

ABSTRACT

Title of Dissertation: **ROLE OF MAGNETIC FORCES
ON REGOLITH BEHAVIOR ON METALLIC ASTEROIDS
WITH A RESIDUAL MAGNETIC FIELD**

Anmol Sikka
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Dissertation Directed by: **Professor Christine M. Hartzell**
Department of Aerospace Engineering

We have visited and observed various traditional (stony) asteroids to study the origin and evolution of terrestrial planets. Recently, the OSIRIS-REx spacecraft returned samples from the asteroid Bennu. These missions and studies have shown that stony asteroids are rubble-pile structures held together by self-gravity and cohesion. This cohesive force among regolith grains influences the geological and morphological features on asteroids' surfaces.

Magnetic fields have also been detected on asteroids such as Braille and Gaspra. While these detections were indirect, the Psyche mission is the first to carry a magnetometer onboard. The spacecraft will detect the potential magnetic field on the metallic asteroid Psyche. It is one of the most unique objects in the solar system, as its main constituents are Iron and Nickel. The leading theory is that Psyche is a protoplanet - the building block of planets. Researchers argue that a magnetic field would be locked into the asteroid during the cooling period post-formation. Studying such M-type asteroids provides insight into planetary formation.

The presence of a magnetic field on Psyche would have significant implications for the behavior of the surface regolith. When placed in a uniform magnetic field, paramagnetic particles experience a mutual force. Therefore, the regolith on metallic asteroids will experience an additional magnetic cohesion. Magnetic forces could influence mass-wasting processes, such as avalanching, which shape the asteroid's surface. Understanding these processes is crucial for interpreting the geological features observed by the Psyche mission and for planning future missions to metallic asteroids, including potential sample return and mining activities. In this dissertation, we investigate the role of magnetic forces in regolith behavior on metallic asteroids with residual magnetic fields.

First, we develop an empirical model for the magnetic force between paramagnetic particles in a uniform magnetic field. We compared various models for the magnetic force existing in the literature. The dipole-dipole model is the most commonly used model for magnetic force, but it is only accurate for particles that are far apart. We find that the dipole-dipole model significantly underestimates the magnetic force when particles are in close proximity, which is the case for regolith grains on asteroid surfaces. We implemented a Spherical Harmonics Approximation (SHA) model for magnetic force, which provides the exact solution for the two-particle case. Using the SHA model, we generated data for the magnetic force between two particles for a range of particle sizes and magnetic field strengths. We then developed an empirical model of magnetic force using a polynomial fit to the SHA data. This empirical model provides a more accurate representation of magnetic forces for computations such as the magnetic bond number, enabling comparisons of forces between regolith grains on small bodies.

Second, we implemented a magnetic force model in LIGGGHTS, an open-source Discrete Element Method (DEM) software, to simulate regolith behavior on metallic asteroids. The model uses the Mutual Dipole Model (MDM) for far-field interactions, and closer-range interactions are calculated using the Spherical Harmonics Approximation (SHA). We also developed a characteristic magnetic time

step for DEM simulations to ensure numerical stability while maintaining accuracy. This inclusion model implementation was validated for two-, three-, and eight-particle chains, as per data available in the literature. We then performed avalanching simulations with steel balls to validate the model against experimental data for the angle of repose with varying magnetic field strengths. All three flow regimes (granular, correlated, and plastic) were observed in the simulations, and the angle of repose and surface roughness trends were consistent with experimental data. These validations confirmed that our implementation of magnetic forces in DEM simulations is accurate and results in the first experimental validation of magnetic forces in granular simulations.

Finally, we performed avalanching simulations of regolith on 16-Psyché, varying the magnetic field strength and the composition of the regolith grains. We find that magnetic forces can significantly influence the angle of repose and the final settled configuration of the regolith after an avalanche. At higher magnetic field strengths, the regolith becomes plastic, potentially leading to steeper slopes and more stable regolith on Psyche's surface. The simulations showed several interesting characteristics of the flow, including unstable, steep cliffs, regolith grains forming chains, and the formation of hanging clusters of regolith. These results suggest that magnetic forces could play a significant role in shaping the surface features of metallic asteroids, and these findings will be crucial for interpreting the data from the Psyche mission and for planning future missions to metallic asteroids.

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WITH A RESIDUAL MAGNETIC FIELD

by

Anmol Sikka

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Advisory Committee:

Professor Christine M. Hartzell, Chair/Advisor
Professor Daniel Lathrop, Dean's Representative
Professor Raymond Sedwick
Professor Tam Nguyen
Professor Alban Sauret

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Preface

Humans have gone to the Moon, and we've sent robotic spacecraft to investigate other rocky planets (Mercury, Venus, Mars), gas and ice giant planets (Jupiter, Saturn, Uranus, Neptune), and icy asteroids and moons (Ceres, Enceladus, Europa, and a couple of comets), but there is one category of solar system object that we have never investigated: the small category of asteroids that we think may be made primarily of metal. Earth's core and the cores of the other rocky planets are metal.

Earth's core is also the source of our magnetic field, the field that may help protect our atmosphere and keep our planet habitable. Metal is clearly a fundamental building block of our habitable planet. But we will never see our own core. To see a metallic world, we think we need to go to Psyche. We won't know with certainty until we get there whether Psyche is a part of a planetesimal core, but Psyche is the only large asteroid in our solar system.

- Lindy Elkins-Tanton in 'A Portrait of the Scientist as a Young Woman, A Memoir'

Dedication

To all the pioneers of space science and technology in India.

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Thanks to my family (Mumma, Papa, Nani Ma, Harshit, Ayushi) for supporting me throughout my life. Mom and Dad, thanks a lot for providing for me and still caring for me from a million miles away. Harshit, thanks for being the ‘elder’ brother and taking care of everything back home so that I can pursue my dreams on the other side of the world. Ayushi, I can stop worrying about my younger brother now that I know he has a constant companion in you. Nani Ma, thank you for your continued

blessings and for being the tech-savvy grandmother who would call me even when I didn't. Thanks also to my Nana Ji for his heavenly blessings and for making me love mathematics as a child. Dadi Ma and Dada Ji, thank you for raising me to be the empathetic and independent person I am. I hope you are proud in heaven. Finally, to my extended family, thanks for making me feel at home whenever I visited and for forgiving me for missing all the important events in everyone's life.

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List of Abbreviations

ALMA	Atacama Large Millimeter/submillimeter Array
DEM	Discrete Element Model/Method
EPSD	Elastic-Plastic Spring Dashpot
FDM	Fixed Dipole Model/Method
FVM	Finite Volume Method/Method
LAMMPS	Large-scale Atomic/Molecular Massively Parallel Simulator
LIGGGHTS	LAMMPS Improved for General Granular and Granular Heat Transfer Simulations
MDM	Magnetic Dipole Model/Method
MRF	Magnetorheological Fluid
NASA	National Aeronautics and Space Administration
SH	Spherical Harmonics
SHA	Spherical Harmonic Approximation
SJKR	simplified JKR - Johnson-Kendall-Roberts
SSDEM	Soft-Sphere Discrete Element Model/Method

Chapter 1: Introduction

M-type asteroids are a class of asteroids that are thought to be composed primarily of metals based on their spectral properties. 16-Psyche is the largest known M-type asteroid and is the target of NASA's upcoming Psyche mission, which aims to explore its surface and composition in detail [7]. The Psyche asteroid is hypothesized to be the exposed metallic core of a planetesimal that was stripped of its outer layers by collisions during the early solar system [8]. This theory is supported by its high density, radar albedo, and spectral characteristics that suggest a composition rich in iron and nickel [9]. Such a planetary body provides a unique opportunity to study the cores of differentiated bodies that are otherwise inaccessible and to gain insights into the processes that shaped the early solar system. Among the various science investigations planned for the Psyche mission, the spacecraft will conduct magnetometric analysis of the asteroid using a magnetometer onboard [10] to gain insights into the history of the dynamo that powered its magnetic field.

A prehistoric dynamo on planetesimals like 16-Psyche would have locked in remanent magnetization into the cooling material in the solar plasma environment [11]. Modeling efforts suggest that the surface magnetic fields on 16-Psyche could have been as high as $200 \mu\text{T}$ [12]. Atacama Large Millimeter/submillimeter Array (ALMA) observations of 16-Psyche have revealed a heterogeneous surface, indicative of a collisionally evolved surface with regolith of varying grain sizes [13]. This remanent magnetization could lead to significant magnetic cohesion between regolith particles on the

surface of 16-Psyche. We know that cohesion plays a crucial role in the morphology and surface processes on small bodies [14]. On metallic bodies with remanent magnetization, magnetic cohesion can increase net cohesion, thereby influencing morphology. For example, magnetic cohesion could lead to steeper slopes and more stable surface features on 16-Psyche than on non-metallic asteroids. Our focus in this study is to investigate the role of magnetic cohesion in regolith behavior on metallic asteroids with residual magnetic fields, and its implications for morphology and surface processes on these bodies.

We aim to answer the following question in this work: *Can magnetic cohesion significantly influence the morphology and surface processes on metallic asteroids, and if so, to what extent?* We employ numerical modeling to simulate regolith behavior on metallic asteroids under the influence of magnetic forces in low gravity. The main contributions of this work are as follows:

- **Analytical Modeling:** Formulated an empirical force model for inter-particle interactions between paramagnetic grains in uniform magnetic fields, specifically tailored for the environmental constraints of M-type asteroids.
- **Computational Framework:** Developed and validated an open-source DEM framework that uses the more accurate Inclusion Model instead of the widely used Mutual Dipole Method (MDM), establishes the characteristic magnetic time-step for numerical stability, and accurately captures the transition to the plastic regime.
- **Geophysical Characterization:** Conducted multi-scenario avalanching simulations to delineate the parameter space (field strengths and particle sizes) where magnetic forces fundamentally dictate the surface morphology and regolith evolution of 16-Psyche.

Thesis Statement

The tools developed in this work will help us understand the interparticle magnetic cohesion in regolith on metallic asteroids and its implications for morphology and surface processes on these bodies. We will either validate or invalidate the hypothesis that magnetic cohesion can significantly influence the morphology and surface processes on metallic asteroids, and, if validated, quantify the extent of this influence. We develop new, more accurate models to perform granular mechanics simulations of magnetic regolith in microgravity conditions and demonstrate their ability to simulate previously unmodeled flow regimes, such as the plastic regime. This work will serve as a stepping stone for future research to understand the surface processes on metallic asteroids and their implications for the upcoming NASA Psyche mission and future missions to metallic asteroids. The tools developed in this work could also be used to understand magnetic cohesion in terrestrial applications such as magnetic powders and magnetorheological fluids.

Thesis Outline

First, we present background and motivation for this work through a literature survey of 16-Psyche, magnetic cohesion, and discrete element method simulations of granular mechanics in Chapter 2. Then, we present the development of an empirical model of the force between paramagnetic particles in a uniform magnetic field on M-type asteroids in Chapter 3. Next, we present the development of an experimentally validated magnetic force model for discrete element modeling of paramagnetic granular media in Chapter 4. Finally, we present the results of discrete element method simulations of avalanching on 16-Psyche in Chapter 5. Chapters 3 - 5 are written in the format of standalone

articles and are intended for publication in peer-reviewed journals (we note the state of publication (published/under review/prepared) at the beginning of each chapter). Finally, in Chapter 6, we present a summary of the conclusions and future work.

Publications

Journal Articles

- A.Sikka, C.Hartzell (2026) *Investigating the Role of Magnetic Cohesion in Avalanching on I6-Psyche: A Discrete Element Modeling Approach*, The Planetary Science Journal (In Preparation).
- A.Sikka, C.Hartzell (2026) *An Experimentally Validated Magnetic Force Model for Discrete Element Modeling of Paramagnetic Granular Media*, Granular Matter (Accepted).
- A.Sikka, I.DesJardin, T.Leps, and C.Hartzell (2023) *Development of an Empirical Model of the Force between Paramagnetic Particles in Uniform Magnetic Field on M-type Asteroids*, en, The Planetary Science Journal, vol. 4, no. 7, p. 129, Jul. 2023, Publisher: IOP Publishing, DOI: 110.3847/PSJ/ace323.

Conferences

- A.Sikka and C.Hartzell. *DEM Simulations of avalanching of metallic regolith under the influence of magnetic forces*. At 56th Annual Meeting of the Division for Planetary Sciences (DPS), Oct. 2024. Talk
- A.Sikka and C.Hartzell. *Magnetic Force Model to simulate Avalanching on Metallic Asteroids*

like 16-Psyche. At Granular Matter Gordon Research Seminar (GRS) and Conference (GRC), Jun. 2024. Poster.

- A.Sikka and C.Hartzell. *Extending LIGGGHTS to Perform Discrete Element Method Simulations of Mass Wasting Events in Uniform Magnetic Field on Psyche (16)-Like Metallic Bodies*. At 54th LPSC, Mar. 2024. Talk.
- A.Sikka and C.Hartzell. *Empirical model of the force between paramagnetic particles in uniform magnetic field on m-type asteroids*. At Asteroids, Comets and Meteors (ACM) Conference, Jun. 2023. Poster.
- A.Sikka, I.DesJardin and C.Hartzell. *Characterizing Magnetic Force Between Paramagnetic Particles of Magnetic Asteroids*. At 52nd Lunar Planetary Science Conference (LPSC), Mar. 2022. Talk.

Invited Talks

- A.Sikka (2025) *Unlocking Metallic Worlds: Granular Mechanics on Asteroid Psyche* at Aerospace Engineering Department, IIT Bombay, India. 21 July 2025.

Chapter 2: Literature Review

Magnetic cohesion on metallic asteroids is a relatively unexplored area of research, and several gaps remain in our understanding of this phenomenon. The relevant work can be broadly categorized into the following areas:

- metallic asteroids with residual magnetic fields
- studies of cohesion in regolith mechanics of small bodies
- studies of discrete element method simulations of granular mechanics in microgravity conditions
- studies of magnetic cohesion in granular media

Metallic meteorites and observations of metallic asteroids like 16-Psyché provide constraints on the regolith environments on these bodies, which are necessary to understand the role of magnetic cohesion in surface processes. Cohesion plays a critical role in the mechanics of regolith on small bodies, and understanding the different sources of cohesion is necessary to understand surface processes on these bodies. Limited work on magnetic cohesion indicates that magnetic forces increase net cohesion, leading to multiple granular regimes similar to those in wet granular media. However, most computational modeling efforts have used inaccurate dipolar-dipolar methods to model magnetic forces, which are more appropriate for distant particle interactions, such as in Magnetorheological Fluids (MRFs). Finally, while several studies have examined discrete element method simulations of granular mechan-

ics in microgravity conditions, none have included magnetic forces, which are necessary to understand the role of magnetic cohesion in surface processes on metallic asteroids. In this chapter, we review the relevant literature in these areas to provide the necessary background and motivation for this work.

2.1 Metallic Asteroids

Metallic asteroids are a class of asteroids that are primarily composed of metallic materials, such as iron and nickel. They are believed to be the remnants of the cores of differentiated planetary bodies that were disrupted by collisions in the early solar system [9]. 16-Psyché is the largest known metallic asteroid, with a diameter of about 225 kilometers, and is the target of NASA's Psyche mission, which is set to arrive at the asteroid in 2029 [7]. Multiple ground-based observations have constrained the shape, size, and gravitational parameters of 16-Psyché [8, 15, 16]. Atacama Large Millimeter/submillimeter Array (ALMA) observations of 16-Psyché have provided constraints on the thermal properties of the asteroid's surface, which can be used to infer the presence of regolith and its properties [17]. Cambioni et al. [13] used these observations to propose a heterogeneous regolith environment on 16-Psyché, which is indicative of the asteroid's complex geological history.

A prehistoric magnetic field is expected to have been generated in the core of the parent body of 16-Psyché, and some remnant magnetization may be present in the regolith on the surface of 16-Psyché [9, 11, 12, 18]. Psyche spacecraft will carry a magnetometer to measure the magnetic field around 16-Psyché, which will provide insights into the presence and strength of remnant magnetization [10]. The presence of remnant magnetization in the regolith can induce magnetic cohesion between particles, thereby influencing surface processes on the asteroid, such as landslides, crater formation, and regolith transport. While some constraints on the magnetic field strength on 16-Psyché can be obtained from

the dynamo evolution studies [12], meteorite data is necessary to constrain the magnetic properties of the regolith, such as the magnetic susceptibility and remanent magnetization of the particles. Terho et al. [19, 20], Kohout et al. [21] have measured the magnetic properties of iron meteorites, which are believed to be analogous to the regolith on metallic asteroids, and found that they can exhibit high magnetic susceptibilities and remanent magnetization, leading to significant magnetic cohesion between particles.

2.2 Cohesion in Regolith on Small Bodies

Scheeres et al. [14] compared different forces acting on particles on the surface of small bodies, such as gravitational forces, electrostatic forces, and cohesive forces, and showed that cohesive forces can dominate over gravitational forces for small particles on small bodies, leading to the formation of cohesive regolith. They defined the Bond number as the ratio of a force to the particle's weight. They showed that, for particles smaller than a few centimeters, cohesive forces such as van der Waals forces can dominate over gravitational forces. Researchers have modeled the effects of cohesion on various surface processes on small bodies, such as the strength of regolith [22], the avalanching of self-cohesive regolith [23], and the creep stability of rubble-pile bodies [24]. NASA's OSIRIS-REx mission to asteroid 101955-Bennu also showcased the need to understand cohesion in regolith on small bodies, as the sample collection mechanism sank into the surface more than expected, which was attributed to the presence of near-zero cohesive regolith [25, 26]. Numerical simulations of the DART mission's impact on 65803-Didymos also showed that regolith cohesion can significantly affect the impact outcome [27]. These missions highlight the importance of understanding cohesion in regolith on small bodies, and its implications for morphological evidence and surface processes.

2.3 Discrete Element Method in Microgravity

Discrete Element Method (DEM) is a numerical technique used to model the behavior of granular materials by simulating the interactions between individual particles. DEM uses a Newtonian framework in which the motion of each particle is governed by the forces acting on it, including contact, gravitational, and other external forces. At each timestep, the forces acting on each particle are calculated from its interactions with neighboring particles and any external fields, and the particle's position and velocity are updated accordingly. There are two main types of DEM: soft-sphere DEM, where particles can overlap, and the contact forces are calculated based on the degree of overlap, and hard-sphere DEM, where particles are treated as rigid bodies that cannot overlap, and collisions are resolved instantaneously. We focus on soft-sphere DEM in this work, as it is more appropriate for dense granular systems. Several studies have used DEM to model granular mechanics in microgravity conditions, such as lunar [28, 29] and small bodies [23, 24, 30, 31].

Multiple different DEM codes have been developed and validated for modeling granular mechanics in microgravity conditions. Schwartz et al. [32] implemented a soft-sphere DEM in the N-body code `pkdgrav`, originally developed for astrophysical simulations. This code has been used in several studies to model granular mechanics on small bodies, such as, creep stability of 65803-Didymos [24, 33, 34] tidal disruption of 99942-Apophis during its close approach to Earth [35, 36], oscillation driven motion of regolith on small bodies [37, 38] and avalanching on 101955-Bennu [39]. Sánchez and Scheeres [40] have developed a soft-sphere DEM code and used it in several studies, such as the disruption of rubble pile bodies [22, 40], simulating avalanching of cohesive powders in microgravity [23], and seismic wave propagation on small bodies [41]. A team of researchers in Japan has also developed an in-house DEM code to model and design their electrostatic [42] and magnetostatic sampler

[28, 43] for lunar regolith. Finally, researchers have combined DEM with other numerical techniques, such as the Finite Element Method (FEM) [44] and Smoothed Particle Hydrodynamics (SPH) [45], to model impact cratering.

A few researchers have modified and used open-source DEM codes, such as LIGGGHTS [46] and CHRONO [47], to model granular mechanics in microgravity conditions. Sunday et al. [31] modified and validated the DEM code CHRONO to model granular mechanics in microgravity conditions by testing it for simple cases and piling experiments. The code has been used in studies like rover wheel interaction with regolith on small bodies [48]. Frizzell and Hartzell [29] used the same test cases to validate the DEM code LIGGGHTS for modeling wave propagation on the lunar surface. They modified the code and used it to demonstrate that seismic waves following impacts can cause regolith to dilate and form Lunar Cold Spots [49, 50]. We aim to implement a magnetic force model in the open-source DEM code LIGGGHTS and use it to model magnetic cohesion in regolith on metallic asteroids.

2.4 Magnetic Cohesion in Granular Media

While Van der Waals forces play a major role in increasing cohesive strength in small particles, other mechanisms can also contribute to cohesion. The presence of interstitial liquid is one of the widely studied methods. Alexander et al. [51] investigated the avalanching of cohesionless glass beads, wet glass beads, and dry cohesive powders using rotating cylinder experiments and DEM simulations. Tegzes et al. [52] performed similar experiments with wet granular media but particularly looked at the dynamics of the cohesive flow and showed that such avalanches showcase a periodic behavior. While Quintanilla et al. [53] showed that the average clump size of avalanches increased with cohesion by

performing statistical analyses of clump size based on the angle of repose (the angle that granular materials form when piled, such as sand in an hourglass) in a rotating cylinder. There is a considerable amount of other literature [54, 55, 56, 57, 58] available on avalanches in both dry and wet cohesive granular media, as these studies find applications in industrial (cement, pharmaceutical) and natural scenarios (snow, wet sand, landslides). Generally, rotating cylinders, column formation, or DEM simulations are used as technical approaches in these studies.

There is a third type of cohesion possible, magnetic interactions between granular particles [59]. Magnetic cohesion occurs when metallic (high magnetic susceptibility) particles are subjected to an external magnetic field. Forsyth et al. [60] conducted experiments with a steel ball bearing to show that the angle of repose changes very little with magnetic field strength. Fazekas et al. [6], Taylor et al. [61] performed DEM simulations to validate the experimental results of [60] and provide varying reasons for a small increase in the angle of repose, even for large cohesive forces. Peters and Lemaire [62] argued that, rather than a uniform magnetic field that results in a highly anisotropic force between particles, a rotating magnetic field is more suitable for control over avalanching of cohesive particles. The possibility of tuning the cohesive forces between granular media is one of the only applications of magnetic cohesion found in the literature.

The earliest experimental work by Forsyth et al. [59, 60] with iron spherical balls placed in a uniform magnetic field established that magnetic cohesion influences granular behavior, such as the packing fraction and angle of repose. They showed that granular properties depend on the ratio of interparticle forces to gravitational forces, defined as the magnetic Bond number (B_m), rather than on the absolute value of the magnetic field or particle size. In their rotating drum experiments [60] observed three flow regimes: (1) a granular regime at low magnetic field strengths where the flow is similar to non-magnetic granular media, (2) a correlated regime at intermediate magnetic field strengths

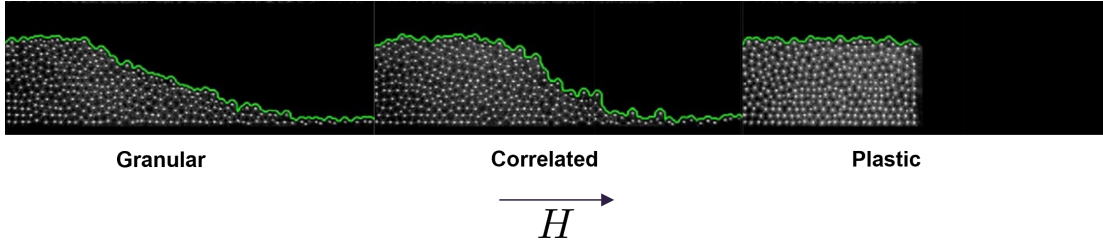


Figure 2.1: Final frames of avalanching experiments performed by Sunday et al. [4] using 8.73 mm steel balls. The magnetic field is increased from left to right. The leftmost frame shows the granular regime, the middle frame shows the correlated regime, and the rightmost frame shows the plastic regime. (Reproduced from Sunday et al. [4])

where the particles form clusters and these clusters influence the flow, and (3) a plastic regime at high magnetic field strengths where the particles are strongly cohesive and the flow is dominated by the breaking of cohesive bonds between particles. More recently, Sunday et al. [4] conducted avalanching experiments with steel and brass particles, where a bounding wall is removed to trigger avalanches, and observed similar regimes to Forsyth et al. [60]. However, in their plastic regime, particles did not move. 2.1 shows the three regimes observed by Sunday et al. [4]. We observe a smooth final profile in the granular regime, a rugged profile in the correlated regime, and a rigid structure in the plastic regime formed by the steel balls. They also analyzed surface roughness parameters, along with the angle of repose, to characterize their dependence on magnetic field strength. A linear increase in the angle of repose with the magnetic bond number was observed in both these studies. Avalanching study by Sunday et al. [4] also showed that the bulk behavior depends on the bond number, as seen in figure 2.2. The two plots show the angle of repose trends for different particle sizes and mixture combinations, which collapse when plotted against the magnetic bond number. However, it is important to note that they could not collapse the mixture data and the monodisperse data into a single plot.

