporating the tribo-charging model. Validation is implemented for the added forces and charge transfer models in addition to the basic dynamics prior to more complex scenarios. Sensitivity analysis is conducted to evaluate the effects of initial charge, tribo-charging, and E-field on the dispersion and velocity of lunar dust. DEM simulations of 500 lunar dust particles for 2 s are implemented with aforementioned forces and charge transfer to more clearly show the effects of electrostatics on charged particles in a near realistic lunar environment. According to the simulations, the charged dust particles can be hovering compared to the uncharged particles that stay close under lunar gravity. The charged particles can fall slower than the uncharged particles due to electrostatic effects. Dust particles have a high dispersion of position and also gain high velocity when charged by rocket plume or other mechanical interactions. The dispersion in position and the high velocity of the charged dust particles due to electrostatic effects become more apparent with increased initial charge, and tribo-charging plays a more important role in the dynamics of charged particles with a large amount of charge. However, the change of E-field does not have a significant effect.

In this dissertation, discrete element modeling is effectively and efficiently implemented to model and simulate the electrostatic effects on the dynamics of lunar dust particles when they are charged and subsequently in motion. The outcome of simulation provides a potential explanation for the phenomena of the approximately 30 s dust hovering after engine cut-off following Apollo Lunar Module landing. The modeling and simulation techniques used in this dissertation can be utilized for studying the inter-particle interactions on dust particles in other environments and thus benefit future space missions.
To accomplish high-fidelity simulation in the future, aspherical geometries with non-uniform charge distributions on particles will be further investigated. More accurate estimations of initial conditions such as initial charge and initial velocity, and properties including individual particle density will be considered. Other factors such as screened electrostatic force and cohesion could also be incorporated.
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