Multiple modeling efforts have been undertaken to simulate magnetic forces between particles using the Discrete Element Method (DEM). DEM requires a force model to calculate the magnetic forces on

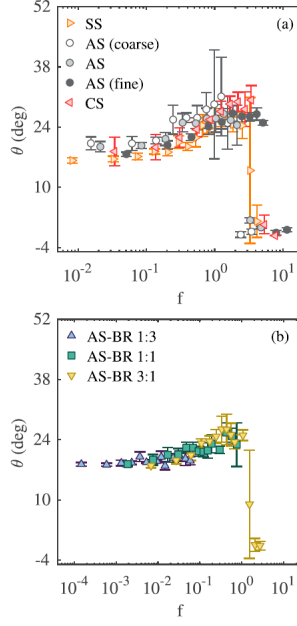


Figure 2.2: Angle of repose trends against magnetic bond number for different experimental materials used by Sunday et al. [4]. The top plot (a) shows that the data from all monodisperse experiments collapse, while the bottom plot (b) shows that the trends from mixture experiments collapse separately. (Reproduced from Sunday et al. [4])

particles. The magnetostatic force between two particles can be calculated by solving Maxwell's equations [63], but this requires appropriate boundary conditions and substantial computational resources. A simplified approach is to assume the particles are point dipoles and use dipole-dipole interactions to calculate the magnetic force, which underlies the Fixed Dipole Model (FDM) [6]. This simple model is computationally efficient and was used in early modeling efforts by Fazekas et al. [6] and Taylor et al. [61]. They reproduced a weak increase in the angle of repose with increasing magnetic field strength, but the different regimes observed in the experiments were not captured in their simulations.

There are two key assumptions in the FDM: (1) the particles are point dipoles, which is only valid when the particles are far apart, and (2) the magnetic field is uniform across the particle, which is only valid for small particles in weak magnetic fields. The Mutual Dipole Method (MDM) [1] is an improvement over the FDM that accounts for the finite size of particles and the non-uniformity of the

magnetic field across them. This model has been used in several studies [64, 65, 66] to model Magnetorheological Fluids (MRFs). Magnetorheological fluids (MRFs) [67] are suspensions of magnetic particles in a carrier fluid, and the particles are typically in the order of microns and are subjected to strong magnetic fields. The MDM is appropriate for modeling magnetic forces in MRFs, as the particles are far apart compared to those in dense granular media formed by regolith on asteroid surfaces. Keaveny and Maxey [1] formulated an Inclusion model that is more accurate than the MDM for modeling magnetic forces by including the exact two-particle solution to Maxwell’s equations for particles that are close together. While more accurate, the Inclusion model is computationally more expensive than the MDM and, to our knowledge, has not been used in DEM simulations of magnetic granular media. We aim to develop an efficient computational framework to implement the Inclusion model in DEM simulations of magnetic granular media and to use it to model magnetic cohesion in regolith on metallic asteroids.

2.5 Summary

In summary, there is a significant gap in our understanding of magnetic cohesion in regolith on metallic asteroids and its implications for surface processes on these bodies. While studies have examined cohesion in regolith mechanics of small bodies and magnetic cohesion in granular media, none have combined these two areas to understand the role of magnetic cohesion in regolith mechanics on metallic asteroids. Scheeres et al. [14] showed that cohesive forces can dominate over gravitational forces for small particles on small bodies due to microgravity conditions. NASA’s Psyche mission to the metallic asteroid 16 Psyche will provide new insights into the regolith environment on metallic asteroids. It is essential to understand the role of magnetic cohesion in regolith mechanics on metallic

asteroids to interpret the data from the Psyche mission and to understand surface processes on these bodies. We believe we are the first to study and characterize the effects of magnetic cohesion for probable scenarios on metallic bodies like 16-Psyche. We start with a detailed comparison of different magnetic models and define an empirical model that is more accurate than the FDM-based force formula used for magnetic bond number in the literature.

Chapter 3: Development of an Empirical Model of the Force between Paramagnetic Particles in Uniform Magnetic Field on M-type Asteroids

This chapter appeared in its original form as: Sikka, A., DesJardin, I., Leps, T. and Hartzell, C. (2023) Development of an Empirical Model of the Force between Paramagnetic Particles in Uniform Magnetic Field on M-type Asteroids. *Planetary Science Journal* 4, 7, 129.

3.1 Introduction

Magnetic fields [$\approx 2\text{nT}$] have been detected around asteroids Gaspra (by the Galileo spacecraft [68]) and Braille [69]. The magnetic field detections at these two bodies are weakened by the fact that they were either close to the measurement sensitivity of the detector (in the case of Braille) or could also be explained by other plasma interactions with the asteroid (in the case of Gaspra) (see discussion in Scheinberg et al. [70]). While these are S-type asteroids, 20% of the main belt [71] is comprised of X-type asteroids (E-type, M-type, P-type) that may have significant magnetic fields. These asteroids, predicted to be constituted primarily of nickel and iron, may be exposed planetesimal cores. A prehistoric dynamo could have caused a magnetic field to be locked into the cooling material [18].

Scheinberg et al. [11] studied the evolution of the dynamo during solidification, particularly in the context of the asteroid Psyche. The Psyche mission to its eponymous asteroid will carry a

magnetometer, the measurements of which will be central to testing the hypothesis that Psyche once was a planetary core [72]. On-going simulation work has modeled the plasma environment around Psyche with magnetic fields ranging from 0-500nT [73], while the strength of the magnetic field will be much higher on the surface. Additionally, it is natural to assume that metallic asteroids will also be subject to the disruption and reaccretion processes that are thought to produce rubble pile asteroids from other taxonomic classes. Thus, metallic asteroids may exist in various sizes and magnetic field strengths.

Previous work by Scheeres et al. [14] showed that the van der Waals cohesion is a the significant force between grains on traditional (non-metallic) asteroids. Subsequently, Sánchez and Scheeres [40, 74] demonstrated the influence of the cohesive force in the evolution of rubble-pile asteroids. Additionally, the surface morphology of the regolith is influenced by the dominant force. The angle of repose (the angle that granular materials form when dropped into a pile, e.g., the sand in an hourglass) is steeper for more strongly cohesive granular materials [75]. A magnetic force between regolith particles can result in an increase or decrease of the net cohesion between particles (depending if the force is attractive or repulsive), thus possibly influencing the surface morphology.

While Iron and Nickel are ferromagnetic substances (the likely constituents of M-type asteroids), their compounds are paramagnetic. Kohout et al. [21] discuss bulk magnetic properties for various classes of meteoroids, including iron and stony-iron, in paramagnetic terms. Paramagnetic particles placed in an external uniform magnetic field are influenced not just by the external magnetic field but also by the induced magnetic moments of their neighboring particles. The differential equations for the magnetic interactions between particles involve the Laplace equation. By applying appropriate boundary conditions, a solution can be generated. The process is cumbersome and cannot be solved for a system of large particles. There are various methods in literature to solve such problems, but

each of these methods has some shortcomings, either being inaccurate or being too computationally expensive. There is a need for a fast and reliable solution to the problem.

We describe the various methods mentioned in the literature [1, 76] for completeness, starting by stating the magnetostatic problem. We implement and utilize the spherical harmonics solver given in [1] to generate force data for a range of different parameters, specifically: applied magnetic field strength, particle size, particle susceptibility, and particle spacing. Finally, an empirical formula is developed using fitting to calculate the force between two identical paramagnetic particles in a uniform magnetic field. This empirical formula is an essential first step to understanding the significance of magnetic forces [14] by providing a quick analytical framework to compare different forces between particles.

3.2 Magnetostatic Problem

First, the magnetostatic problem is described (based on [1]). Consider N spherical particles of radius a and magnetic volume susceptibility χ , neglecting free and displacement currents. The permeability μ is then defined as $\mu = (1 + \chi)\mu_0$, where μ_0 is the free space permeability. Each n^{th} particle is placed at position $\mathbf{X}_n$ in a uniform magnetic field $\mathbf{H}_0$. The Maxwell's equations [63], therefore, are

$$\nabla \cdot \mathbf{B} = 0, \tag{3.1}$$

$$\nabla \times \mathbf{H} = \mathbf{0}, \tag{3.2}$$

with magnetic flux density $\mathbf{B} = \mu\mathbf{H}$ inside the particles and $\mathbf{B} = \mu_0\mathbf{H}$ outside the particles. Scalar potentials can be introduced based on equation 3.2, such that $\mathbf{H} = -\nabla\phi_{out}$ outside the particles and

$\mathbf{H} = -\nabla\phi_{in}^{(n)}$ inside the particles $n = 1, 2, \dots, N$. We can now use the relations between $\mathbf{B}$ and $\mathbf{H}$ along with equation 3.1 to find Laplace's equations

$$\nabla^2\phi_{out} = 0, \quad (3.3)$$

$$\nabla^2\phi_{in}^{(n)} = 0. \quad (3.4)$$

For a spherical coordinate system defined at the center of each sphere such that $\mathbf{r}_n = \mathbf{x} - \mathbf{X}_n$ with $r_n = |\mathbf{r}_n|$,

$$\phi_{in}^{(n)} = \phi_{out}, \quad (3.5)$$

$$\mu \frac{\partial\phi_{in}^{(n)}}{\partial r_n} = \mu_0 \frac{\partial\phi_{out}}{\partial r_n}. \quad (3.6)$$

at $r_n = a$ for each $n = 1, 2, \dots, N$. Additionally, as $r_n \rightarrow \infty$,

$$\phi_{out} \rightarrow \mathbf{H}_0 \cdot \mathbf{r}_n. \quad (3.7)$$

Based on boundary conditions (eqs. 3.5-3.7), the potential is solved, and the field is computed. The total magnetic force $\mathbf{F}_n$ on n^{th} particle is computed using the Maxwell Stress Tensor:

$$\mathbf{T} = \mu_0 \left(\mathbf{H}\mathbf{H} - \frac{1}{2}H^2\mathbf{I} \right), \quad (3.8)$$

$$\mathbf{F}_n = \int_{V_i} \nabla \cdot \mathbf{T} dV, \quad (3.9)$$

where V_n is the total volume of the n^{th} particle. The general solution to equations 3.3 and 3.4 can be written as a sum of potential due to the external magnetic field and a sum of spherical harmonic

expansions for each particle. One can also solve the equations using numerical methods such as finite volume method and finite difference method. The boundary conditions (eqs. 3.5 and 3.6) pose complications in finding all parameters for the general solution. Most models are based on this general solution.

3.2.1 Fixed Dipole Moment (FDM) Model

To compare the different models, the solution to a two-particle magnetostatic problem (Figure 3.1) is considered. Consider the magnetostatic problem with $\mathbf{X}_1 = (0, 0, sep)$, $\mathbf{X}_2 = (0, 0, 0)$ and the applied magnetic field $\mathbf{H}_0 = (H_\perp, 0, H_\parallel) = H_0(h_\perp, 0, h_\parallel)$ where $(h_\perp, 0, h_\parallel)$ is unit vector.

The fixed dipole moment model (described in [76]) is the simplest and most commonly used solution

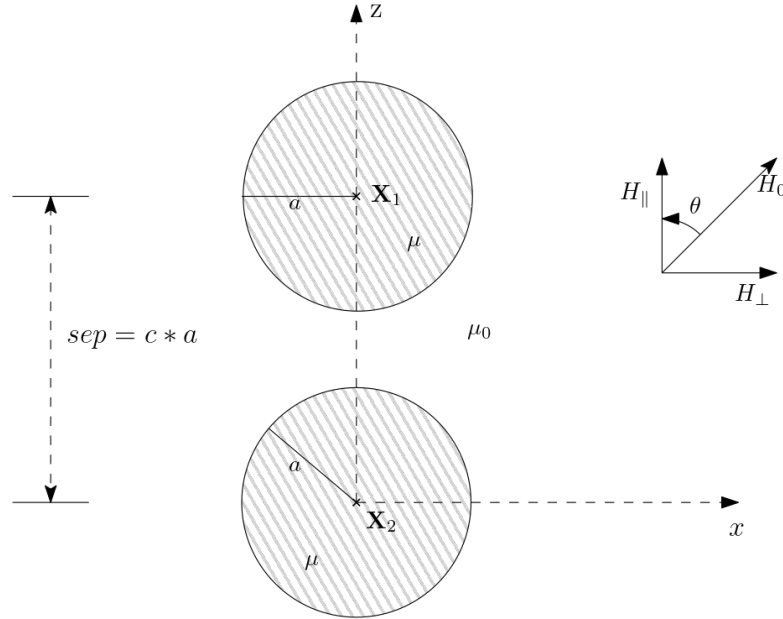


Figure 3.1: Two identical grains in an external uniform magnetic field

to estimate force between paramagnetic particles. The model is based on the general solution for a single particle magnetostatic problem. Consider a single spherical paramagnetic particle in a uniform

magnetic field, $\mathbf{H}_0$. The particle is uniformly magnetized and acquires a magnetic dipole moment

$$\mathbf{m} = \frac{4\pi a^3 \chi_{eff}}{3} \mathbf{H}_0, \quad (3.10)$$

where $\chi_{eff} = \frac{3\chi}{\chi+3}$ is the effective magnetic susceptibility of the particle. The magnetic field around this particle is then computed as

$$\mathbf{H}_{dip}(\mathbf{r}) = \frac{1}{4\pi} \left(\frac{3\mathbf{r}(\mathbf{m} \cdot \mathbf{r})}{r^5} - \frac{\mathbf{m}}{r^3} \right). \quad (3.11)$$

In this method, only this magnetization of a single particle in a uniform magnetic field is considered. Based on this, if a second particle is placed at distance $sep = c * a$, both particles will experience a force:

$$\begin{aligned} \mathbf{F}_1 &= \mu_0 \nabla (\mathbf{m}_1 \cdot \mathbf{H}_{dip}(\mathbf{X}_1 - \mathbf{X}_2)) \\ &= \frac{3\mu_0}{4\pi c^5 a^4} \left[(\mathbf{m}_1 \cdot \mathbf{c}) \mathbf{m}_2 + (\mathbf{m}_2 \cdot \mathbf{c}) \mathbf{m}_1 + (\mathbf{m}_1 \cdot \mathbf{m}_2) \mathbf{c} - \frac{5(\mathbf{m}_1 \cdot \mathbf{c})(\mathbf{m}_2 \cdot \mathbf{c})}{c^2} \mathbf{c} \right] \end{aligned} \quad (3.12)$$

where $\mathbf{F}_1$ is the force experienced by particle 1, $\mathbf{m}_1$ is the dipole moment of particle 1, $\mathbf{m}_2$ is the dipole moment of particle 2, $\mathbf{c}$ is the connector vector between the two particles and $\mathbf{H}_{dip}(\mathbf{X}_1 - \mathbf{X}_2)$ is the dipolar magnetic field generated by particle 2. Further reduction of equation 3.12 for two special cases $\mathbf{H}_0 \parallel \mathbf{c}$ and $\mathbf{H}_0 \perp \mathbf{c}$ gives

$$\mathbf{F}_{FDM} = \begin{cases} \frac{3\mu_0 m^2}{4\pi c^4 a^4} (-2\hat{\mathbf{c}}), & \mathbf{H}_0 \parallel \mathbf{c} \\ \frac{3\mu_0 m^2}{4\pi c^4 a^4} (1\hat{\mathbf{c}}), & \mathbf{H}_0 \perp \mathbf{c} \end{cases}. \quad (3.13)$$

It can be seen that the magnitude of the force between two particles as a function of separation distance

c is

$$\begin{aligned} F_{FDM}(c) &\propto a^2, \\ &\propto H_0^2, \end{aligned} \tag{3.14}$$

where separation distance c is measured in terms of particle radius a .

3.2.2 Mutual Dipole Moment (MDM) Model

The fixed dipole model (FDM) considered magnetization only due to the external field. In the mutual dipole model (MDM), the field generated by other magnetized particles is also considered. Consequently, the dipole moment of particle 1 is

$$\mathbf{m}_1 = \frac{4\pi a^3 \chi_{eff}}{3} \left(\mathbf{H}_0 + \mathbf{H}_{dip}(\mathbf{X}_1 - \mathbf{X}_2) \right), \tag{3.15}$$

where $\mathbf{H}_{dip}$ is the same as described in equation 3.11. The calculation is iterated until the dipole moments converge. The mutual dipole model solves the issue of interaction between the particles, but the effect of higher-order multipole terms is still not included. Both FDM and MDM diverge from the exact solution, particularly at low separation distances, as seen in figures 3.2 and 3.3. To include the higher-order multipole terms, we need to estimate the solution to Laplace's equations.

3.2.3 Finite Volume Method (FVM)

Equations 3.1 and 3.2 describe a Laplace equation with prescribed boundary conditions given at the interface (eqs. 3.5 and 3.6), and at infinity (eq. 3.7). This problem can be solved numerically

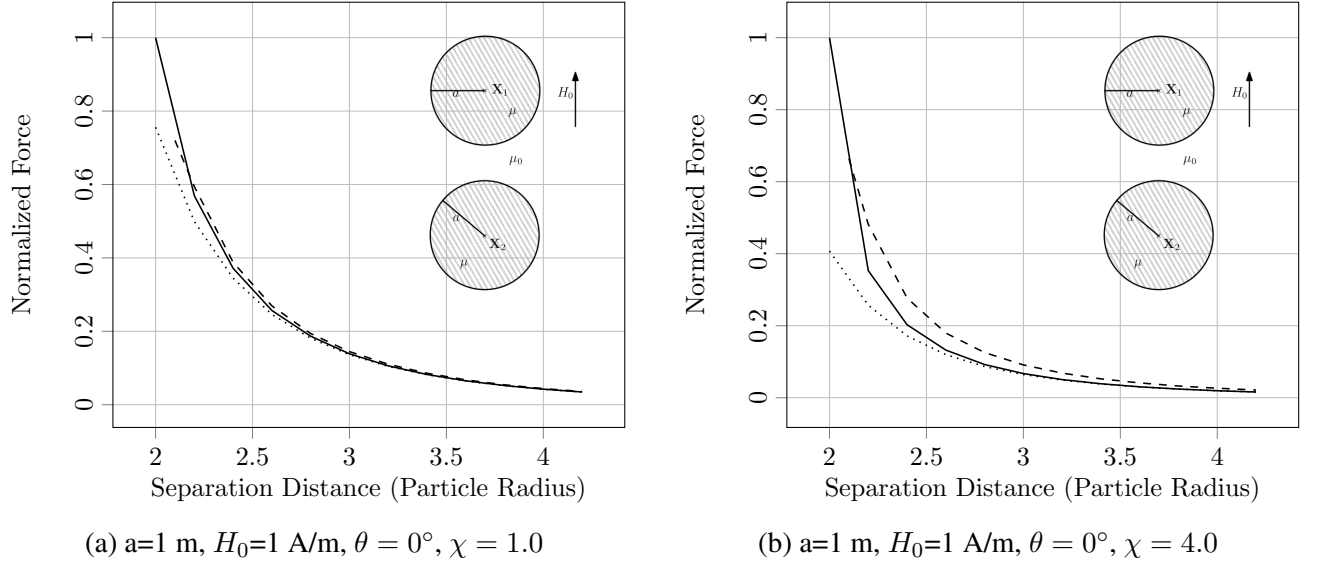


Figure 3.2: Comparison curves for different models for the two body problem (external magnetic field is parallel to the particles: ($\theta = 0^\circ$)). The force is normalized by the value (fig a: $-5.57\text{E-}07$ N and fig b: $-6.46\text{E-}06$ N) when the particles are touching. For higher susceptibility, the mutual dipole moment underestimates the force when particles are closer. In the plots: (.....) Mutual Dipole Moment; (---) Finite Volume Method; (—) Spherical Harmonics Solver.

through the FVM in three dimensions using the smoothed profile method as outlined in [76, 77]. The magnetic susceptibility μ inside and outside the grains is given by

$$\mu = \begin{cases} \mu & r_n > a, \\ \mu_0 & r_n \leq a. \end{cases}$$

A smoothed profile is generated for the susceptibility by approximating the true μ as a smooth differentiable function given by

$$\mu_{\text{approx}}(\mathbf{x}) = \frac{\mu_0}{s(\mathbf{x}) (\mu_0/\mu) + (1 - s(\mathbf{x}))}, \quad (3.16)$$

where $s(\mathbf{x})$ approximates the step function using tanh given by

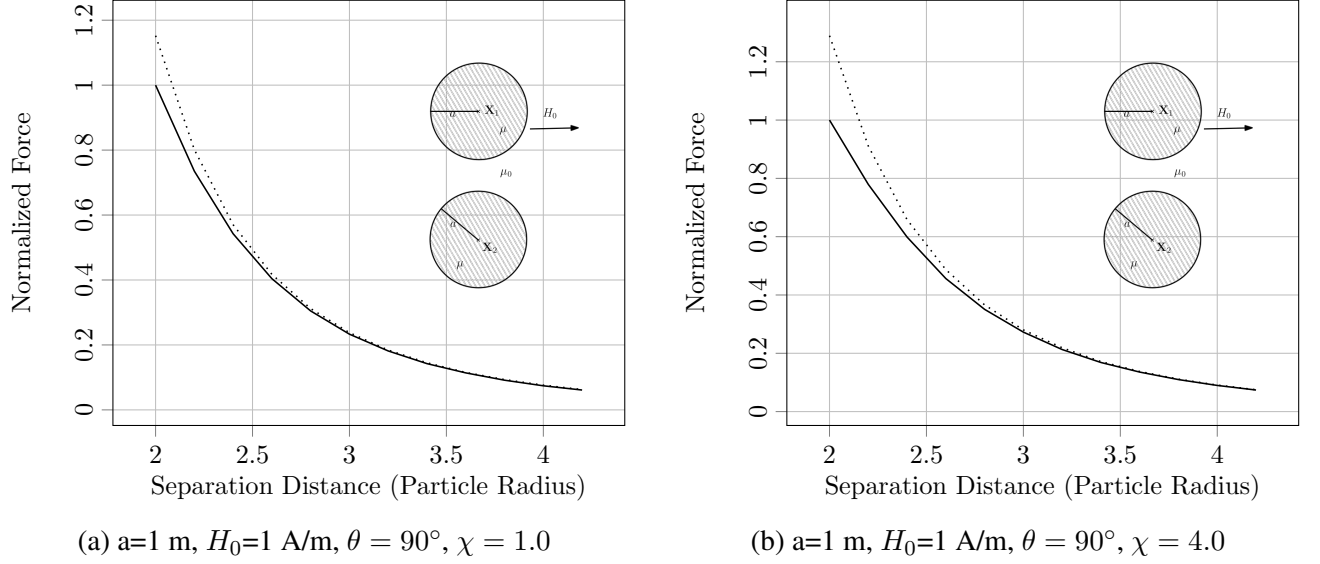


Figure 3.3: Comparison curves for different models for the two body problem (external magnetic field is perpendicular to the particles: $\theta = 90^\circ$). The force is normalized by the value ((a): $1.51\text{E-}07$ N and (b): $6.53\text{E-}07$ N) when the particles are touching. For higher susceptibility, the mutual dipole moment underestimates the force when particles are closer. In the plots: (.....) Mutual Dipole Moment; (—) Spherical Harmonics Solver.

$$s(\mathbf{x}) = \sum_i \frac{1}{2} \left[\tanh \left(\frac{1 - \|\mathbf{x} - \mathbf{X}_i\|_2}{\alpha \min(ds, dz)} \right) + 1 \right], \quad (3.17)$$

α is a thickness ratio that defines the steepness for the transition from $\mu_0 \rightarrow \mu$. The value of α determines the accuracy of the smoothed profile for the FVM. Kang and Suh [78] show that α values between 0.2 – 0.6 work well and recommend 0.4 value for a range of susceptibilities. ds and dz are the grid sizes in the axial and longitudinal directions. The grid sizes are determined by performing a convergence study. In the limit of $\mathbf{x} = \mathbf{X}_i$, $s \approx 1$, and $\mu_{\text{approx}} = \mu$. Likewise, when $\|\mathbf{x} - \mathbf{X}_i\|_2 \rightarrow \infty$, $s \rightarrow 0$, and $\mu_{\text{approx}} \rightarrow \mu_0$. Figure 3.4c shows the smoothed profile approximation of μ normalized to μ_0 in the simulation domain.

Du et al. [76] used a full 3D code with an iterative linear system solver. The study first finds a coarse solution which is then used as the initial guess for the fine solution. These methods are

necessary because in 3D, for a symmetric grid of size $n \times n \times n$, the connectivity matrix is of size $\mathcal{O}(n^3) \times \mathcal{O}(n^3)$. For a 2D grid of size $n \times n$, the connectivity matrix is of size $\mathcal{O}(n^2) \times \mathcal{O}(n^2)$. Solving the full 3D system in full resolution is not yet practical for small-sized, high-performance computing systems. For this reason, initial simulations were conducted with a 2D axisymmetric formulation.

The test problem considered for benchmarking against later described numerical methods is a set of stacked particles where the stack is parallel to the externally applied magnetic field H_0 (see Fig 3.1). Along the axis of the stacked grains, the field solution is cylindrically symmetric. The axisymmetry is not valid for any other case of applied magnetic field direction. Consider an evenly spaced rectangular grid along a slice of the cylinder in the radial and axial directions. Figure 3.4a illustrates this style of the grid. The FV formulation discretizes the system as fluxes between the different cells. In the cylindrical formulation, the s direction flux depends on s itself while the z flux is constant. Simulations were performed with a grid number of $n = 1200$ with domains ranging $16a$ in each direction, where a is the grain radius. Once ϕ is solved for using the FVM over the entire domain,

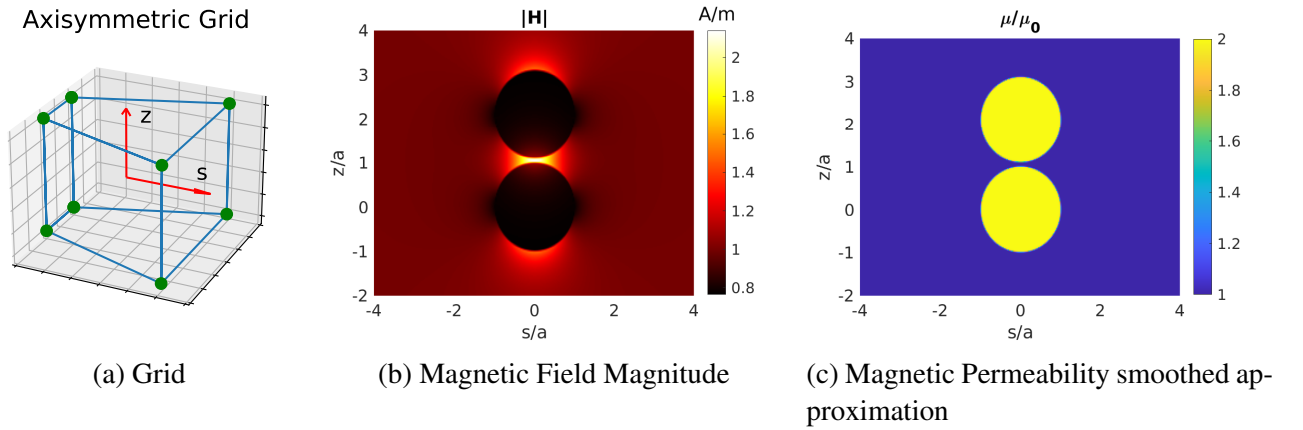


Figure 3.4: (a) shows the axisymmetric cylindrical mesh used in the FVM formulation. The 2D grid is in the sz plane, but the flux between cells in the s direction is a function of the radius from the $s = 0$ axis. (b) shows the magnetic field magnitude around two particles. (c) shows the smoothed representation of $\mu(\mathbf{r})$. The results in (b) and (c) are for particle diameter $a = 1\text{m}$, magnetic susceptibility $\chi = 1$, and applied external magnetic field $H_0 = 1\text{A/m}$ parallel to the particles.

$\mathbf{H}$ and $\mathbf{T}$ are calculated using numerical approximations of the outer product and gradient operators. The force is found by summing $\nabla \cdot \mathbf{T}$ near the grain boundary as in equation 3.8. Figure 3.4b shows the $|H|$.

3.2.4 Spherical Harmonics (SH) Solver

The Laplace problem (eqs. 3.3-3.7) is solved in [1] using a sum of spherical harmonics.

$$\phi_{in}^{(n)} = \sum_{l=0}^{\infty} \sum_{m=0}^1 \alpha_{lm}^{(n)} r_n^l P_l^m(\cos \theta_n) \cos m\phi, \quad (3.18)$$

$$\phi_{out} = -H_0(h_{\perp}x + h_{\parallel}z) + \sum_{n=1}^2 \sum_{l=0}^{\infty} \sum_{m=0}^1 \beta_{lm}^{(n)} \frac{P_l^m(\cos \theta_n)}{r_n^{(l+1)}} \cos m\phi, \quad (3.19)$$

where (x, y, z) are the Cartesian coordinates of the system and (r_n, θ_n, ϕ_n) are the spherical coordinates of a system with the origin at the center of sphere n . The associated Legendre function is defined as

$$P_l^m(\cos \theta) = (-1)^m (1 - \cos^2 \theta)^{\frac{m}{2}} \frac{d^m P_l(\cos \theta)}{(\cos \theta)^m}. \quad (3.20)$$

The coefficients $\alpha_{lm}^{(n)}$ and $\beta_{lm}^{(n)}$ are found by satisfying the boundary conditions. We need the Hobson formula to describe the general solution in a single coordinate system:

$$\frac{P_l^m(\cos \theta_1)}{r_1^{l+1}} = \sum_{s=m}^{\infty} (-1)^{s+m} (-1)^{l+s} \binom{l+a}{s+m} \frac{r_2^s}{c^{l+s+1}} P_s^m(\cos \theta_2), \quad (3.21)$$

$$\frac{P_l^m(\cos \theta_2)}{r_2^{l+1}} = \sum_{s=m}^{\infty} (-1)^{s+m} \binom{l+a}{s+m} \frac{r_1^s}{c^{l+s+1}} P_s^m(\cos \theta_1). \quad (3.22)$$

On substituting the general solution into the boundary conditions, using the Hobson formula and eliminating $\alpha_{lm}^{(n)}$, we find for each $m = 0, 1$,

$$((\chi + 2)l + 1)\beta_{lm}^{(1)} + \sum_{s=1}^{\infty} \beta_{sm}^{(2)} (-1)^{l+m} \chi l \binom{l+s}{s-m} \frac{a^{2l+1}}{c^{l+s+1}} = \delta_{1j} a^3 \chi H_0 (\delta_{0m} h_{\parallel} - \delta_{1m} h_{\perp}), \quad (3.23)$$

$$((\chi + 2)l + 1)\beta_{lm}^{(2)} + \sum_{s=1}^{\infty} \beta_{sm}^{(1)} (-1)^{l+s} (-1)^{l+m} \chi l \binom{l+s}{s-m} \frac{a^{2l+1}}{c^{l+s+1}} = \delta_{1j} a^3 \chi H_0 (\delta_{0m} h_{\parallel} - \delta_{1m} h_{\perp}). \quad (3.24)$$

Considering only a finite number of multipoles, $l = 0, \dots, L$, we arrive at $2L \times 2L$ linear systems of equations. For each $m = 0, 1$

$$\begin{pmatrix} \mathbf{X} & \mathbf{\Delta}_m \\ \mathbf{\Gamma}_m & \mathbf{X} \end{pmatrix} \begin{pmatrix} \beta_m^{(1)} \\ \beta_m^{(2)} \end{pmatrix} = \begin{pmatrix} \mathbf{q}_m \\ \mathbf{q}_m \end{pmatrix} \quad (3.25)$$

where

$$\beta_m^{(1)} = (\beta_{1m}^{(1)}, \beta_{2m}^{(1)}, \dots, \beta_{Lm}^{(1)})^T, \quad \beta_m^{(2)} = (\beta_{1m}^{(2)}, \beta_{2m}^{(2)}, \dots, \beta_{Lm}^{(2)})^T, \quad (3.26)$$

$$\mathbf{q}_0 = (H_0 h_{\parallel} a^3 \chi, 0, \dots, 0)^T, \quad \mathbf{q}_1 = (-H_0 h_{\perp} a^3 \chi, 0, \dots, 0)^T, \quad (3.27)$$

and the $L \times L$ matrices are

$$X_{ij} = \delta_{ij}((\chi + 2) i + 1), \quad (3.28)$$

$$\Delta_{ij;m} = (-1)^{i+m} \chi^i \binom{i+j}{j-m} \frac{a^{2i+1}}{c^{i+j+1}}, \quad (3.29)$$

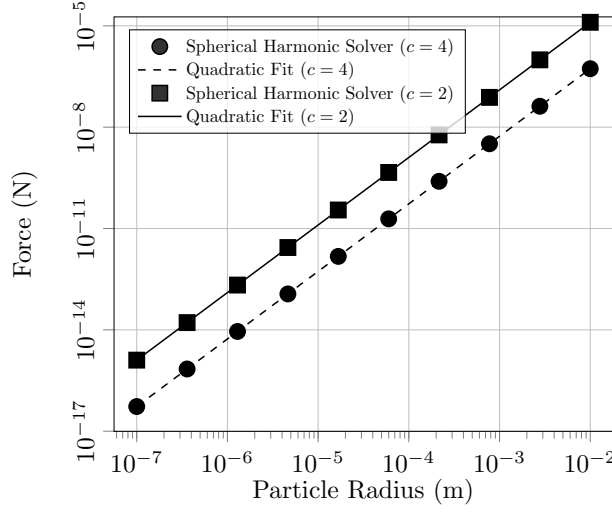
$$\Gamma_{ij;m} = (-1)^{i+j} \delta_{ij;m}. \quad (3.30)$$

After solving the system of equations, with $\beta_{lm}^{(n)}$ known, the contribution of the magnetic field from the particles is found by taking the gradient of the scalar potential ϕ_{out} . The interaction force between particles can, therefore, be calculated using equations 3.8 and 3.9.

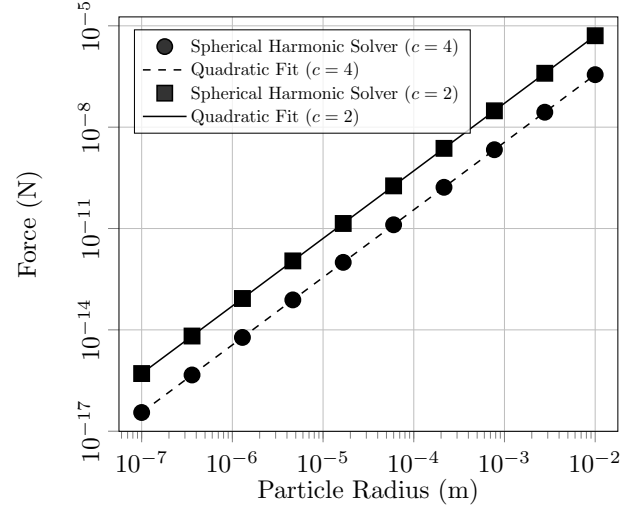
Looking at the formulation of equations 3.25, we can conclude that each coefficient $\beta_{sm}^{(1)}$ and $\beta_{sm}^{(2)}$ is proportional to H_0 . Therefore, the scalar potential outside the particles is proportional to H_0 , which in turn implies the force between particles is proportional to H_0^2 . This relation is the same as the one achieved through the FDM method (Eq. 3.14). Similarly, looking at particle radius variation in figure 3.5, we find that the magnitude of force between two particles as a function of separation distance c is proportional to particle radius a . The spherical harmonic solver is unable to accurately calculate force for lower particle radii ($< 10^{-2}$ m) for higher susceptibilities as the condition number for matrix in equation 3.25 becomes very high. We instead verified the quadratic relation with particle radii using meter-sized radii.

$$\begin{aligned} F(c) &\propto a^2, \\ &\propto H_0^2, \end{aligned} \quad (3.31)$$

where separation distance c is measured in terms of particle radius a .



(a) $\theta = 0^\circ, \chi = 1, B_0 = 6 \text{ G}$



(b) $\theta = 90^\circ, \chi = 1, B_0 = 6 \text{ G}$

Figure 3.5: Magnetic force follows a quadratic relation with particle radius.

A comparison for different models is seen in Figures 3.2 and 3.3. The Mutual Dipole Moment underestimates the forces when particles are closer together. The error at short distances increases for higher susceptibilities. However, the FVM and SH Approximation solutions are comparable.

The FDM and MDM models require very little computational power and run time but fail at low particle separation distances. The FVM, while providing an exact solution for the whole range of separation distances, requires high computational power and cannot solve the case when particles are touching. The SH solver provides good results but takes a long computational time. A faster and more reliable method is needed to compute the magnetic force between particles. Therefore, an empirical model of force between two particles is developed. The model would provide an essential step to understanding the magnetic force by providing an analytical framework.

3.3 Development of the Empirical Model

The force between two identical spherical particles in a uniform magnetic field is dependent on the following parameters: magnitude H_0 and direction of the applied magnetic field $\hat{\mathbf{H}}_0$, particle radius a , separation distance c , and particle volume magnetic susceptibility χ . We already showed the relation to the magnitude of the applied magnetic field H_0 and particle radius a (Eq. 3.31).

First, force data for different parameters were generated using the SH solver. Two different equations (Eq. 3.32 and eq. 3.33), inspired from [76] were then fitted over a range of separation distance (sep) for a given susceptibility (χ)

$$F = \mu_0 H_0^2 a^2 \sum_{i=0}^3 \frac{p_i(\chi)}{c^{4+i}}, \quad (3.32)$$

$$F = F_{FDM} + \mu_0 H_0^2 a^2 \sum_{i=1}^3 \frac{p_i(\chi)}{c^{4+i}}, \quad (3.33)$$

where F_{FDM} is the force between particles when only a fixed dipole model is considered (Eq. 3.13), $c = sep/a$ and parameters $p_i(\chi)$ are unique parameters for each susceptibility. Negative means attractive, while positive means repulsive force. This resulting data of $p_i(\chi)$ for each $i = 0 - 3$ was then fitted on different polynomial functions in either magnetic susceptibility (χ) or effective susceptibility (χ_{eff})

$$p_i = q_3^i \chi^3 + q_2^i \chi^2 + q_1^i \chi^1 + q_0^i \quad i = 1, 2, 3 \quad (3.34)$$

$$p_i = q_3^i \chi_{eff}^3 + q_2^i \chi_{eff}^2 + q_1^i \chi_{eff}^1 + q_0^i \quad i = 1, 2, 3 \quad (3.35)$$

Therefore, for each of the force fits (Eq. 3.32 and eq. 3.33) and the best fitting p_i equation was derived. This exercise resulted in four different complete empirical fit for the force function. Finally, we check each of the four empirical fits over the whole data and optimize it to maximize the total R^2 value. The empirical formula, thus mentioned in the section below, had the best fit (highest R-squared value). Python's Scipy library was used as the fitting algorithm.

3.4 Empirical Model

The empirical fit was developed for two special cases of applied magnetic field direction: magnetic field parallel ($\theta = 0^\circ$) and perpendicular ($\theta = 90^\circ$) to the line joining the particles. Kohout et al. [21] measured bulk magnetic susceptibility and bulk densities for over 700 meteorite samples. The volume magnetic susceptibility range for stony-iron and iron meteorites is 4-160, with a majority of them between 7-80 (Fig. 1 in [21]). Therefore, we chose susceptibilities [7, 10, 15, 20, 25, 30, 35, 40, 45, 50, 55, 60, 65, 70, 75, 80] for the parallel and [7, 10, 12, 20, 30, 40, 50, 60, 70, 80] for the perpendicular case in our study.

For the susceptibility range considered (7-80), forces corresponding to both MDM and SH solver converge at 4.2 particle radii separation distance. As the relation to H_0 and a are known, both are assumed to be unity, while the separation distances from 2 to 4.2 particle radii (where 2 corresponds to the case where the two particles are touching) are considered.

Amongst the four combinations of equations 3.32-3.33 and 3.34-3.35, the following combination produced the best empirical fit for both the cases.

$$F = F_{FDM} + \mu_0 H_0^2 a^2 \sum_{i=1}^3 \frac{p_i(\chi)}{c^{4+i}} \quad (3.36)$$

$$p_i = q_3^i \chi_{eff}^3 + q_2^i \chi_{eff}^2 + q_1^i \chi_{eff}^1 + q_0^i \quad i = 1, 2, 3 \quad (3.37)$$

where F_{FDM} is the force between particles when only a fixed dipole model is considered (Eq. 3.13), $c = sep/a$ and parameters p_i are effective susceptibility polynomials. Tables 3.1 and 3.2 give the values of the q_i parameters. Figure 3.6 shows the empirical fits for a few selected susceptibilities.

Table 3.1: Empirical model (Parallel case, $\theta = 0^\circ$, $c > 2$).

	q₃	q₂	q₁	q₀
p₁	-497.952	2671.567	-5718.948	4061.883
p₂	2944.524	-16054.067	33639.652	-23897.555
p₃	-4317.452	23490.267	-48875.994	34745.551

Table 3.2: Empirical model (Perpendicular case, $\theta = 90^\circ$).

	q₃	q₂	q₁	q₀
p₁	2.766	-7.992	1.807	8.525
p₂	-11.914	28.931	9.020	-28.672
p₃	12.478	-46.440	-6.332	24.884

While fitting the force data for the parallel case ($\theta = 0^\circ$), a different behavior was noticed. When the particles are touching and parallel to the magnetic field, the force is an order of magnitude higher than the cases when the particles aren't touching. Therefore, the polynomial fit in equations 3.36 and 3.37 don't capture this sensitivity. Various polynomial and exponential fits were tried for this special case. A cubic fit could give high R-squared accuracy while having low enough parameters. Therefore, a separate cubic fit (Eq. 3.38 and table 3.3) in magnetic susceptibility is generated for the case when

particles are touching and parallel to the applied magnetic field.

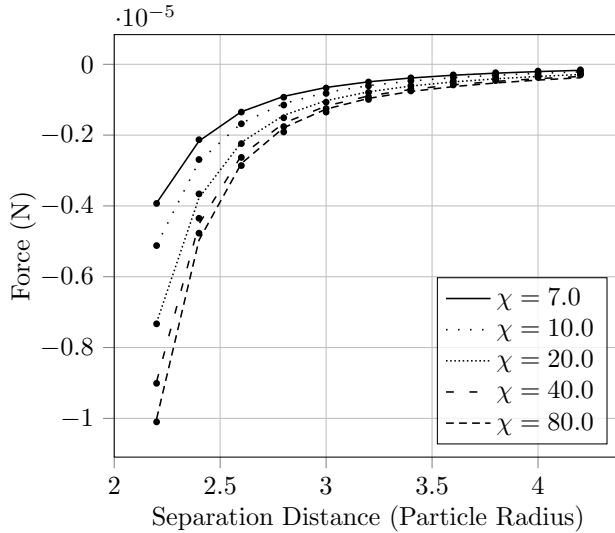
$$F = a^2 H_0^2 (q_3 \chi^3 + q_2 \chi^2 + q_1 \chi + q_0) \quad (3.38)$$

Table 3.3: Empirical model (Parallel case, particles touching, $\theta = 0^\circ$, $c = 2$).

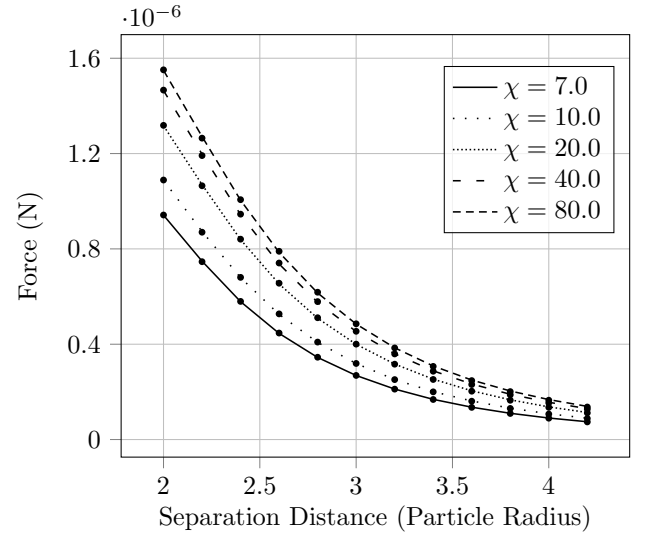
q_3	q_2	q_1	q_0
5.70975153e-10	-1.05822795e-07	-1.75194410e-06	-2.57928572e-06

The empirical model, thus generated, is accurate for susceptibilities ranging 7-80 and separation distances up to 4 particle radii. For separation distances higher than 4.2 radii, fixed dipole or mutual dipole moment methods can be used. MDM gives a closer value to the SH method, but the difference between MDM and FDM is less than 5% for a magnetic susceptibility of 80 and is less than 1% for single-digit susceptibilities.

The empirical model was also tested for lower susceptibilities. The R^2 value for the model decreases



(a) $a=1$ m, $H_0=1$ A/m, $\theta = 0^\circ$



(b) $a=1$ m, $H_0=1$ A/m, $\theta = 90^\circ$

Figure 3.6: Empirical model curves. The ticks represent the SH data, and the lines represent the empirical model.

quite fast as the susceptibilities lower. The model overestimates the force value for lower separation distances. For higher susceptibilities, testing was only done up to 100 susceptibilities. The model provides good accuracy up to those susceptibilities.

3.4.1 Extension for multiple particles

All methods were discussed in the two-particle context so far given in figure 3.1. Now, we discuss the extension for multiple particles for each case. FDM is easily tackled. As before, we assume each particle generated a magnetic field ($\mathbf{H}_{dip}$) given by equation 3.11. Therefore, the force on n^{th} particle due to total N particles is given by modifying equation 3.12.

$$\mathbf{F}_n = \mu_0 \nabla (\mathbf{m}_1 \cdot \left(\sum_{i=1, i \neq n}^{i=N} \mathbf{H}_{dip}(\mathbf{X}_n - \mathbf{X}_i) \right)) \quad (3.39)$$

Similarly, the MDM is extended to include the magnetic field from each particle in the dipole moment calculation.

$$\mathbf{m}_n = \frac{4\pi a^3 \chi_{eff}}{3} \left(\sum_{i=1, i \neq n}^{i=N} \mathbf{H}_{dip}(\mathbf{X}_n - \mathbf{X}_i) \right) \quad (3.40)$$

The FVM directly solves the Maxwell equations numerically. Therefore, it inherently can solve multiple particle systems. The smoothed profile can be modified for the entire system by an overall step function ($s(\mathbf{x})$) given by the sum of individual step functions for each particle.

The SH approximation is valid only for a two-particle system. Both Du et al. [76] and Keaveny and Maxey [1] show that for particles that are close to each other two-body effects are dominant. Keaveny and Maxey [1] give a technique called inclusion model to extend the model by using either fixed or mutual dipole method for far-field effects along with the spherical harmonics for particles that

are close enough to account for higher multipoles.

The comparison of different models, as discussed in section 3.2.4, still holds. The FDM and MDM fail at lower separation distances, while the FVM is too computationally expensive. Therefore, we aim to utilize the inclusion model given by Keaveny and Maxey [1] for our granular mechanics (discrete element) simulations. The empirical model presented in this work provides an analytical framework to perform comparison calculations such as done in [14] and section 3.5. Future work is needed to reach this intended model.

3.5 Implications

To understand the significance of magnetic effects [14] on asteroid surface processes, we compare the force between two particles to attractive forces of various surface gravities (Eq. 3.41), self-gravity (Eq. 3.42) and van der Waals cohesive force (Eq. 3.43) for clean ($S = 1$) and dirty surface ($S = 0.1$). The magnetic force is maximum for particles touching and parallel to the external magnetic field (Eq. 3.38), therefore, that case is considered for Figures 3.7 and 3.9. The case of particles being perpendicular to the external magnetic field is considered in Figure 3.8.

$$F_{gSurface} = \rho \frac{4}{3} \pi a^3 g \quad (3.41)$$

$$F_{gSelf} = G \left(\rho \frac{1}{3} \pi a^2 \right)^2 \quad (3.42)$$

$$F_{cohesion} = 3.6 \times 10^{-2} S^2 a \quad (3.43)$$

Plots in figures 3.7 and 3.8 represent lines for equal surface gravity and magnetic force. Figure 3.7 shows the case where the magnetic field is parallel to the line of contact between the particles. Below

these lines, the magnetic cohesive force dominates over the gravitation force. Individual plots also show the variation with external magnetic field strength, particle susceptibility, and particle density. The plots also mark asteroid Psyche’s mean expected surface gravity, $g = 0.144 \text{ m/s}^{-2}$ [79]. Figure 3.9 compares different forces on particles with magnetic susceptibility $\chi = 40.0$ and density $\rho = 5 \text{ g cm}^{-3}$ from surface gravity, self-gravity, van der Waals cohesion, and magnetic attraction. Identical-sized particles in contact and parallel to the external magnetic field are considered. Magnetic force is the highest for mid-sized particles ($10^{-4} - 1 \text{ m}$). For larger sizes, the gravitational force is dominant.

Kohout et al. [21] suggests that 40 is a reasonable estimate of the magnetic susceptibility of iron and stony-iron asteroid materials. Additionally, Elkins-Tanton et al. [9] list Psyche’s predicted bulk densities from various studies ranging from 2.5 to 11.0 g cm^{-3} , with a majority of them in the 3.5 to 4.5 g cm^{-3} range. We assume a particle density of 5 g cm^{-3} in the plots. Simulations by Fatemi and Poppe [73] assume surface magnetic fields on $5.0 \times 10^{-7} \text{ T}$. At this level of magnetization and particle parameters, the magnetic attraction would equal the gravitational acceleration for particles less than 0.01 microns. However, we note that the magnetic field at the surface of Psyche may be significantly larger as predicted magnetic fields [69] over Gaspra and Braille’s surface are $\mathcal{O}(10^{-5}) \text{ T}$, which would result in the magnetic force matching the gravitational force for particles $\mathcal{O}(100)$ microns. Additionally, if small asteroids with remanent magnetic fields and surface gravities of $\mathcal{O}(10^{-6})\text{G}$ ’s exist, then even weak remanent magnetic fields ($5.0 \times 10^{-7} \text{ T}$) would result in significant forces on 100-micron particles.

Figure 3.7c shows that decreasing the particle density from 5 g cm^{-3} to 1 g cm^{-3} (likely an underestimate) would increase the max size of particles influenced by magnetic forces by an order of magnitude. Similarly, Figure 3.7b shows the range of susceptibilities considered (5-80) resulting in about a two-order of magnitude variation in the particle size significantly influenced by magnetic

forces.

Figure 3.8 shows the case where the magnetic field is perpendicular to the line of contact between the particles. Plots in Figure 3.8 provide a lower bound for particle radius where gravity and magnetic attraction are balanced. At susceptibility $\chi = 40.0$, the magnetic force for the perpendicular case is two orders of magnitude lower than that in the parallel case. Therefore, all curves in Figures 3.8a and 3.8c are shifted by $\mathcal{O}(10^{-2})$ as compared to Figures 3.7a and 3.7c. Additionally, Figure 3.8b shows that the magnetic force is less sensitive to susceptibility for the perpendicular case, as compared to the parallel case.

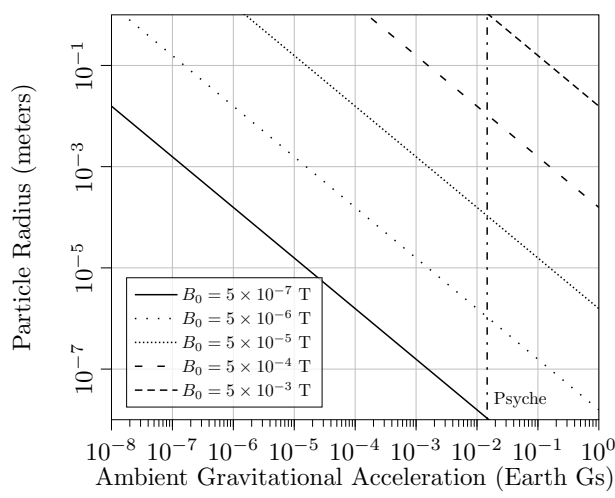
The conditions on asteroids may not be uniform. There would be variations in size, shape, and magnetic susceptibilities of the regolith, and even magnetic field strength would vary. The effects of these variations are not known and are hard to predict. While the presented work provides a technique to model uniform particles in a uniform magnetic field for a specific set of conditions, future investigations are planned to study the complex nature of the anticipated variation. We have only discussed two different orientations of particles and magnetic fields. It is important to note for different morphological structures, the scale of simulations may change, and therefore local variation in the magnetic field will need to be considered. Future works will attempt to answer these questions with both computational and experimental investigations.

If Psyche has retained its submicron particles, given current predictions for the expected remanent magnetic field, the particles are likely to be strongly influenced by magnetic forces. Strong inter-particle forces may influence the larger regolith structure since these very small particles are predicted to ‘cement’ larger particles or boulders together [23]. Additionally, the magnetic attraction between particles may serve as an additional cohesive force, influencing macroscale regolith properties like the angle of repose, which may be observable by visiting spacecraft.

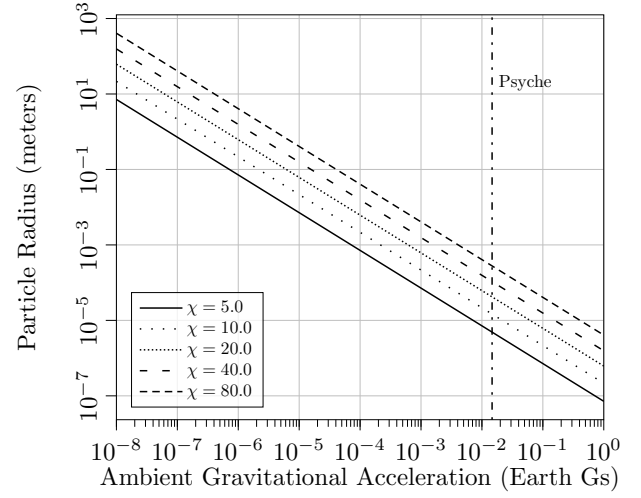
3.6 Conclusions

We have implemented and compared the results of MDM, FVM, and SH models of the magnetic interaction of two identical spherical particles in an externally applied magnetic field, considering magnetic susceptibilities that are representative of the materials expected on M-type asteroids. We have presented an empirical model of these results that is computationally faster and simpler to use than the full numerical solutions albeit for magnetic fields parallel and perpendicular to the axis of contact between two particles considered. The empirical model provides an analytical framework to perform quick balance type calculations. For example, in [14], analytical approximations of different forces are used to compare the significance of different forces on asteroid regolith particles. Researchers can utilize this empirical model to make decisions regarding the need for a magnetic field model in their granular mechanics simulations.

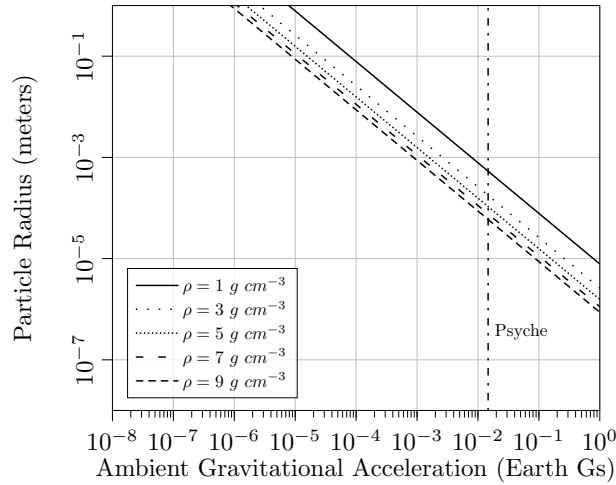
Additionally, the results presented here enable preliminary evaluation of the significance of magnetic interaction for regolith particles on asteroids of varying surface gravities, particle densities, and magnetic susceptibilities. For Psyche, we predict that submicron - 100-micron grains will be strongly influenced by these forces (depending on the surface magnetic field strength, particle susceptibility, and particle density), which could influence the surface morphology of the asteroid.



(a) $\chi = 40.0$ and $\rho = 5 \text{ g cm}^{-3}$

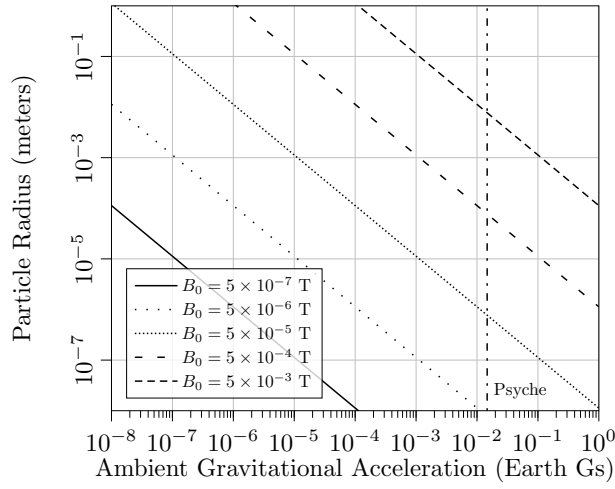


(b) $B_0 = 5 \times 10^{-5} \text{ T}$ and $\rho = 5 \text{ g cm}^{-3}$

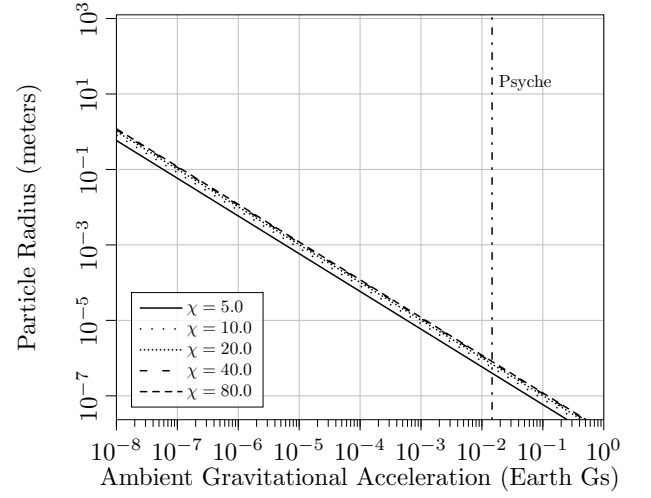


(c) $B_0 = 5 \times 10^{-5} \text{ T}$ and $\chi = 40.0$

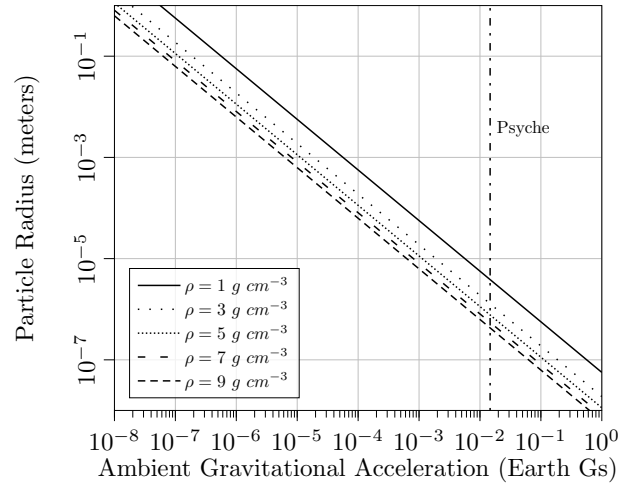
Figure 3.7: Lines of equal force between surface gravity and magnetic attraction between two paramagnetic particles in an external magnetic field. Magnetism dominates under the various lines. Particles are parallel to the external magnetic field.



(a) $\chi = 40.0$ and $\rho = 5 \text{ g cm}^{-3}$



(b) $B_0 = 5 \times 10^{-5} \text{ T}$ and $\rho = 5 \text{ g cm}^{-3}$



(c) $B_0 = 5 \times 10^{-5} \text{ T}$ and $\chi = 40.0$

Figure 3.8: Lines of equal force between surface gravity and magnetic attraction between two paramagnetic particles in an external magnetic field. Magnetism dominates under the various lines. Particles are perpendicular to the external magnetic field.

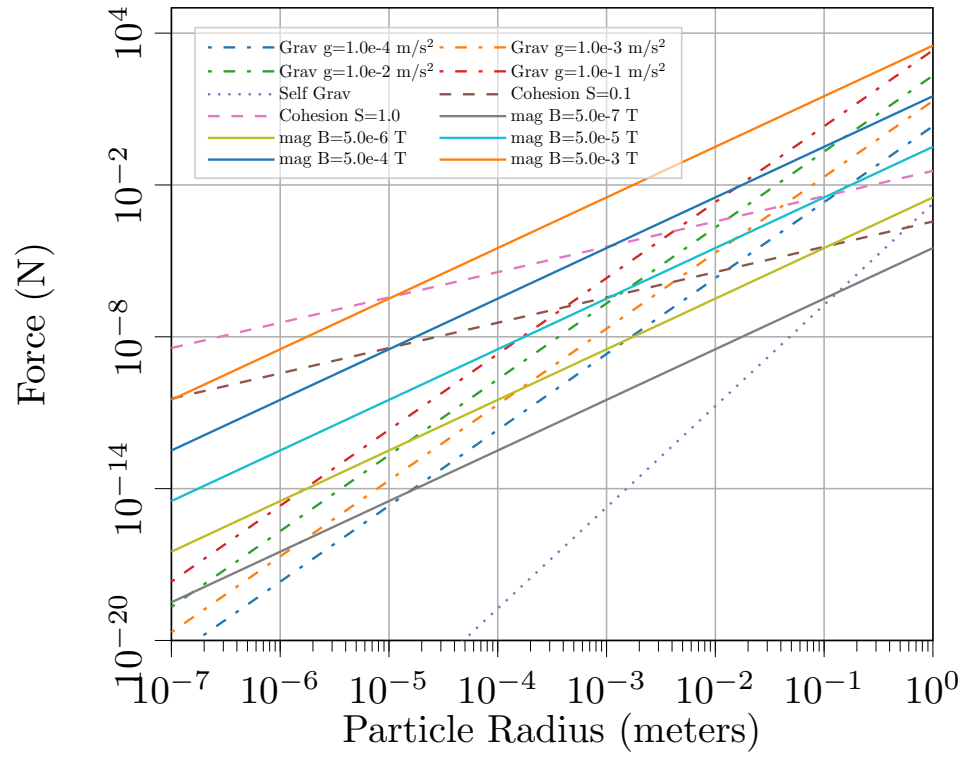


Figure 3.9: Forces on particles with magnetic susceptibility $\chi = 40.0$ and density $\rho = 5 \text{ g cm}^{-3}$ from surface gravity, self-gravity, van der Waals cohesion, and magnetic attraction. Identical-sized particles in contact and parallel to the external magnetic field are considered.

Chapter 4: An Experimentally Validated Magnetic Force Model for Discrete Element Modeling of Paramagnetic Granular Media

This chapter is accepted in its original form as: Sikka, A. and Hartzell, C. (2026) An Experimentally Validated Magnetic Force Model for Discrete Element Modeling of Paramagnetic Granular Media. to the *Granular Matter* journal.

4.1 Introduction

Magnetic interactions between metallic granular particles can result in magnetic cohesion [59]. Various theoretical, experimental, and numerical studies have looked at the effect of magnetic cohesion on the angle of repose and flow characteristics of granular media for Magneto-Rheological Fluids (MRF)[1, 62, 64, 66, 80] and Planetary Science [4, 81] applications. Forsyth et al. [60] conducted experiments with steel ball bearings to show that the angle of repose changes linearly but slowly with increasing magnetic field strength. Fazekas et al. [6] & Taylor et al. [61] performed Discrete Element Modeling (DEM) simulations to validate the experimental results of [60] and provide varying reasons for a slight increase in the angle of repose, even for large cohesive forces. Peters and Lemaire [62] argued that, rather than a uniform magnetic field that results in a highly anisotropic force between particles, a rotating magnetic field is more suitable for control over the avalanching of cohesive particles.

Sunday et al. [4] conducted avalanching experiments with varied particle sizes and two materials to show transitions between three different flow regimes: the granular regime, where particles move independently, the correlated regime, where particles move in clusters, and the plastic regime, where the entire assembly acts as a single block. They showed that the linear increase of the angle of repose with applied magnetic field only holds in the granular regime, while surface roughness parameters: Root-Mean-Square (RMS) height and RMS slope continue to increase in the correlated regime.

Discrete Element Model (DEM) based numerical studies are used to model forces on each particle to simulate magnetic interactions between granular particles using various methods. Fazekas et al. [6] & Taylor et al. [61] used the Fixed Dipole Model (FDM) based on single particle dipoles for magnetic interactions between granular particles. However, various studies [1, 76, 81] have shown that dipolar models, such as FDM, are quite inaccurate when particles are sufficiently close, especially in dense assemblies. In this work, we seek to implement a more accurate magnetic force model for DEM simulations. We build upon the work of Keaveny and Maxey [1] who proposed the Inclusion Model. We present the first experimentally validated DEM model of magnetic interactions of granular materials.

4.1.1 Planetary Science Motivation

Due to surface gravities up to 1 million times smaller than that on Earth, surface grains on traditional (non-metallic) asteroids are significantly affected by van der Waals cohesion [14]. Multiple studies considered the role of cohesion in simulations related to NASA’s successful Double Asteroid Redirection Test (DART) Mission. DART impacted the smaller satellite object Dimorphos in the binary pair of 65803 Didymos and Dimorphos to demonstrate the potential to change an asteroid’s

trajectory for planetary defense. Zhang et al. [24] studied the role of cohesion in the bulk structural stability to maintain the fast rotational spin of the primary asteroid Didymos. Raducan et al. [27] evaluated different values for momentum change for the impact on the satellite Dimorphos to show that Dimorphos must have a weaker cohesive strength than the larger parent Didymos. The OSIRIS-REx mission experienced unexpected behavior due to near-zero cohesion [26] during the sample collection on asteroid 101955 Bennu. Sánchez and Scheeres [82] looked at the cohesive properties of different fine powders in the context of rubble-pile asteroids. These studies demonstrate the need to model and simulate cohesion for asteroid regolith research.

NASA's Psyche spacecraft, launched in October 2023, is headed to the main-belt asteroid 16-Psyche. A predominantly metallic body, 16-Psyche, is assumed to be a remnant core of a protoplanet [9]. A dynamo could have existed in the initial cooling period of the asteroid [11]. This dynamo would result in a magnetic field being locked in the body. Anand et al. [83] model possible magnetic field of 16-Psyche due to Solar Wind Induced Magnetization (WIM). Courville et al. [12] theorizes volcanic dykes on 16-Psyche with magnetic field signatures. Solar plasma wind interaction simulations by Fatemi and Poppe [73] assume surface magnetic fields up to 500 nT. These various theories suggest the possibility of a local surface magnetic field on 16-Psyche. The spacecraft is carrying a magnetometer [10, 72] to measure the magnetic field from orbit.

The likely constituents of M-type asteroids are iron and nickel. These ferromagnetic substances will have paramagnetic ores, resulting in a paramagnetic regolith. Kohout et al. [21] measured magnetic susceptibilities of multiple iron and stony-iron meteorites. When placed in a uniform magnetic field, paramagnetic grains develop a magnetic moment. This moment results in a magnetic force acting between the particles, increasing the net cohesion. Sikka et al. [81] argued that on metallic bodies like 16-Psyche, magnetic cohesion can dominate over surface gravity for sub-micron-sized grains, while

noting that a higher magnetic field strength would further enhance this effect for larger particles.

Robinson et al. [84] showed different gravity-driven morphological features on Eros 433's three craters: Psyche, Himeros, and Shoemaker. Avalanching on the Moon was compared to the same on Earth by Kokelaar et al. [85]. They showed that Lunar avalanches only involve dry-flowing grains, while terrestrial avalanches involve both dry and fluidized grains. Sugita et al. [86] demonstrated evidence of mass-wasting on asteroid 162173 Ryugu using Hayabusa2 observations. The role of volatiles in mass wasting on Vesta and Ceres was studied by Parekh et al. [87]. They concluded that dry granular flows dominate Vesta's mass-wasting, while Ceres shows evidence of fluidized flows. Tang et al. [39] studied mass-wasting on Bennu's Bralguh crater using DEM simulations. All these studies have shown the importance of cohesion in understanding mass wasting and granular flows on small planetary bodies.

Based on granular mechanics, DEM simulations have been used to model the regolith on small bodies. Researchers have used DEM in multiple studies for rubble pile asteroids ranging from reshaping & disruption [22], avalanching [23], and wave transmission [41]. Maurel et al. [38] simulated the Brazil-nut effect on asteroid regolith. DeMartini et al. [30] used a proprietary software PKDGRAV to study and simulate the 2029 tidal encounter of Apophis 99942 with Earth. Frizzell and Hartzell [29, 49], Frizzell et al. [50] simulate wave transmission on regolith to study the cold spot formation around lunar craters. Marohnic et al. [88] looked at the effect of particle shape on rubble-pile dynamics with a new approach to model non-spherical particles. Tang et al. [39] uses the PKDGRAV code to study mass-wasting on the asteroid 101955 Bennu's Bralguh Crater. Many researchers studied the various aspects of the DART mission target: the Dimorphos and Didymos system, including the impact momentum enhancement factor using an integrated smoothed particle hydrodynamics (SPH) and DEM code [45] and the effect of cohesion on the structural stability of Didymos using PKDGRAV

[24].

4.1.2 Magneto-Rheological Fluids Motivation

Magneto-Rheological Fluids (MRF) are suspensions of micron-sized, magnetizable particles in a carrier fluid [89]. Without an external magnetic field, the particles are randomly distributed in the fluid, and the fluid behaves like a Newtonian fluid. When subjected to an applied magnetic field, the particles become magnetized and form chain-like structures along the field lines, thereby altering the bulk rheological properties, such as viscosity. This property of MRFs is exploited in various applications, including dampers, clutches, and prosthetics. Bica et al. [67] provide a comprehensive review of MRF applications in various industries. Understanding the behavior of MRF in various magnetic environments is crucial for optimizing these applications.

Modeling and simulation of MRFs is crucial for predicting their behavior under various conditions. There are two primary approaches to modeling MRFs: continuum models and discrete models. Ghaffari et al. [90] provide a review of both the modeling and simulation techniques used for MRFs. Continuum models treat the system as a continuous medium modeled with rheological equations that describe fluid flow, magnetization, structural formation, and stress-strain relationships. These models are computationally faster but are limited by the rheological equation used and cannot capture particle-level interactions for every application. Finding an accurate rheological equation for MRFs is an ongoing area of research. Discrete models, on the other hand, simulate the behavior of magnetized particles independently of the carrier fluid, enabling a more detailed understanding of particle interactions and dynamics. While these models can be computationally expensive, they provide valuable insights into the microstructural behavior of MRFs. Modeling inter-particle magnetic forces is a key

research area for discrete models. Various methods have been proposed to model magnetic interactions between particles in discrete models.

Han et al. [64] reviewed different magnetic force models used in DEM simulations of MRFs. Most commonly, dipolar models like the Fixed Dipole Method (FDM) and the Mutual Dipole Method (MDM) are employed due to their simplicity and computational efficiency. However, these models have limitations in accuracy, especially when particles are in close proximity. Keaveny and Maxey [1] proposed the Inclusion Model, which improves upon dipolar models, but Han et al. [64] & Ghaffari et al. [90] note that it is highly computationally expensive and therefore not widely adopted. We introduce a critical magnetic time step that allows the Inclusion Model to be run at a larger time step than the Hertzian collision time, making it more computationally feasible for DEM simulations. Our model is implemented in LIGGGHTS, an open-source DEM software, and validated against experiments. This work is the first experimentally validated Inclusion model for magnetic interactions in DEM simulations.

4.1.3 Soft-Sphere Discrete Element Model

Our simulations utilize a Soft-Sphere Discrete Element Modeling (SSDEM) technique to model the interactions between thousands of grains. In discrete element models, equations of motion are integrated at each time step for every particle in the system. Soft-sphere, in particular, means that particles themselves can deform during collisions. Various force models are used to model the different physics of the problem, such as a spring-dashpot for collision dynamics.

Consider a system with a total of N particles. The dynamical equations for a the i^{th} particle (Figure 4.1) are given as

$$m_i \dot{\mathbf{v}}_i = m_i \mathbf{g} + \sum_{j=1}^N (\mathbf{F}_{n,i} + \mathbf{F}_{c,i} + \mathbf{F}_{t,i}) , \quad (4.1)$$

$$I_i \dot{\boldsymbol{\omega}}_i = \sum_{j=1}^N (\mathbf{T}_i - \mathbf{M}_{f,i}) , \quad (4.2)$$

where m_i , I_i , $\mathbf{v}_i$, $\boldsymbol{\omega}_i$ are mass, moment of inertia, translational and rotational velocity respectively of i^{th} particle. $\mathbf{F}_{n,i}$, $\mathbf{F}_{c,i}$, $\mathbf{F}_{t,i}$ are normal, cohesive and tangential forces respectively on the i^{th} particle. Finally, $\mathbf{T}_i$ and $\mathbf{M}_{f,i}$ are the torque and frictional moment on i^{th} particle. The torque is given by $\mathbf{T}_i = a_i \mathbf{F}_{t,i} \times \hat{\mathbf{n}}$ where a_i is the radius of the particle and $\hat{\mathbf{n}}$ is the direction of the normal as shown in the Figure 4.1.

For collision dynamics, we use the Hertz contact model, where the contact force experienced by the particles depends on the overlap ‘ δ ’ (Fig. 4.1) as a power law $\delta^{3/2}$. The Hertz contact model requires the simulation time step (dt) to be less than the Hertzian collision time (τ_{hc}) [91], that is usually in 10^{-6} order of magnitude. Along with the contact model, we use an elastic spring and dashpot-based static and rolling friction model [92]. The cohesion is a simplified JKR - Johnson-Kendall-Roberts (SJKR) model [93] based on cohesion energy density. The cohesive force is given by $\mathbf{F}_c = kA\hat{\mathbf{n}}$ where k is the cohesion energy density in J/m^3 units, and A is the contact area between the two particles.

4.1.4 Paper Overview

This paper presents the implementation of the modified Inclusion model for magnetic interactions of spherical particles, as proposed by Keaveny and Maxey [1], implemented in the open-source

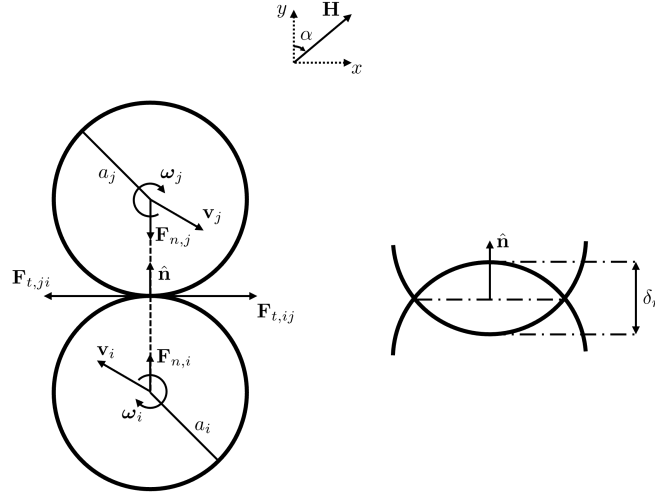


Figure 4.1: Soft-sphere discrete element model. a represents the particle radius, $\hat{n}$ represents the normal at the point of contact, $\mathbf{H}$ is the applied magnetic field, $\mathbf{v}$ and $\boldsymbol{\omega}$ are the particle velocity and angular velocity respectively, and $\mathbf{F}_t$ and $\mathbf{F}_n$ are the tangential and normal forces on each particle. Subscripts i and j represent the two particles. δ_n is the overall distance between the particles during collision. The applied magnetic field is at an angle α to the line joining the two particles. Velocities and forces are not in the same plane as the magnetic field necessarily.

DEM software LIGGGHTS [46] and validated with experimental results from Sunday et al. [4]. Section 4.2 reviews the magnetostatics equations and the theoretical background for magnetic force models for granular particles.

Section 4.3 describes the implementation of the magnetic force model in the open-source DEM software LIGGGHTS. We detail the numerical methods, including the Mutual Dipole Method (MDM) and the Inclusion Model, and discuss computational considerations for efficient simulation. We also introduce the critical magnetic time step, which allows the magnetic force model to be run at a larger time step than the Hertzian collision time.

Section 4.4 presents validation of the implemented models against analytical and published results for simple particle systems, demonstrating the accuracy and limitations of each approach.

Section 4.5 applies the model to simulate avalanching of metallic grains under varying magnetic field strengths, comparing simulation outcomes to experimental results. We replicate flow regimes

along with trends for angle of repose, surface roughness, and root mean square (RMS) slope, demonstrating the model's effectiveness in capturing magnetic cohesion effects.

Section 4.7 concludes with a summary of contributions, limitations, and directions for future work.

4.2 Magnetostatics

Consider a system of N spherical particles placed in a uniform magnetic field $\mathbf{H}_0$. Each particle has a radius a and a magnetic susceptibility χ . Neglecting free and displacement currents, we can write Laplace's equations [63] using scalar magnetic potential Φ such that $\mathbf{H} = -\nabla\Phi$:

$$\nabla^2\phi_{out} = 0 \quad \nabla^2\phi_{in,i} = 0, \quad (4.3)$$

where ϕ_{out} is the potential outside the particle and $\phi_{in,i}$ is the potential inside the i^{th} particle. The boundary conditions for the Laplace equations at particle surfaces ($r_n = a$) are given by:

$$\phi_{out} = \phi_{in,i} \quad \mu \frac{\partial\phi_{in,i}}{\partial r_n} = \mu_0 \frac{\partial\phi_{out}}{\partial r_n}, \quad (4.4)$$

where μ is the permeability of the particle and μ_0 is the permeability of free space. Additionally, as $r_n \rightarrow \infty$, $\phi_{out} \rightarrow -\mathbf{H}_0 \cdot \mathbf{r}_n$.

The general solution to the Laplace equations (equation 4.3) is an infinite sum of spherical harmonics. Magnetic force models are based on an approximation of this infinite series.

Earlier studies [6, 61] employed the Fixed Dipole Method (FDM) to model magnetic interactions between granular particles. Recent studies [43, 64, 66, 80] pivot to the more accurate Mutual Dipole

Model (MDM). Sikka et al. [81] compared different models of magnetic force, such as the Mutual Dipole Method (MDM) [1], the Finite Volume Model (FVM) [76], and the Spherical Harmonic Approximation (SHA) [1]. They concluded that SHA presents the most accurate results while being fairly computationally efficient. FVM can provide comparable accuracy to the SHA, but it is significantly slower. While being fast, the MDM loses accuracy when particles are closer than 3 particle radii. However, the SHA only applies to a two-particle system and, therefore, cannot be applied to a system of multiple particles. Keaveny and Maxey [1] provided an Inclusion model to calculate the force on each particle placed in a uniform magnetic field by combining dipole-based models such as FDM and MDM, with SHA, thereby providing a potential framework for multi-particle systems. However, to the best of our knowledge, the Inclusion model has not been implemented in any DEM software. We specifically implemented and compared the Inclusion model to the MDM.

4.2.1 Mutual Dipole Method

The Mutual Dipole Model (MDM) extends the Fixed Dipole Method (FDM), the simplest model. In both cases, the magnetic moment of a particle is assumed to be dipolar. The FDM only uses the external magnetic field to calculate the magnetization for each particle. A single particle placed in the uniform magnetic field $\mathbf{H}_0$ gains a dipole moment,

$$\mathbf{m} = C\mathbf{H}_0, \quad C = \frac{4}{3}\pi a^3 \chi_{eff}, \quad (4.5)$$

where a is the particle radius and $\chi_{eff} = \frac{3\chi}{\chi+3}$ is particle effective susceptibility.

FDM assumes that every particle is dipolar and doesn't affect the others. MDM addresses the second assumption by incorporating the effect of the magnetic field generated by every other particle.

A particle with dipole moment $\mathbf{m}$ changes the magnetic field around it by $\mathbf{H}_{dip}$ [1],

$$\mathbf{H}_{dip}(\mathbf{r}) = \frac{1}{4\pi} \left(\frac{3\mathbf{m} \cdot \mathbf{r} \mathbf{r}}{r^5} - \frac{\mathbf{m}}{r^3} \right), \quad (4.6)$$

where $\mathbf{r}$ denotes a coordinate system centered at the particle. MDM accounts for this change in the magnetic field when calculating the dipole moments. For the i^{th} particle, the moment $\mathbf{m}_i$ is then given by [1]:

$$\mathbf{m}_i = C_i \left(\mathbf{H}_0 + \sum_{j=0, j \neq i}^N \mathbf{H}_{dip,j}(\mathbf{r}_{i,j}) \right), \quad (4.7)$$

where $\mathbf{r}_{i,j}$ is the separation distance vector from i^{th} particle to j^{th} particle. Equations 4.6 and 4.7 result in a $3N \times 3N$ linear system of equations. The moments of all the particles are coupled and must be solved simultaneously. We discuss numerical methods to solve this system in section 4.3.2. The calculated moment is then used to calculate the dipolar force ($\mathbf{F}_i^{dip}$) on each particle [1],

$$\mathbf{F}_i^{dip} = -\mu_0 \nabla \left(\mathbf{m}_i \cdot \sum_{j=0, j \neq i}^N \mathbf{H}_{dip,j}(\mathbf{r}_{i,j}) \right). \quad (4.8)$$

4.2.2 Inclusion Model

The Inclusion model provided by Keaveny and Maxey [1] removes the assumption of considering only dipoles. When particles are closer together, other multipoles, in addition to the dipole, become significant. The Inclusion model improves MDM by calculating the SHA solution, which accounts for ‘ L ’ multipoles, for particle pairs with separation distances less than a cutoff distance. Below, we give a brief description of the Inclusion model.

Step 1: Calculate forces using a dipolar approach like MDM.

Step 2: Identify the particle pairs with separation distances lower than the cut-off distance.

Step 3: Calculate force using the SHA on the selected particle pairs. There are some important considerations when applying SHA here. The MDM already included the dipolar terms for the selected particle pair. Therefore, Keaveny and Maxey [1] provides some corrective measures to ensure that no calculation is performed twice. Along with dipolar corrections, a component of the magnetic field due to the out-of-plane component of the dipole moment from the MDM needs to be added to the Maxwell Stress Tensor [63]:

$$\mathbf{T} = \mu_0 \left(\mathbf{H}\mathbf{H} - \frac{1}{2} H^2 \mathbf{I} \right), \quad (4.9)$$

$$\mathbf{F}_i = \int_{V_i} \nabla \cdot \mathbf{T} dV. \quad (4.10)$$

With the corrective terms calculated, the magnetic field is now known. We can use the equations 4.9 and 4.10 to calculate the force.

4.3 Magnetic Model Implementation

We use LIGGGHTS, an extensively validated SSDEM solver, for our work. In addition to being open-source, multiple force models are available for contact, rolling friction, and cohesion. Various researchers have extended LIGGGHTS with different models, showcasing its ease of adding new models. Finally, the software can scale with parallel processing on High-Performance Computing servers. Therefore, we could focus on implementing the magnetic force model. To ensure correctness, we validated the force models in LIGGGHTS by running unit test cases [31]. The tangential history model needed corrections [29] as a particle didn't stop at the theoretical distance after sliding on a wall.

LIGGGHTS is based on the C++ language and some legacy Fortran-based codes. Users only

need to add the corresponding source and header files with the same class style to add a new capability. Various class styles in LIGGGHTS provide a base structure to extend the functionality. For example, the `atom` class deals with all particle-centric properties like position, velocity, force, and such. For all computations, the source code uses simple C-style data structures. We instead build LIGGGHTS with `eigen` and `boost` libraries to access efficient linear algebra and numerical integration functions.

We defined a new `fix` for the magnetic force model in LIGGGHTS called `fix magnetic`. A `fix`, in LIGGGHTS, is a modular component applied during time integration to modify particle behavior [94]. It takes six arguments along with the `fix ID` and `group-ID`. The first three arguments define the components of the applied magnetic field $\mathbf{H}_0$ in A/m units in the simulation coordinate frame. Next, we define the magnetic time step (*mag_steps*), followed by model type (could be `mdm` or `inclusion`) and finally the dipole moment calculation method (could be `convergence` or `linalg`). An example magnetic `fix` is as follows:

```
fix mag all magnetic 0 0 1 100 mdm convergence
```

The `fix` currently only works with SI units. It also needs the `atom_style` to be `hybrid granular dipole` as the particles need to be granular and dipolar. Per particle type, the property called `magneticSusceptibility` needs to be defined for this magnetic `fix`. To run the magnetic model at a different time step (dt_{mag}), we modified the LIGGGHTS `atom` class to add another variable called `mag_f` similar to the existing total force variable `f`. This variable stores the magnetic force for each particle each time a new force is calculated. At all other time steps, the same force is propagated. All the modified `atom` classes and magnetic code (folders `src/DIPOLE` and `src/MAGNETIC`) can be found at our public LIGGGHTS fork [95].

4.3.1 Critical Magnetic Time

The computation time for the magnetic model is comparatively the highest among the different force models. With the time step being on the order of microseconds ($dt \rightarrow \mathcal{O}(10^{-6})$), the magnetic model can be run at a larger time step. The particles don't move much in a single time step, resulting in minimal change to the magnetic force. This variable time step can help reduce the computational load of the magnetic model. There are different formulations for critical time steps for the Hertzian force model. LIGGGHTS uses the Hertzian collision time (τ_{hc}), which is based on the maximum possible relative velocity of a particle pair v_{max} ,

$$v_{max} = 2 \max_i^N |\mathbf{v}_i|, \quad (4.11)$$

where $\mathbf{v}_i$ is the the velocity of i^{th} particle.

$$\tau_{hc} = \min_{i,j}^N \left[2.87 * \left(\frac{m_{eff}^2}{a_{eff} * E_{eff}^2 * v_{max}} \right)^{0.2} \right], \quad (4.12)$$

where effective mass is $m_{eff} = \frac{m_i m_j}{m_i + m_j}$, effective radius $a_{eff} = \frac{a_i a_j}{a_i + a_j}$ and effective Young's Modulus is given using poisons ratio ν

$$\frac{1}{E_{eff}} = \frac{1 - \nu_i^2}{E_i} + \frac{1 - \nu_j^2}{E_j}. \quad (4.13)$$

Using a similar formulation, we defined a critical time step for the Magnetic force model. Sikka et al. [81] developed an empirical model for the force between two identical sphere paramagnetic particles. They provide three simplified formulas for calculating the magnetic force between particles in specific orientations: parallel to the magnetic field, perpendicular to the field, and touching while

parallel to the field. The formula (Equation 4.14) for particles parallel to the field provides the maximum possible force between a particle pair. We use this empirical model in our definition of critical magnetic time

$$F = F_{DM} + \mu_0 a^2 H_0^2 \sum_{i=1}^3 \frac{p_i(\chi)}{c^{4+i}}, \quad (4.14)$$

$$p_i(\chi) = \sum_{j=0}^4 q_j^i \chi_{eff}^j \quad i = 1, 2, 3. \quad (4.15)$$

where $c = r/a$ and the coefficients q_j^i are given in [81]. Given this force, we can find $\frac{dF}{dr}$. We know that the values of F and $\frac{dF}{dr}$ are maximum at $r = 2$ for a given susceptibility. First, we find the change in relative position Δr for which the magnetic force changes by 100%,

$$\Delta r(\chi) \approx \left[\frac{1}{F(\chi)} \frac{dF}{dr}(\chi) \right]^{-1}. \quad (4.16)$$

Now, we can use the maximum relative velocity to define the critical magnetic time (τ_{mag}),

$$v_{max} \tau_{mag} \approx \left[\frac{1}{F(\chi)} \frac{dF}{dr}(\chi) \right]^{-1}. \quad (4.17)$$

We have implemented this into our LIGGGHTS model using a `fix check/timestep/mag` command. The user inputs the tolerable $\frac{\Delta F}{F}$ and the time step at which they want to check the magnetic time. It is worth noting that the empirical formula is based on a spherical harmonic approximation. Therefore, the critical magnetic time τ_{mag} would be much smaller than the exact definition using the FDM or MDM model. A larger tolerance is advised when using the MDM model. We compare the critical magnetic time with the Hertz collision time in one set of our simulations as discussed in section

4.5.4.

4.3.2 MDM Implementation

The MDM method described in section 4.2.1 requires a solution to $3N \times 3N$ linear system. For large systems with $\approx 1000s$ of particles, even optimized C++ libraries like `eigen` require a lot of computational resources. One possible solution is to limit the dipole influence of each particle (eq. 4.6) as it directly scales with the cube of the distance from the particle (r^3). Fazekas et al. [6] employ a similar technique for force calculation using the FDM by keeping the magnetic force cutoff at $\approx 6.25D$ where D is the particle diameter. Han et al. [64] show that for an infinite chain of particles, a force cutoff of $\approx 6a$ gives less than 5 % relative error. While force cutoff is a possible solution for the FDM model and dispersed/special systems, we observed that the aggregate of all small interactions from far-field particles becomes significant for a large particle system. Leps and Hartzell [66] implemented an MDM solver in LIGGGHTS while using a cut-off distance. They used a convergence algorithm instead of solving the linear system.

However, their convergence algorithm is not guaranteed to converge each time. Han et al. [64] proposed a convergence algorithm using the Gauss-Seidel method. This method uses the latest dipole moment value rather than the value from the last step as described in the following equation.

$$\mathbf{m}_i^{k+1} = \mathbf{m}_i^0 + C_i \sum_{j=0, j \neq i}^N \frac{(3\hat{\mathbf{r}}_{ij} \cdot \hat{\mathbf{r}}_{ij}^T - \mathbb{I})}{4\pi r_{ij}^3} \mathbf{p}, \quad (4.18)$$

$$\text{where } \mathbf{p} = \begin{cases} \mathbf{m}_j^{k+1} & \text{if } j < i \\ \mathbf{m}_j^k & \text{if } j > i. \end{cases} \quad (4.19)$$

By stacking the dipole moments of each particle, we can create a stacked moment vector $\mathbf{m} = [\mathbf{m}_i]^T$, and we can define a new $3N \times 3N$ matrix called $\mathbb{R}$ whose 3×3 elements at $3i, 3j$ can be defined as $\mathbb{R}_{3i,3j} = C_i \frac{(3\mathbf{f}_{ij} \cdot \mathbf{f}_{ij}^T - \mathbb{I})}{4\pi r_{ij}^3}$ to result in the following linear discrete-time system,

$$\mathbf{m}_{k+1} = \mathbf{m}_0 + \mathbb{L} \mathbf{m}_{k+1} + \mathbb{U} \mathbf{m}_k , \quad (4.20)$$

where $\mathbb{L}$ and $\mathbb{U}$ are lower and upper triangular matrices of $\mathbb{R}$ respectively. As $\mathbb{R}$ has a zero diagonal, $\mathbb{L}$ and $\mathbb{U}$ are strictly triangular matrices. By applying the same technique to this system, we need to examine the eigenvalues of $(\mathbb{I} - \mathbb{L})^{-1}\mathbb{U}$. Using that $\mathbb{L}$ and $\mathbb{U}$ are strictly triangular with all eigenvalues equal to zero. It can be shown that $(\mathbb{I} - \mathbb{L})^{-1}\mathbb{U}$ has all eigenvalues equal to 0. Therefore, the system converges.

In our implementation (Algorithm 1), we use this discrete-time system given in equation 4.18. Different columns of the $\mathbb{R}$ matrix are calculated by individual processors as per their local particles. Then, the convergence algorithm is applied on processor 0, after which the converged moments are distributed to all the processors. We also implement another algorithm to solve the $3N$ linear systems of equations described in equations 4.6 and 4.7. It follows the same principle as the convergence algorithm. The $3N \times 3N$ linear system can be written in terms of the earlier defined $\mathbb{R}$ matrix by modifying the discrete-time system,

$$\mathbf{m} = \mathbf{m}_0 + \mathbb{R} \mathbf{m} , \quad (4.21)$$

$$(\mathbb{I} - \mathbb{R})\mathbf{m} = \mathbf{m}_0 . \quad (4.22)$$

Each processor calculates the corresponding components (for local particles) of both $(\mathbb{I} - \mathbb{R})$ and

Algorithm 1 Convergence-based Mutual Dipole Method for LIGGGHTS

```
initialization;
each local processor calculates column matrices for  $\mathbb{R}$  matrix
for every  $i^{th}$  local particle do
  for  $j = 0$  to  $N - 1$  do
    if  $i \neq j$  then
      calculate the  $3 \times 3$  matrix  $\mathbb{R}_{3j,3i}$ ;
    end if
  end for
  stack  $\mathbb{R}_{3j,3i}$  for  $j = 0$ 
end for
Gather all local matrices to create the  $\mathbb{R}$  matrix on proc 0;
if proc == 0 then
   $k_{max} = \text{max number of convergence steps};$ 
   $\epsilon = \text{convergence threshold};$ 
  for  $k = 0$  to  $k_{max} - 1$  do
    for  $i = 0$  to  $N - 1$  do
       $\mathbf{m}_i^0 = C_i \mathbf{H}_0;$ 
       $\mathbf{m}_i^k = \mathbf{m}_i^0;$ 
      for  $j = 0$  to  $N - 1$  do
        if  $i < j$  then
           $\mathbf{m}_i^k = \mathbf{m}_i^k + \mathbb{R}_{i,j} \mathbf{m}_j^{k-1};$ 
        else if  $i > j$  then
           $\mathbf{m}_i^k = \mathbf{m}_i^k + \mathbb{R}_{i,j} \mathbf{m}_j^k;$ 
        end if
      end for
       $m_{dif}(i) = \frac{\|\mathbf{m}_i^k - \mathbf{m}_i^{k-1}\|}{C_i \|\mathbf{H}_0\|};$ 
    end for
    if  $\max_i m_{dif}(i) < \epsilon$  then
      break ;
    end if
  end for
end if
```

m_0 . These are gathered on processor 0, and the linear system is solved using the `eigen` library's `ColPivHouseholderQR` algorithm, which is based on the Householder rank-revealing QR decomposition of a matrix with column pivoting. The calculated moments are then scattered to the respective processors for housekeeping.

LIGGGHTS uses neighbor lists to track particle pairs and potential interactions between them. These lists are generated by each processor for its local particles. Therefore, every processor only stores information for local particles and their neighbors. While this setup is both memory and computationally efficient for other DEM force models, our magnetic model requires all particle pairs to be considered. We modify the neighbor parameters for our simulations to generate neighbor lists that include all particle pairs.

To ensure all particle pairs are considered, we need the neighbor cutoff distance, known as `neighbor_skin` distance in LIGGGHTS, to encompass the whole simulation domain. We refer to a neighbor list with all particle pairs as a complete neighbor list. This larger `skin` distance has some drawbacks. Each processor has its own neighbor list for each local particle. If neighbors for a particle are local to another processor, information pertaining to those particles is shared between the processors. With a complete neighbor list, there is a significant communication overhead. Therefore, it is essential to optimize the number of processors used.

Another critical parameter is the frequency of neighbor list generation. For a complete neighbor list, we could, in theory, never update the neighbor list after the simulation setup. However, LIGGGHTS also decides if a particle should be moved between processors during neighbor list generation. If the neighbor list is not updated, all particles remain associated with their initial processors, even if they have moved significantly within the simulation domain. At the end of the simulation run, LIGGGHTS identifies the particles that have moved significantly, determines they are behaving abnor-

mally, and deletes them. Any restart file generated after the run would not contain the said particles. Therefore, the frequency of neighbor list generation also needs to be optimized.

4.3.3 Force Calculation

Once the moments are calculated with either `linalg` or `convergence` (Algorithm 1), we can calculate the dipolar force between particles. The force between two dipolar particles can be calculated as [76]:

$$\mathbf{F}_{i,j}^{dip} = \frac{3\mu_0}{4\pi r^4} \left[(\mathbf{m}_i \cdot \hat{\mathbf{r}}) \mathbf{m}_j + (\mathbf{m}_j \cdot \hat{\mathbf{r}}) \mathbf{m}_i + (\mathbf{m}_i \cdot \mathbf{m}_j) \hat{\mathbf{r}} - 5(\mathbf{m}_i \cdot \hat{\mathbf{r}})(\mathbf{m}_j \cdot \hat{\mathbf{r}}) \hat{\mathbf{r}} \right] \quad (4.23)$$

where $\mathbf{r} = \mathbf{r}_j - \mathbf{r}_i$, $r = |\mathbf{r}|$ and $\hat{\mathbf{r}} = \mathbf{r}/r$.

Therefore, the force on a single particle is the sum of the forces on all other particles,

$$\mathbf{F}_i^{dip} = \sum_{j=0, j \neq i}^{N-1} \mathbf{F}_{i,j}^{dip}. \quad (4.24)$$

The force due to the spherical harmonics approximation ($\mathbf{F}_i^{sha}$) for the Inclusion model (discussed more in the next section) is calculated for particle pairs with separation distances less than four radii ($r_{i,j}/a_i = c < 4$). Therefore, the total magnetic force on the i^{th} particle (Algorithm 2) is calculated,

$$\mathbf{F}_i^{mag} = \mathbf{F}_i^{dip} + \mathbf{F}_i^{sha}. \quad (4.25)$$

The calculated force $\mathbf{F}_i^{mag}$ is then assigned to `atom` class variables for total force (`f`) and magnetic

force (mag_f).

Algorithm 2 Force Calculation

```

initialization;
if  $dt \bmod mag\_steps$  then
    for every  $i^{th}$  local particle do
         $f[i] += mag\_f[i];$ 
    end for
else
    for every  $i^{th}$  local particle do
        for  $j = 0$  to  $N - 1$  do
            if  $i \neq j$  then
                calculate  $\mathbf{F}_{i,j}^{dip}$ 
                 $\mathbf{F}_i^{dip} = \mathbf{F}_i^{dip} + \mathbf{F}_{i,j}^{dip}$ 
                if  $r_{i,j} < 4a_i$  and  $model\_type == 'inclusion'$  then
                    calculate  $\mathbf{F}_{i,j}^{sha}$ 
                     $\mathbf{F}_i^{sha} = \mathbf{F}_i^{sha} + \mathbf{F}_{i,j}^{sha}$ 
                end if
            end if
        end for
         $\mathbf{F}_i^{mag} = \mathbf{F}_i^{dip} + \mathbf{F}_i^{sha}$ 
         $mag\_f[i] = \mathbf{F}_i^{mag}$ 
         $f[i] += mag\_f[i]$ 
    end for
end if

```

4.3.4 Inclusion Model Implementation

As described in the force calculation algorithm 2, the `model_type inclusion` only affects the calculation of $\mathbf{F}_{i,j}^{sha}$. We use a cutoff distance to ascertain when to incorporate multipoles for a particle pair by calculating the SHA force. Sikka et al. [81] and Figure 4.5 show that MDM and SHA converge quickly for a two-particle case. Therefore, we finalized a cutoff distance of three radii ($3a$). We have a separate class called `sphericalharmonics` to calculate the SHA force. The initializer takes six input arguments: the particles' radius (a), the particles' susceptibility (χ), the applied magnetic field vector ($\mathbf{H}_0$), the separation distance vector ($\mathbf{r}_{i,j}$) and finally the respective

dipole moments ($\mathbf{m}_i$ and $\mathbf{m}_j$).

The `spherical_harmonics` class initializes the two $2L \times 2L$ linear systems needed for spherical harmonics approximation. Table 4.1 is used to find the number of multipoles L to be used for a given susceptibility χ . The corrections to the system are added to account for the dipolar force that has already been calculated.

In a two-body isolated case, each particle would only have in-plane components (plane with the two particles and the external magnetic field) of the dipole moments. We therefore need to ensure that the corresponding spherical harmonics (β_{11} and β_{10} in equation A.2) don't have the dipolar force calculated twice. The bulk scenario, instead, would have an out-of-plane component of dipole moment. Keaveny and Maxey [1] include a new term in the Inclusion model based on this out-of-plane component. One can think of this as adding a β_{12} into the equation A.2. But, there are no such terms in any other multipoles in the SHA formulation; therefore, it results in non-physical phenomena in bulk simulations. This phenomenon is further discussed in detail in the sub-section 4.3.4.1. The validation cases discussed in [1] are all particle chains with all out-of-plane components equal to zero. We remove this term in our implementation.

The linear system is then solved using the `ColPivHouseholderQR` algorithm mentioned earlier. The surface integral of the Maxwell stress tensor (equation 4.10) was first reduced analytically using Mathematica. The reduced polynomial dependence is then solved with `boost` library's Gaussian Konrod algorithm. The Spherical Harmonics Approximation and the reduced polynomials are discussed in detail in the Appendix A.

4.3.4.1 Out-of-plane Dipolar Correction

The out-of-plane dipole correction is applied to the SHA force to add additional information from the out-of-plane component of the dipole moment calculated during the MDM method. The scalar potential $\Phi_{out-plane}$ is given by [1]:

$$\Phi_{out-plane,i} = \frac{\mathbf{m}_i \cdot \hat{\mathbf{y}}}{4\pi a^3} \frac{P_l^m \cos \theta_i \sin \phi_i}{r_i^2}, \quad (4.26)$$

where P_l^m is the associated Legendre polynomial, $\mathbf{m}_i$ is the dipole moment and r_i , θ_i and ϕ_i are the spherical coordinates of the i^{th} particle respectively. The correction to the magnetic field is then the sum of the gradient of scalar potentials of the two particles, i and j :

$$\mathbf{H} = -\nabla \Phi_{out-plane,i} - \nabla \Phi_{out-plane,j}. \quad (4.27)$$

We can use simple geometric relations to convert the spherical coordinates of one particle to another by including the separation vector $\mathbf{c}$. We observed a unique non-physical phenomenon once we implemented these equations into our model. The top particles are further from the center of the box in a spiral motion. To understand this phenomenon, we simulated boxes of different sizes. We used three different box sizes: Size 1: $35 \times 35 \times 130$ mm, Size 2: $85 \times 85 \times 130$ mm, and Size 3: $120 \times 120 \times 130$ mm with the same particle size (6.35 mm diameter) and susceptibility ($\chi = 3.6$). The magnetic field is applied in the $+z$ direction, with all other parameters held constant across the three boxes.

Figure 4.2 shows the dipolar moments of the particles. We see that the x-component of dipole moment (Figures 4.2a, 4.2d, 4.2g) have opposite signs near opposing x-walls while the y-component of

Table 4.1: Number of Multipoles (L) for a given magnetic susceptibility (χ). These values were obtained by testing the two-particle configuration (section 4.4.1) for different susceptibilities and finding the minimum number of multipoles required for convergence.

χ	(0, 4)	[4, 7)	[7, 12)	[12, 20)	[20, 35)	[35 – 55)	[55, 75)	[75 – 100)
L	10	20	30	40	45	50	75	80

dipole moment (Figures 4.2b, 4.2e, 4.2h) have opposite signs near opposing y-walls. The z-component of the dipole moment is aligned in the positive z-direction, the same as the applied magnetic field. These dipole moments contribute to the out-of-plane term, leading to a spiral motion.

In Figure 4.3, we plot the specific angular momentum about the center of the box of top particles against their distance from the center for each of the three boxes. Most particles have positive angular momentum, indicating rotational motion about the center of the box. For the smallest box, the top particles quickly settle out of the spiral motion because the walls are too close for the given particle radius. We can observe that the particles at the center (further away from the wall) have almost zero velocities for other sizes. In contrast, the particles closer to the walls have higher velocities. Particles closest to the walls have lower angular momentum because they are slowed down by friction with the walls. Therefore, we observe a peak in angular momentum at some distance between the center and the wall.

We conclude that including the out-of-plane term in the SHA implementation leads to this non-physical rotation because the MDM model lacks the corresponding out-of-plane terms. This could be achieved by including another multipole in the far-field calculation and the MDM. We remove this out-of-plane correction term, as the aim of this study is to implement a more accurate model than dipolar models such as MDM.

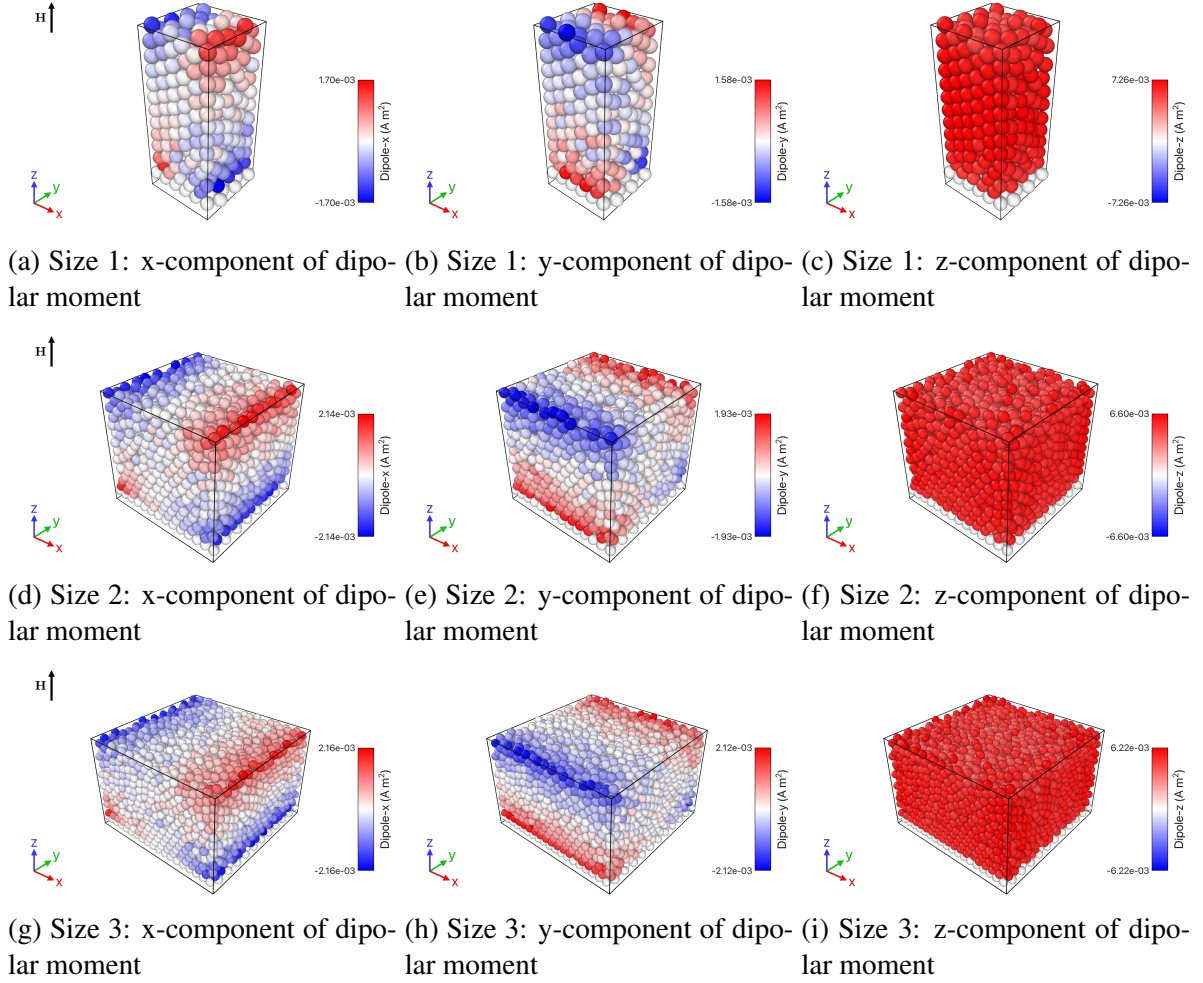


Figure 4.2: Dipolar moments of particles for three different sizes: Size 1: $35 \times 35 \times 130$ mm, Size 2: $85 \times 85 \times 130$ mm, and Size 3: $120 \times 120 \times 130$ mm. The applied magnetic field is in the positive z-direction (upwards). The x-component of the dipole moment is shown to be opposite near opposing x-walls (4.2a, 4.2d, 4.2g), while the y-component is opposite near opposing y-walls (4.2b, 4.2e, 4.2h). These figures illustrate the effect of the out-of-plane dipolar moment term in the Inclusion model, leading to spiral motion. Therefore, we require the modification of removing the out-of-plane correction term as described in section 4.3.4.1.

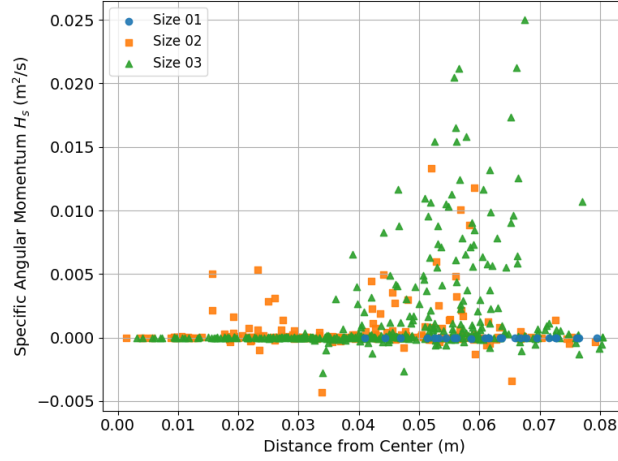
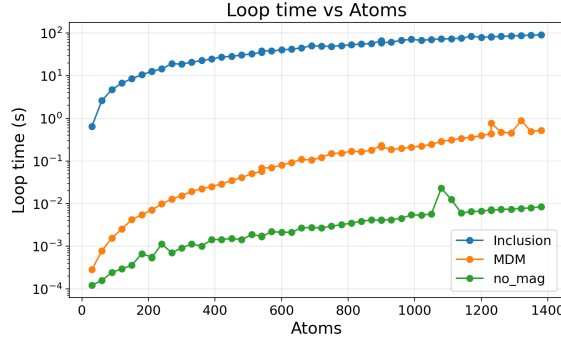


Figure 4.3: Specific Angular Momentum about the center of the box of top particles against their distance from the center for three different box sizes at a representative time step. The H_s increases as the distance of the particles from the center increases, indicating the spiral motion around the center of the box. Size 01: $35 \times 35 \times 130$ mm, Size 2: $85 \times 85 \times 130$ mm and Size 3: $120 \times 120 \times 130$ mm.

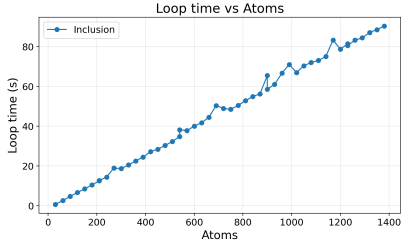
4.3.5 Computational Comparison

We compared the computation cost of the MDM (convergence-based) and the Inclusion model by systematically increasing the number of particles in hexagonal close-packed (HCP) configurations. A box of dimensions $10 \times 10 \times 100$ m was used for this comparison study. The particles were arranged in an HCP configuration with a particle radius of 1 m and a susceptibility of $\chi = 1$. The magnetic field was applied in the z-direction, and the force was calculated twice for each configuration and each model. We increased the number of particles by increasing the number of layers in the z-direction while keeping the x and y dimensions constant. There is no particle motion in this computational comparison. The results for loop times (total run-time in LIGGGHTS output file) are shown in the Figure 4.4. We also include the computational effort of the no-magnetic force calculation for reference.

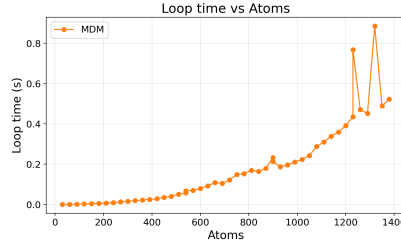
It is clear that the MDM model is much more computationally efficient than the Inclusion model.



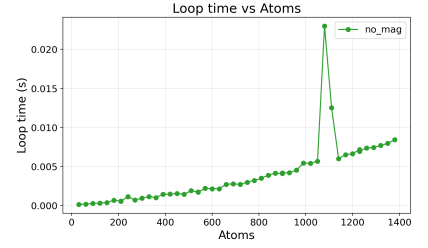
(a) Logarithmic scale of loop time for all three cases.



(b) Loop time for Inclusion model.



(c) Loop time for MDM model.



(d) Loop time for no magnetic force case.

Figure 4.4: Computational effort of the MDM and Inclusion model for different numbers of particles in an HCP configuration. The computational effort of no magnetic force calculation is also included for reference. The MDM model is more computationally efficient than the Inclusion model and scales quadratically with the number of particles, while the Inclusion model scales linearly. The loop times for the Inclusion model are approximately two orders of magnitude higher than the MDM model, while the MDM model is approximately one order of magnitude higher than the no magnetic force case.

The loop times for the Inclusion model are approximately two orders of magnitude higher than the MDM model, while the MDM model is approximately one order of magnitude higher than the no magnetic force case. The computational effort for the Inclusion model is linear, while the MDM model is quadratic with the number of particles, as expected. These results are for a specific configuration and may vary for different configurations, but they provide a general idea of the computational effort required for each model. The MDM model, being more computationally efficient, is suitable for larger simulations with sparse particle configurations as the accuracy of the MDM model is comparable to the Inclusion model for such cases, as shown in the validation cases in the next section. For dense particle configurations, the Inclusion model is more accurate, but the computational effort may be prohibitive for larger simulations.

4.4 1-D Validations

We validated the model against simple 1-D test cases for which the results are available in the literature [1, 76, 81]. We tested both algorithms (`convergence` & `linalg`) for the MDM model. Results for these always matched; therefore, for the rest of the paper, MDM refers to the convergence-based algorithm only.

4.4.1 Two-Particle Case

We first tested the magnetic force model for two particles in two configurations by varying the inter-particle distance to compare it with [1] and [81]. We also show (Figure 4.5) the results for the SHA model. The angle α is varied to test different orientations of the magnetic field with respect to the line joining the two particles. We tested two orientations: parallel ($\alpha = 0^\circ$) and perpendicular

($\alpha = 90^\circ$). SHA is considered to be an exact result for the two-particle case when a large number of multipoles are considered ($L \approx 20$ & 40 for $\chi = 1$ & 4 respectively) [1]. The Inclusion model matches exactly with SHA, as no other far-field force exists. The MDM underestimates the force when particles are closer together in the case of parallel magnetic field orientation, while it overestimates the force for perpendicular orientation. We also tested the quadratic dependence [81] on particle radius (a) and applied magnetic field magnitude (H_0) as other test cases consider unit values for these parameters.

4.4.2 Three-Particle Case

For the three-particle configuration, we fix two particles to be touching, and the third particle's distance is varied along the line connecting all three particles. The force on the moving particle is plotted. The results of this test case, shown in Figure 4.6, match with [1] where they suggest a pairwise Spherical Harmonic Approximation with more multipoles ($L = 20$ for $\chi = 1$ and $L = 30$ for $\chi = 4$) is equivalent to the exact force. The Inclusion model closely matches the exact force for all four cases considered. The MDM model is very inaccurate for higher susceptibilities ($\chi = 4$) in both external magnetic field orientations (parallel and perpendicular to the line joining the particles).

4.4.3 Eight-Particle Case

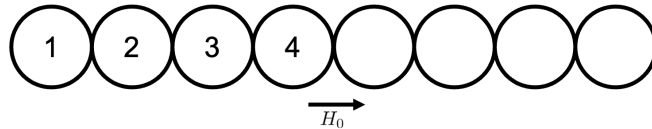
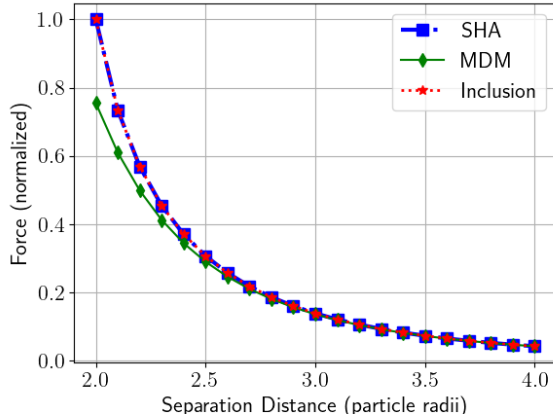
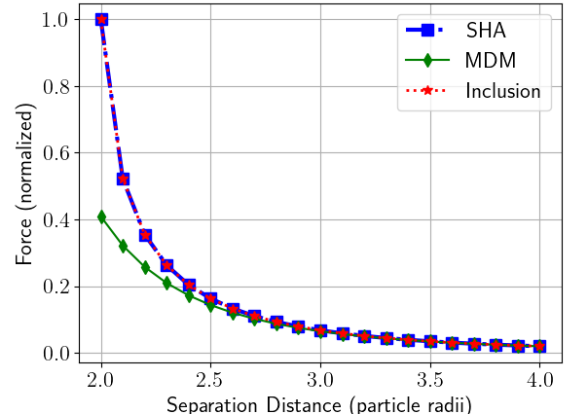


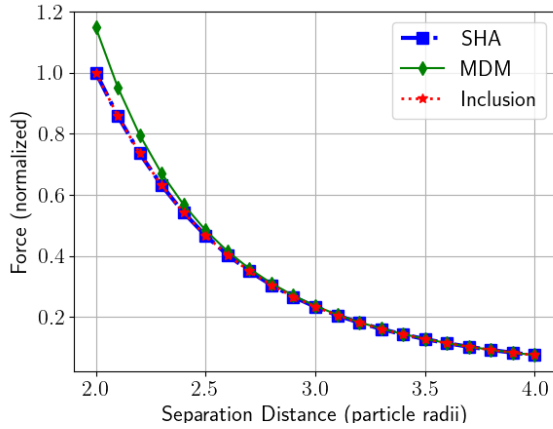
Figure 4.7: Eight-particle chain; applied with aligned with axis of the chain ($\chi = 1$; $H_0 = 1$)



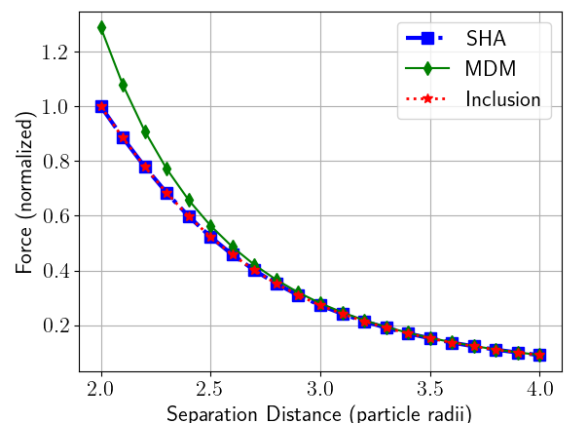
(a) $a = 1$ m, $H_0 = 1$ A/m, $\alpha = 00^\circ$, $\chi = 1.0$



(b) $a=1$ m, $H_0=1$ A/m, $\alpha = 00^\circ$, $\chi = 4.0$



(c) $a=1$ m, $H_0=1$ A/m, $\alpha = 90^\circ$, $\chi = 1.0$

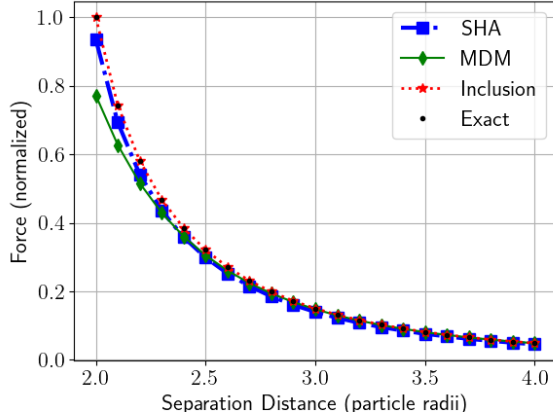


(d) $a=1$ m, $H_0=1$ A/m, $\alpha = 90^\circ$, $\chi = 4.0$

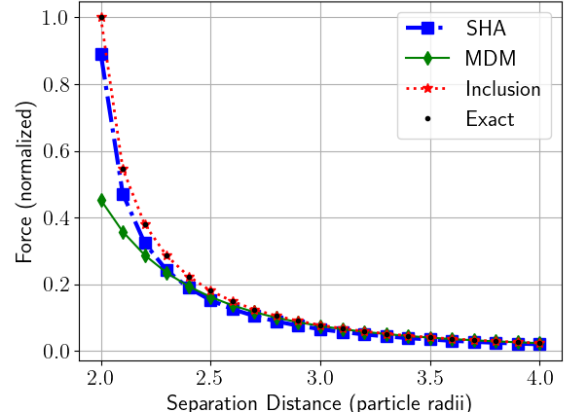
Figure 4.5: Validation curves for a two-particle configuration. The force is normalized by the value when the particles are touching. For higher susceptibility, the MDM underestimates the force when particles have a separation distance less than 2.5 particle radii. SHA is considered the exact force in this two-particle case.

Table 4.2: MDM Results for 8 particle chain configuration: Expected force (N) [1] and percentage error (against expected force) for the various particles (Figure 4.7) for different average neighbors. The error percentage is calculated as $\frac{F_{expected} - F_{calculated}}{F_{expected}} \times 100\%$

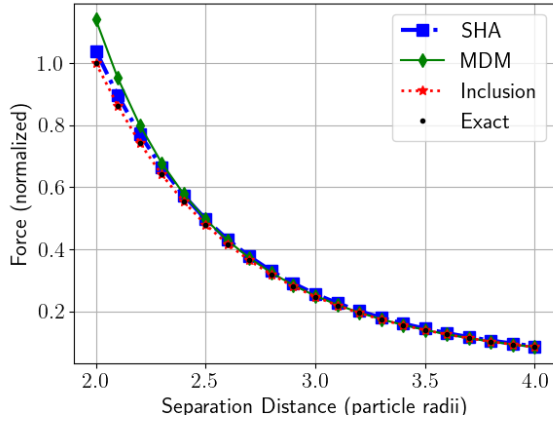
Particle Number	Expected Force (N)	Average number of neighbors per particle				
		4.5	5.5	6.25	6.75	7
1	5.0252E-07	-1.04%	-0.45%	-0.19%	-0.06%	0.00%
2	7.5187E-08	-4.09%	-1.30%	-0.21%	0.11%	0.00%
3	1.8014E-08	-12.60%	-1.82%	0.90%	0.06%	0.00%
4	3.9195E-09	-39.78%	6.44%	0.46%	0.06%	0.01%



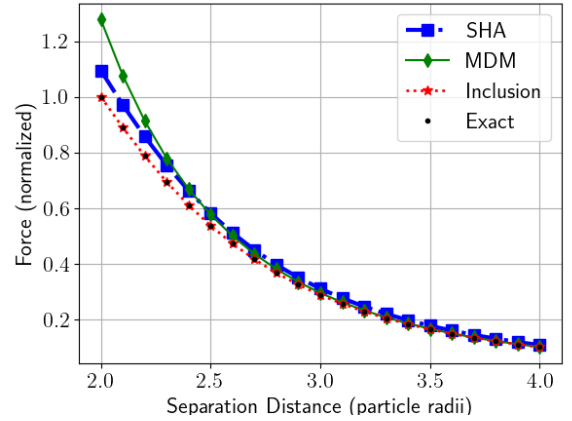
(a) $a=1$ m, $H_0=1$ A/m, $\alpha = 00^\circ$, $\chi = 1.0$



(b) $a=1$ m, $H_0=1$ A/m, $\alpha = 00^\circ$, $\chi = 4.0$



(c) $a=1$ m, $H_0=1$ A/m, $\alpha = 90^\circ$, $\chi = 1.0$



(d) $a=1$ m, $H_0=1$ A/m, $\alpha = 90^\circ$, $\chi = 4.0$

Figure 4.6: Validation curves for a three-particle configuration. The force is normalized by the value when the particles are touching. For higher susceptibility, the MDM underestimates the force when particles are closer than 2.5 particle radii, while the SHA is closer to the exact solution, and the Inclusion model matches the exact force closely.

Table 4.3: Inclusion Results for 8 particle chain configuration: Expected force (N) [1] and percentage error (against expected force) for the various particles (Figure 4.7) for different average neighbors. The error percentage is calculated as $\frac{F_{expected} - F_{calculated}}{F_{expected}} \times 100\%$

Particle Number	True Force (N)	Expected Force (N)	Average number of neighbors per particle				
			4.5	5.5	6.25	6.75	7
1	6.38E-07	6.4659E-07	-1.01%	-0.53%	-0.31%	-0.21%	-0.16%
2	7.07E-08	7.9784E-08	-3.84%	-1.20%	-0.18%	0.10%	-0.02%
3	1.72E-08	1.8894E-08	-11.75%	-1.48%	0.93%	0.03%	-0.03%
4	3.84E-09	4.0966E-09	-37.25%	6.88%	0.43%	0.02%	-0.02%

Keaveny and Maxey [1] also tested the Inclusion model for an eight-particle chain depicted in Figure 4.7. We reproduce the results with our model here in Tables 4.2 and 4.3. We tried different neighbor skin distances (Force cut-off in LIGGGHTS), resulting in different average number of neighbors per particle. These tests were our first indication that a force cut-off for magnetic force could result in an inaccurate calculation. Considering a lower number of average neighbors results in higher error percentages. Especially when the cut-off distance was less than 4 particle diameters (average neighbors: 5.5), the error percentages were close to 40% for the middle particles. Both the MDM and Inclusion models exhibited this behavior. When all particles are considered as each other’s neighbors (average neighbors: 7.0), we observed that our model matches the expected force value [1]. Therefore, we concluded that the magnetic force model is sensitive to the neighbor skin distance. In our subsequent simulations, we considered all particle neighbor pairs.

4.5 Avalanching of Metallic Grains

After validating the magnetic force model with simple 1-D cases, we tested the model against more complex scenarios. Sunday et al. [4] performed avalanching experiments with brass and steel balls placed between two Helmholtz coils to simulate a uniform magnetic field. We modeled the same setup in LIGGGHTS to reproduce the bulk behavior of metallic grains with our model. Previous avalanche studies have examined the effects of magnetic cohesion on the angle of repose of steel grains through experimental [60] and numerical [6, 61] investigations. Sunday et al. [4] performed experiments with different particles and a larger range of magnetic field strength than Forsyth et al. [60]. Fazekas et al. [6] & Taylor et al. [61] used a dipolar algorithm for force calculation, which is inaccurate at closer distances, as shown in Section 4.4. They could not reproduce the increase

in angle of repose or the bulk flow regimes, such as the correlated and uncorrelated regimes. Our implementation can be used with either the dipolar algorithm or the Inclusion model. We tested both algorithms to compare their results.

4.5.1 Setup

Sunday et al. [4] uses 3.18 mm, 6.35 mm, and 8.73 mm-sized grains. We looked at the experiments with 8.73 mm grains, as fewer particles provide a reasonable computational time. Figure 4.8 shows the simulation setup. An avalanche is triggered by removing the middle partition wall. The length of the box (x -axis) is 280 mm, with a middle partition at 130 mm. The width (y -axis) is 85 mm while the height (z -axis) is initially set to 130 mm. The floor is modeled with brass particles (Figure 4.9a) that are frozen in a hexagonal closed packing to simulate a coarse floor. We use fixed boundaries in LIGGGHTS with granular walls (`fix wall/gran`) to keep particles within the simulation box. The magnetic susceptibility for walls is set to zero to simulate non-magnetic walls. The middle partition wall is also modeled similarly. The gravity is in the downward ($-z$) direction while the applied magnetic field is in the upward ($+z$) direction. Once particle assembly is prepared, we change the ceiling (`change_box`) to a shrink-wrapped boundary condition to have fewer idle processors. The middle partition is removed (`unfix`) to initiate the avalanche.

4.5.2 Material Properties

We used three materials in the simulation: alloy steel for magnetic particles, brass for the floor particles, and acrylic for the walls, including the middle partition. The material properties are given in Table 4.4. The densities (ρ) for alloy steel and brass are modeled the same as [4]. Multiple DEM

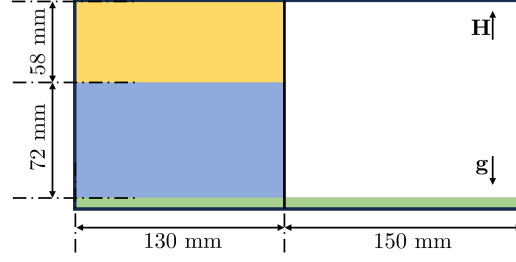


Figure 4.8: Mass wasting setup: Green section are the fixed floor particles in a hexagonal packing, blue section is filled with the magnetic particles for avalanching and the yellow section is used to insert particles while preparing the particle assembly.

studies [5, 29] have shown that using a factor of 0.01-0.0001 to the actual Young's modulus (E_0) does not affect bulk flow behavior. The Hertz collision time, and therefore time-step (dt), however, directly depends on Young's modulus ($dt \propto \sqrt{E}$). We use a 0.01 to E_0 factor for our E values to keep computation time reasonable. The mechanical properties of the walls were based on PMMA material [5].

The interaction properties between different materials, the coefficient of restitution (e), and the rolling friction coefficients (μ_r , $\gamma_{d,r}$) were based on DEM studies by Hlosta et al. [5]. The friction coefficient varied between 0.3 [5] and 0.7 [6]. We start with the values by [5] for all interaction properties. We then calibrate the interaction properties' values to match the angle of repose of experiments [4] in the absence of any magnetic field. The calibrated values are mentioned in Table 4.5.

We set the magnetic susceptibility for the walls and the brass particles to zero because they are assumed to be non-magnetic. Two types of susceptibility values are mentioned in the literature: bulk susceptibility and material susceptibility. Material susceptibility is intrinsic to the material, while bulk susceptibility depends on the shape and size of the material sample. Sunday et al. [4] mentions the bulk effective susceptibility of the coarse alloy grains to be 3.59 ± 0.12 . However, the material susceptibility is mentioned to range between 13 and 100. Sunday et al. [4] observed that the steel particles demonstrated plastic flow behavior starting at 25 mT field strength. We varied the material

Table 4.4: Material Properties for Avalanching [2, 3, 4]

Quantity	Symbol	Units	Steel	Floor (Brass)	Wall (Acrylic)
Density	ρ	(kg/m ³)	7800	8500	1250
Young’s modulus	E	(MPa)	2100	1100	30
Poisson ratio	ν	(-)	0.3	0.375	0.4
Magnetic Susceptibility	χ	(-)	3.6 – 40.0	0	0

Table 4.5: Interaction Properties for Avalanching [5, 6]

Quantity	Symbol	Units	Steel-Steel	Steel-Floor	Steel-Wall
Coeff. of restitution	e	(-)	0.80	0.70	0.40
Friction coefficient	μ_s	(-)	0.2	0.15	0.10
Rolling friction coeff.	μ_r	(-)	0.02	0.015	0.01
Rolling visc. damping	$\gamma_{d,r}$	(-)	0.02	0.02	0.02
Cohesion energy density	k_c	(mJ/m ³)	2	2	2

susceptibility between 3.6 and 40.0 at a field strength of 25 mT. With the Inclusion model, we could reproduce the flow behavior with a material susceptibility of 20.0.

4.5.3 Particle Assembly Preparation

Each simulation starts with preparing a particle assembly. We use the same particle size for the floor (brass) and the bulk (steel) particles. The particles are modeled as spheres with a diameter of 8.73 mm (coarse). We arrange the floor particles in a hexagonal packing using LIGGGHTS’ `lattice` command (Figure 4.9a). The left half is filled by pouring particles and allowing them to settle under gravity, as it provides more control over the packing fraction (φ) [29]. The packing fraction is defined as the ratio of the volume of particles to the total bulk volume. For packing fraction calculation, we only consider the assembly region up to the height of 72 mm (blue in Figure 4.8). The particles are inserted using `ins/rate/region fix` in LIGGGHTS. We define an insertion region (yellow in Figure 4.8), insertion rate, total number of particles inserted, and a random seed. The particles are



Figure 4.9: Different stages of particle assembly preparation to obtain a desired packing fraction.

inserted at a rate of 2 per time step (dt). A slow insertion rate facilitates a higher packing fraction of the assembly and, therefore, a compact particle assembly. We aim for a packing fraction of $\varphi \approx 0.59$ to match experiments [4]. The extra particles are then deleted to ensure a fixed height (72 mm).

In some cases, we tap the assembly to achieve the required packing fraction (Figure 4.9c). The assembly floor is provided with a sinusoidal vibration: $z_t = z_0 + A \sin(2\pi ft)$ [29]. We use the same amplitude ($A = 0.5$ mm) and frequency ($f = 30$ Hz) as used by Frizzell and Hartzell [29]. The tapping is done for fixed intervals, and the packing fraction is calculated. Once the desired packing fraction is achieved, we stop the tapping. The final particle assembly (Figure 4.9d) is then used to perform various avalanching simulations using a restart file (`write_restart` command). We provide input scripts and restart files in our dataset [96]. Multiple seeds are used to generate different assemblies for the same packing fraction.

For each simulation, we first allow the particles to settle after switching on the external magnetic field. By ‘settle’, we mean particles should reach a steady state. We define the steady state by observing the simulation and the total kinetic energy plots. The total kinetic energy becomes negligible for cases

Table 4.6: Critical magnetic time step (τ_{mag}) and hertz collision time (τ_{hc}) for different field strengths at 0.1ms magnetic time step (mag_t) for our time sensitivity analysis. The ratio of the two is also shown.

H (mT)	τ_{hc} (s)	τ_{mag} (s)	Ratio ($\frac{\tau_{mag}}{\tau_{hc}}$)
5.0	2.176272e-05	1.121155e-01	5.151722e+03
15.0	2.215137e-05	1.224906e-01	5.529708e+03
30.0	2.414839e-05	1.885994e-01	7.810023e+03

with lower magnetic cohesion (lower susceptibility and field strength), as all particles stop moving. However, in some cases with higher magnetic cohesion, not all particles come to a complete stop. Some particles fall into a steady state around local magnetic fields, oscillating around a local minimum.

Once the assembly is settled, we use this simulation frame as our *pre-avalanche state*. Then, an avalanche is initiated by deleting (using `LIGGGHTS unfix` command) the middle partition wall. The particles are then allowed to fall freely under the influence of gravity. We run each simulation for at least 1.5 seconds more, after which we start checking for the steady state. Once a steady state is reached, we treat the last frame as the *post-avalanche state*.

4.5.4 Sensitivity Analysis for Magnetic Time step

Table 4.7 shows the various time-steps used. Each simulation's time step (dt) is kept to $5\mu s$. The magnetic time step (mag_t) refers to the time step used for a new magnetic force calculation. The magnetic steps value used for the `fix magnetic` is calculated as $mag_steps = \frac{mag_t}{dt}$. Neighbor time step is a similar value used to calculate how often LIGGGHTS constructs a new neighbor list.

We performed a sensitivity analysis for the magnetic time step (mag_t) to ensure that this parameter does not affect our results. MDM simulations were conducted with 6.35 mm particles, magnetic susceptibility of 40.0 (the highest in our study), and applied field strengths of 5.0 mT, 15.0 mT, and

Table 4.7: Time steps used in the simulations.

Quantity	Symbol	Units	Value
Time step	dt	μs	5
Magnetic time step	mag_t	ms	1
Neighbor time step	(-)	ms	10

30.0 mT, as these parameters provide the most magnetic cohesion and therefore are critical for our analysis. The three magnetic time-steps considered were 10.0 ms, 1.0 ms, and 0.1 ms while keeping all other simulation parameters and particle properties (Tables 4.4 & 4.5) the same. Figure 4.10 shows the total kinetic energy at each frame for the three different magnetic time steps. Table 4.6 shows the critical magnetic time and hertz collision time along with the ratio of the two for each case.

The 10.0 ms magnetic time step never settled from a 30 mT field strength, while the 1.0 ms and 0.1 ms magnetic time steps settled for all three field strengths. The 1.0 ms and 0.1 ms magnetic time steps have similar kinetic energy profiles for all three field strengths. τ_{mag} is much higher than τ_{hc} for all three field strengths, which is expected. The order of magnitude of the ratio of τ_{mag} to τ_{hc} is around 10^3 for all three field strengths. We concluded that a magnetic time step of 1.0 ms (three orders of magnitude higher than the simulation time step of $5 \mu s$) is suitable for our simulations, providing a good trade-off between accuracy and computational time. In all our subsequent simulations, we used a magnetic time step of 1.0 ms or 2.0 ms when particle velocities were low to speed up the simulations.

4.5.5 Data Analysis

To analyze the simulation results, we examine three different granular flow parameters: Flow Behavior, Angle of Repose, and Surface Roughness [4]. Surface roughness is determined using the root-mean-squared (RMS) height and the RMS slope. Python, with the NumPy, SciPy, and Pandas

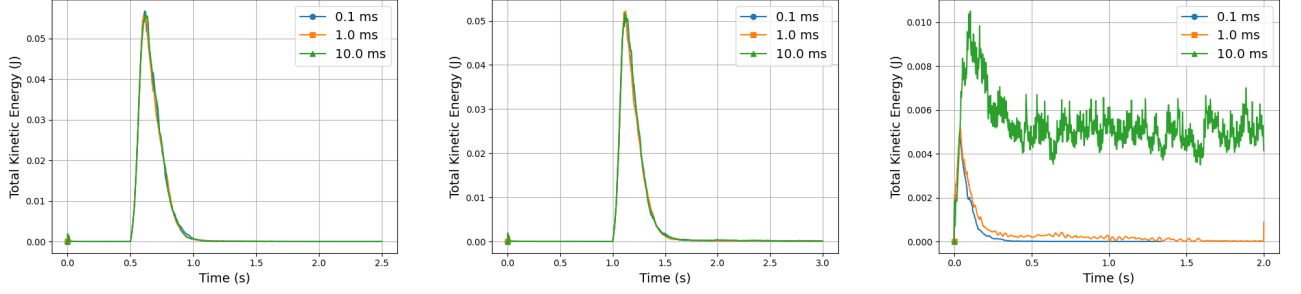


Figure 4.10: Sensitivity analysis for magnetic time step (mag_t) with 6.35 mm particles, susceptibility of 40.0, and field strengths of 5.0 mT (Left), 15.0 mT (Middle), and 30.0 mT (Right). The magnetic time step of 10.0 ms never settles for a 30 mT field strength, while the 1.0 ms and 0.1 ms magnetic time steps settle for all three field strengths. The 1.0 ms and 0.1 ms magnetic time steps have similar kinetic energy profiles for all three field strengths.

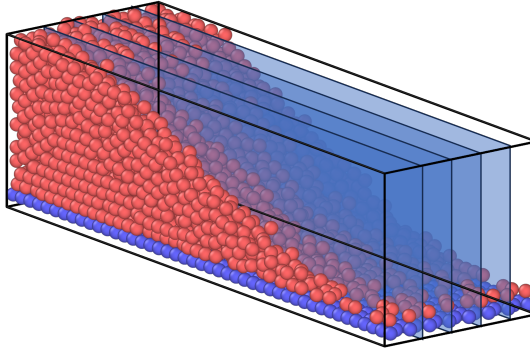


Figure 4.11: Different slices to analyze the angle of repose, RMS height, and RMS slope. The simulation width is divided into five equal slices.

libraries, is used for data analysis, and Ovito Pro [97] is used for visualization. We visually analyze the flow behavior to assess whether our model can recreate the three flow regimes: granular, correlated, and plastic. The angle of repose and surface roughness were analyzed by comparing the top particles in the pre-avalanche and the post-avalanche state. To find the top particles, we divide the simulation box into a grid along the x axis with cells of particle radius size ($a \times w \times h$, where a is the particle radius, w is the simulation width, and h is the height of the simulation box). We then find the highest particle in each grid cell and look at any particle with vertical displacement less than half the particle radius $\Delta y < \epsilon = a/2$ to find the list of stationary particles that haven't moved between the two frames.

We look at two different values for the angle of repose (θ) and surface roughness (RMS height ξ and RMS slope θ_{rms}). First, as in Sunday et al. [4], we collapse the y -dimension (width) of the simulation and find general values. Second, we also analyze the variation of these parameters in the y -axis (width) by calculating them for different slices (Figure 4.11). We divide the simulation width into five equal y -slices and compute the angle of repose, RMS height, and RMS slope for each y -slice. Therefore, we are able to obtain multiple unique values for each of our three data analysis parameters: 3 or 4 from different seeds and 5 within each seed from the y -slicing.

4.5.5.1 Angle of Repose

We measured the angle of repose (θ) by fitting a line through the centers of the top-most particles in the final post-avalanche frame. Some particles were removed from the left and the right side before fitting the line. Stationary particles between the pre-avalanche and post-avalanche frames are removed from fit consideration. We find the stationary particles by comparing only the y -displacement ($\Delta y < a/2$). The right side is trimmed to the furthest particle, resulting in the best fit (R^2 value).

4.5.5.2 Surface Roughness

Both RMS height (ξ) and RMS slope (θ_{rms}) are calculated for all the top particles in the post-avalanche state without any trimming. The RMS height is given by

$$\xi = \left[\frac{1}{n-1} \sum_{i=1}^n (z_i - \bar{z})^2 \right]^{1/2}, \quad (4.28)$$

where n is the number of particles considered, z_i is the height of the i^{th} particle and $\bar{z}$ is the mean height of the n particles. The RMS slope is calculated by

$$\theta_{rms} = \tan^{-1} \left(\frac{v(\Delta x)}{\Delta x} \right), \quad (4.29)$$

where Δx is the difference in x -coordinate of consecutive particles and

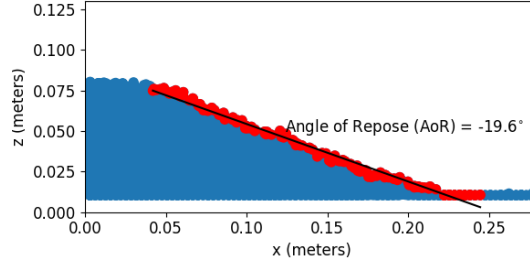
$$v(\Delta x) = \left[\frac{1}{n} \sum_{i=1}^n [z_i - z_{i+1}]^2 \right]^{1/2}. \quad (4.30)$$

The difference in x -coordinate (Δx) remains constant as the particle radius (a).

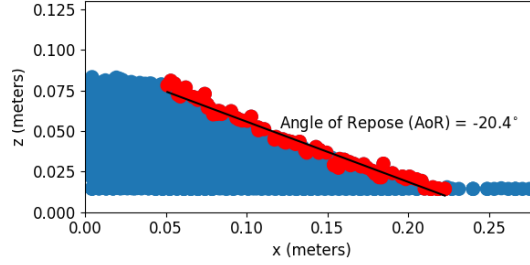
4.5.6 Non-Magnetic Results

Figure 4.12 shows the final frames when no external magnetic field is applied. We performed non-magnetic simulations with both particle sizes (6.35 mm and 8.73 mm) to validate our interaction properties (Table 4.5). The fine particles (6.35 mm) were simulated first to calibrate the interaction properties by matching the angle of repose to approximately 19° [4]. Based on our four different seeds with 6.35 mm particles with a packing fraction of $\varphi = 0.62 \pm 0.01$, we calculated the angle of repose as $19.97^\circ \pm 0.67^\circ$. The surface roughness parameters were: RMS height $\xi = 5.33 \pm 0.50$ mm and RMS slope $\theta_{rms} = 23.46^\circ \pm 1.12^\circ$.

We then used the same interaction properties for the coarse particles (8.73 mm). The angle of repose was calculated as $20.12^\circ \pm 1.02^\circ$, which is within the experimental range of $20.15^\circ \pm 0.17^\circ$ [4]. The surface roughness parameters were calculated: RMS height $6.53 \text{ mm} \pm 0.96 \text{ mm}$ and RMS slope $26.06^\circ \pm 1.00^\circ$. These values validated the calibrated interaction properties (Table 4.5) for both



(a) 6.35 mm particles



(b) 8.73 mm particles

Figure 4.12: Final frame for seed 1 with no applied magnetic field. (a) 6.35 mm particles, (b) 8.73 mm particles.

particle sizes. Table 4.8 summarizes the angle of repose and surface roughness values for both particle sizes.

4.5.7 Magnetic Results

We performed avalanching simulations with both the MDM and Inclusion magnetic models. The magnetic susceptibility was calibrated to 20.0 based on simulations matching the flow behavior to experiments [4] as explained in section 4.5.2. The magnetic field was varied from 2.5 mT to 25 mT for both models.

Table 4.8: Angle of repose and surface roughness values for both particle sizes with no applied magnetic field.

a (mm)	φ (-)	θ (°)	ξ (mm)	θ_{rms} (°)
6.35	0.62	19.97 ± 0.67	5.33 ± 0.50	23.46 ± 1.12
8.73	0.59	20.12 ± 1.02	6.53 ± 0.96	26.06 ± 1.00

We used three different seeds for 8.35 mm particles with the Inclusion model for each simulation to account for variability in the initial packing. Figure 4.13 shows the final frames for the Inclusion model with different field strengths. The results reproduced the three flow regimes: granular, correlated, and plastic at different field strengths. The correlated regime was observed at 15-20 mT, while the plastic regime was observed at 25 mT. Figure 4.14 shows the angle of repose and surface roughness trends with increasing field strength for MDM and the Inclusion model, along with the experimental data in Sunday et al. [4]. We demonstrate the same quantitative increase in the angle of repose and surface roughness parameters as observed in experiments [4]. The angle of repose increased from $20.12^\circ \pm 1.02^\circ$ (no field) to $31.03^\circ \pm 3.00^\circ$ (20 mT). The RMS height increased from 6.53 ± 0.96 mm (no field) to 11.04 ± 1.38 mm (15 mT). The RMS slope increased from $26.06^\circ \pm 1.00^\circ$ (no field) to $42.15^\circ \pm 1.62^\circ$ (20 mT). The surface roughness trends are shifted between the experimental and Inclusion models. We attribute this to different data analysis techniques. Sunday et al. [4] used image processing to find the profile of the top of the avalanche pile. We, on the other hand, use particle center data for analysis. This discrepancy results in shifts in the trends for surface roughness parameters, while the percentage increase remains the same. Therefore, the modeling matches the experimental results.

We do not include the RMS slope data from the 5 slices, as the RMS slope is sensitive to the number of particles considered, and the slices significantly reduce the number of particles. The RMS

slope values from the slices were all over 40° . Figure 4.15 shows the top particles considered in each slice for the no field case. Each slice has a different number of top particles considered, resulting in higher RMS slope values compared to the collapsed width case.

We performed MDM simulations for a single seed to compare the results to the Inclusion model. Figure 4.13 shows the final frames for the MDM model with different field strengths, while Figure 4.14 shows the angle of repose and surface roughness trends with increasing field strength. The figures show that the MDM model cannot reproduce the three flow regimes. We could not reach the plastic regime even at the highest field strength of 25 mT. Moreover, the MDM model continued to exhibit a granular flow regime at the fields, where the Inclusion model showed a correlated and plastic regime (15-25 mT). We observed that, at higher fields, even a single moving particle can disrupt the entire pile. This behavior led to longer settling times ($> 5s$) while all Inclusion simulations reached steady state within 2s. Without the correlated and plastic regimes, the surface roughness parameters did not show a significant increase with increasing field strength. The angle of repose instead showed a slight decrease, $20.34^\circ \pm 0.81^\circ$ (no field) to $17.96^\circ \pm 1.33^\circ$ (25 mT).

We were not able to perform Inclusion simulations with 6.35 mm particles and higher susceptibilities due to computational limitations. Therefore, simulations with a single seed were performed with a magnetic susceptibility of 3.6. At the same time, we varied the field strength from 5 mT to 100 mT to achieve similar magnetic cohesion as the 8.73 mm particles with a susceptibility of 20.0 at 25 mT. We were able to reproduce the three flow regimes with the Inclusion model for 6.35 mm particles. We observed a granular flow regime at 5 mT, a correlated flow regime at 30-65 mT, and a plastic flow regime at 80-100 mT. Figure 4.16 shows the final frames for the Inclusion model with different field strengths, while Figure 4.17 shows the angle of repose and surface roughness trends with increasing field strength. The slight increase in angle of repose from $18.81^\circ \pm 0.17^\circ$ (no field) to $20.50^\circ \pm 0.20^\circ$ (30

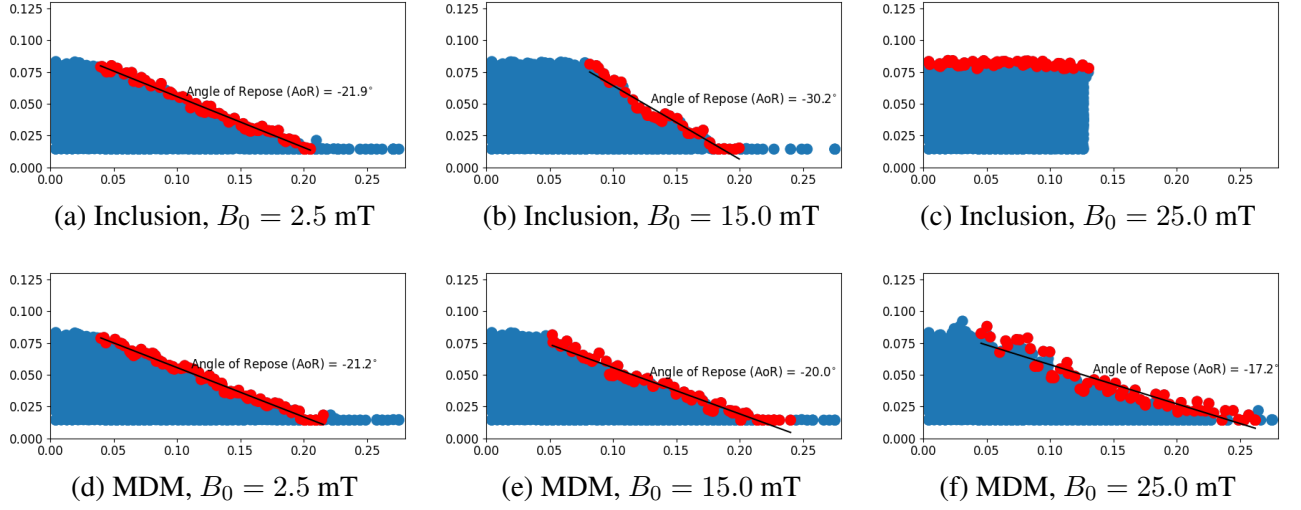


Figure 4.13: Magnetic Results (8.73 mm diameter and 20.0 magnetic susceptibility): Post-avalanche state for different magnetic field strengths. The top row shows the Inclusion model results, while the bottom row shows the MDM model results. Inclusion Model transitions to correlated regime at 15.0 mT (middle) before turning plastic at 25.0 mT (right) in agreement with the experiments [4], while MDM model remains in a granular state even at 25.0 mT.

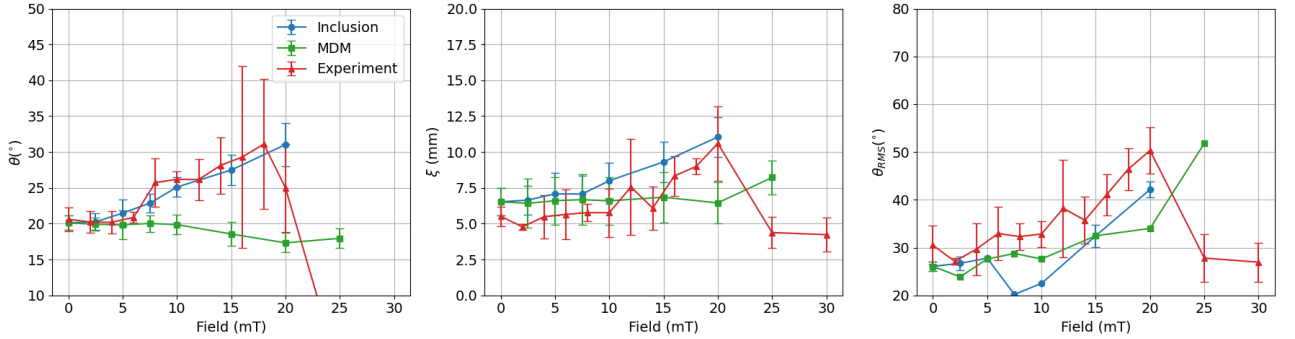


Figure 4.14: Magnetic Results (8.73 mm diameter and 20.0 magnetic susceptibility): Plots showing the relationship between applied magnetic field and various parameters for both the Inclusion and MDM simulations, along with the experimental data from [4]. The Inclusion model (our implementation) and the experimental data agree on all three parameters. Surface roughness plots are shifted as compared to the experimental data. We attribute this shift to differences in data analysis techniques as discussed in section 4.5.7.

mT) is attributed to the lower susceptibility. While 8.73 mm simulations validated the model against experimental results, the 6.35 mm simulations showcase the three flow regimes for another particle size and susceptibility pair, providing further confidence that the Inclusion model accurately models

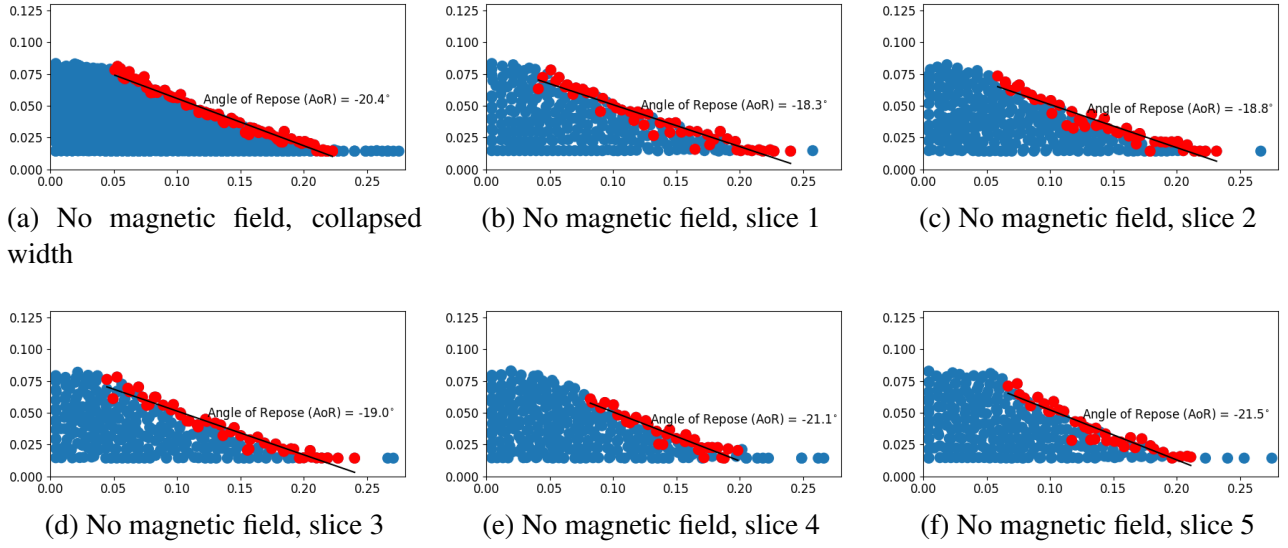


Figure 4.15: Slice Variability (8.73 mm diameter): Post-avalanche state for no applied magnetic field case with different slices.

the magnetic interactions.

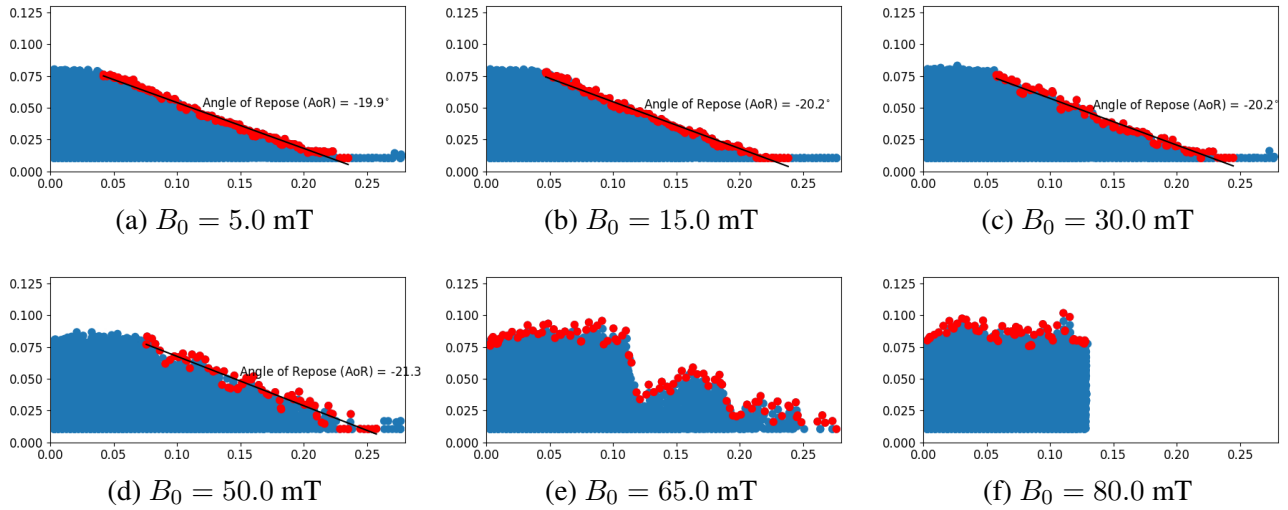


Figure 4.16: Inclusion Results (6.35 mm diameter and 3.6 magnetic susceptibility): Post-avalanche state for different magnetic field strengths. Fields 5 mT to 50 mT (a-d) show a granular regime, while 65 mT (e) shows a correlated regime, and 80 mT (f) shows a plastic regime.

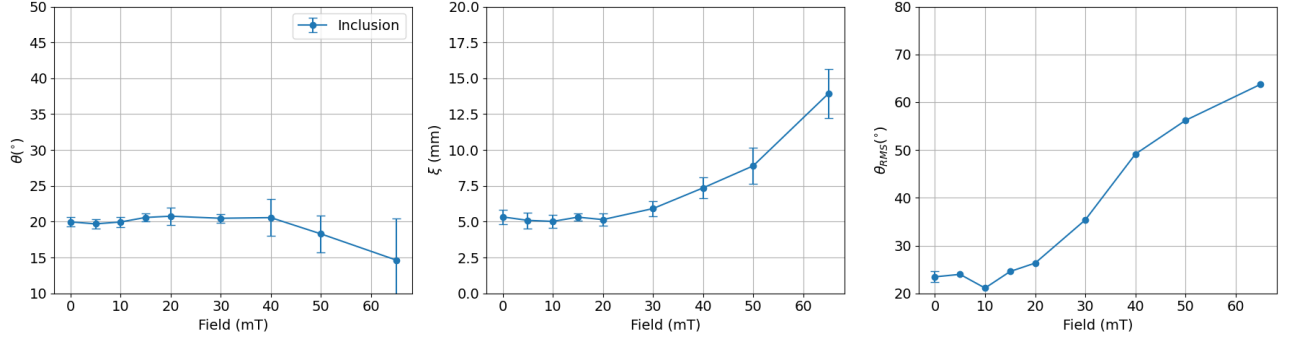


Figure 4.17: Inclusion Results (6.35 mm diameter and 3.6 magnetic susceptibility): Plots showing the relationship between applied magnetic field and various parameters.

4.6 Limitations

A few limitations of the current implementation in LIGGGHTS are worth noting. LIGGGHTS processor mapping in large simulations leads to a non-uniform distribution of particles across processors. This results in an inefficient use of processor resources and longer computation times. Changing the LIGGGHTS processor distribution or using a different DEM software like LAMMPS (`balance` command) helps achieve a more uniform distribution and therefore faster computation times. This could also enable us to run the Inclusion model with larger multipoles to achieve higher magnetic susceptibilities.

LIGGGHTS calculates forces between particle neighbor pairs only. The current implementation circumvents this limitation by using a large neighbor skin distance to include all particles as neighbors. This leads to issues with neighbor list construction requiring more computational resources. The assignment of particles to processors is carried out whenever a neighbor list is constructed, which can lead to a significant slowdown in the simulation. Future work could include optimizing the neighbor list construction to reduce the computational overhead.

A very quirky behavior was observed while using multiple `run` commands in LIGGGHTS. The

`run` command in LIGGGHTS is used to advance the simulation by a specified number of time-steps. Each `run` command starts with a pre-construction of neighbor lists and forces. We observed an influx of energy into the system whenever a subsequent `run` command was used after the first one. This was not observed when using a single `run` command for the entire simulation. We suspect this is due to the large neighbor skin distance that includes all particles as neighbors. We tried using the `run pre no` command, which does not reconstruct the forces, but it did not work as expected. This issue can be avoided by using a single `run` command for the entire simulation. But this is not always feasible for longer simulations, for example, removing the middle wall requires at least two `run` commands. We therefore experimented with the `run` command and found that the influx of energy is dissipated within 1-10 dump time-steps, which is set to 1 ms in our simulations. Therefore, we can safely ignore the influx of energy if we use `run` commands with time steps larger than an order of magnitude of 10 ms.

Along with the limitations in LIGGGHTS, the Inclusion model itself has some limitations. The model is based on the assumption that all particles are identical (same magnetic susceptibility and size) and spherical. Therefore, this model cannot simulate a more complex particle shape or distribution. While the particle shape effects can be modeled by varying friction parameters, different magnetic susceptibilities cannot be modeled. We can, however, use the MDM model to simulate different magnetic susceptibilities and particle sizes.

4.7 Conclusions

We have presented an accurate and experimentally validated magnetic force model for discrete element method (DEM) simulations of metallic grains. The model is based on the Inclusion model of

Keaveny and Maxey [1] and is implemented in the open-source software LIGGGHTS. We also defined a new critical magnetic time to calculate the magnetic force at a lower frequency than the DEM time step. This new model is more accurate than the readily used Mutual Dipole Model (MDM), as shown in our comparisons. We validated the model against simple 1-D test cases and then used it to simulate avalanching of metallic grains. Earlier studies by Fazekas et al. [98] and Taylor et al. [61] using dipolar models did not reproduce the plastic regime. Our model replicated the bulk behavior of metallic grains in avalanching experiments by Sunday et al. [4], showcasing three distinct flow regimes: granular, correlated, and plastic. While earlier computational studies did showcase an increase in the angle of repose with an external magnetic field, they did not compare the trends with experimental results. We demonstrated a quantitative increase in the angle of repose and surface roughness parameters with increasing magnetic field strength, in agreement with the experimental data.

4.7.1 Future Work

The current Angle of Repose (AoR) and surface roughness analysis were primarily done in a 2D manner by collapsing the y -dimension. We sliced the simulation width into five equal slices to analyze the variation of these parameters in the y -axis. Future work should include a more detailed 3D analysis of the angle of repose and surface roughness parameters. The current analysis is limited to comparing the pre-avalanche and post-avalanche states. An advantage of simulations over experimental work is the ability to track the trajectory of each particle, along with the force data. We can use this information to analyze avalanche dynamics in more detail by looking at force chains and particle interactions.

The new magnetic force model enables us to simulate more accurate and complex scenarios for

magnetic cohesion in granular materials. We can use the Inclusion model to simulate the effect of particle shape on avalanching behavior by varying the rolling friction parameters. We can also model the effect of gravity on the change in angle of repose and surface roughness. These simulations would enable us to better understand the behavior of metallic regolith in microgravity environments on asteroids like 16-Psyché. The future work could also include modeling different avalanching experiments, such as the ones by Tang et al. [39]. With minor tweaks, the model can also be used to simulate magnetic manipulation of lunar regolith to design magnetism-based technologies as proposed by Kawamoto et al. [43]. Along with planetary applications, the model can also simulate metallic grains for industrial applications such as powder metallurgy and additive manufacturing.

Chapter 5: Investigating the Role of Magnetic Cohesion in Avalanching on 16-Psyche: A Discrete Element Modeling Approach

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5.1 Introduction

The surfaces of small bodies are covered with regolith, a layer of loose, unconsolidated material that can range from fine dust to large boulders. Scheeres et al. [14] compared various forces acting on regolith particles on small bodies, such as gravitational, electrostatic, Van der Waals cohesion, and solar radiation pressure. They found that for small particles (less than a few centimeters), cohesive forces can dominate over gravitational forces, especially in micro-gravity environments. Many researchers [22, 24, 26, 31, 41, 50] have studied the role of cohesion in small body regolith dynamics. Sikka et al. [81] recently proposed that magnetic cohesion could be a significant force for regolith particles on metallic asteroids, such as 16-Psyche, which is the target of NASA's upcoming Psyche mission. They developed a magnetic force model [99] for Discrete Element Modeling (DEM) simulations, which can be used to study the effects of magnetic cohesion on regolith dynamics, including avalanching, landslides, and crater formation. We aim to use this model to simulate regolith avalanching on Psyche

under different magnetic field strengths and material compositions, to understand the role of magnetic cohesion in these processes.

5.1.1 Avalanching on Small Bodies

Evidence of mass wasting and avalanching processes has been observed on multiple small bodies. Kokelaar et al. [85] showed diverse mechanisms of dry-granular avalanches on craters of the moon and compared them to terrestrial analogs. Mass wasting on Vesta and Ceres was studied heavily by the Dawn mission, which observed landslides and slumps on Vesta [100] and Ceres [87]. Ceres showed more complex mass-wasting processes due to the presence of sublimation of volatiles [87]. Sugita et al. [86] observed landslides on the surface of 162173-Ryugu, which were attributed to thermal fatigue and seismic shaking. Tang et al. [39] modeled the effects of boulders in mass-movement on the surface of asteroid 101955-Bennu. For cometary bodies, the mass wasting processes are more complex as the regolith is more cohesive and there is the presence of volatiles as observed in landslides on comet 67P/Churyumov-Gerasimenko [101]. All these studies showcase the presence of mass-wasting and avalanching processes on small bodies and their link to interparticle cohesion.

5.1.2 16-Psyche: A Metallic Asteroid

16-Psyche is a large main-belt asteroid that is believed to be the exposed metallic core of a differentiated protoplanet [9]. Multiple radar observations [16, 79] have constrained Psyche's shape, size, and gravitational parameters, as shown in table 5.1. de Kleer et al. [17] used Atacama Large Millimeter/submillimeter Array (ALMA) observations to derive a global best-fit thermal inertia and dielectric constant for Psyche. Cambioni et al. [13] used these observations to propose a very heterogeneous

Table 5.1: Psyche Properties.

Quantity	Units	Value	Ref.
Bulk Density	g/cm^3	4172 ± 145	[8]
Gravitational Parameter	km^3/s^2	1.601 ± 0.017	[15]
Volume	km^3	$(5.75 \pm 0.19) \times 10^6$	[16]
Surface gravity	m/s^2	0.13	(calculated assuming a sphere)

surface for Psyche, with a mixture of metallic and non-metallic materials, which is consistent with the radar observations. They assumed Psyche’s surface to be a mixture of iron oxides/sulfides and rocks, constraining the local bulk density of the surface between 1500 and 4500 kg/m^3 . They propose three different scenarios to explain the statistically low thermal inertia of lowlands compared to highlands on Psyche: “thin mantle of fine regolith covering the lowlands; presence of fractures induced by impacts; and/or silicate materials implanted by impacts”, which is indicative of a collisionally evolved surface. These observations suggest that Psyche, like other asteroids, is subject to a range of processes, including impacts, thermal fatigue, and space weathering.

A prehistoric dynamo could have locked a magnetic field into the cooling material [18]. Scheinberg et al. [11], Courville et al. [12] have studied the evolution of this dynamo in the context of Psyche. The Psyche spacecraft will conduct a comprehensive magnetic survey [10] of Psyche’s environment, providing insights into the history and origins of this metallic world. [12] simulated the thermal evolution of Psyche’s core for two different scenarios: one with a smaller core radius and a thicker mantle, and another with a larger core radius and a thinner mantle. They found that the second scenario produces a shorter-lived dynamo but with stronger surface fields of up to 200 μT , while the first scenario produces a longer-lived dynamo but with weaker surface fields of up to 50 μT . While the actual conditions on Psyche remain uncertain, these simulations suggest that its surface could be exposed to magnetic fields of up to 200 μT , which could have significant implications for regolith dynamics on

Psyche, especially for smaller particles that are more susceptible to cohesive forces.

5.1.3 Magnetic Cohesion

Magnetic cohesion is the force that arises when paramagnetic or ferromagnetic particles are exposed to an external magnetic field, causing them to become magnetized and to attract one another. Magneto-rheological fluids are a well-known example of magnetic cohesion, where the application of a magnetic field can change the fluid's viscosity and yield strength [67, 102]. In these fluids, magnetic particles are suspended in a carrier fluid, and when a magnetic field is applied, the particles form chain-like structures, increasing the fluid's resistance to flow. In contrast, on small bodies like Psyche, we deal with dry, dense granular flows in which particles are in direct contact with one another, and magnetic forces can significantly affect their behavior. Very limited work has been done to understand the role of magnetic cohesion with dense granular flows.

Forsyth et al. [60] performed rotating drum experiments with magnetic particles and observed that the angle of repose increased linearly with the applied magnetic field strength in the granular flow regime, where particles move independently. They also observed a correlated and a plastic flow regime, where the surface flow is clumped and smooth, respectively. More recently, Sunday et al. [4] conducted experiments in which they filled a box with steel and brass balls and removed a boundary wall to trigger avalanches. They observed similar flow regimes and a linear increase in the angle of repose and surface roughness parameters with increasing magnetic field. Fazekas et al. [6], Taylor et al. [61] did Discrete Element Method (DEM) simulations of magnetic particles and observed the granular and correlated flow regimes, but not the plastic regime. They used dipolar models to calculate the magnetic forces between particles, which are only accurate for particles with a higher separation

distance than 3 – 4 particle radii [1, 76, 103].

Keaveny and Maxey [1] developed an inclusion model for calculating magnetic forces between particles in close proximity, which is more accurate for simulating regolith dynamics on small bodies. Du et al. [76] used a smoothed profile to resolve boundary conditions and solved the Maxwell equations using a grid-based method to calculate magnetic forces between particles, which is also accurate for close proximity. Sikka et al. [81] compared these models for magnetic parameters relevant to small bodies and found that the inclusion model is the most accurate for simulating regolith dynamics on small bodies. They argued that dipolar models are unable to capture magnetic forces accurately and therefore don't observe the plastic flow regime in simulations. They implemented the inclusion model [99] in LIGGGHTS, an open-source DEM software, and validated it against experimental data [4] across all three flow regimes. We use this implementation to simulate avalanching on Psyche and understand the role of magnetic cohesion in these processes.

5.2 Methodology

We use Discrete Element Modeling (DEM) to simulate regolith avalanching on Psyche under different magnetic field strengths and material compositions. DEM simulations resolve particle dynamics by integrating the equations of motion for each particle separately with a small time step ($\mathcal{O}10^{-7}$ s). Many researchers have used DEM to simulate mass-wasting processes on small bodies, such as landslides and avalanches, to understand their surface evolution [23, 35, 39, 40]. We use the same approach to simulate avalanching on Psyche, incorporating magnetic forces to understand the role of magnetic cohesion in these processes. This section describes the different contact models we use to simulate particle interactions, the simulation setup, the particle properties, and the data analysis

techniques used to analyze our results.

5.2.1 Contact Models

We are using LIGGGHTS [46], an open-source Discrete Element Modeling (DEM) software, for our simulations. It has multiple force models that can simulate particles using the Soft-Sphere Discrete Element Method (SSDEM), a method used by researchers for Lunar and Small bodies studies. Frizzell et al. [50] validated these models and applied them to simulate wave transmission through lunar regolith, testing their effectiveness for generating cold spots around smaller craters. They also compare lunar results with asteroid-like regolith by modeling the properties of ‘thermally fatigued boulders’. They use the Hertzian contact model between the spherical regolith particles. The force between colliding particles is calculated based on the overlap distance between them. Along with the Hertzian model, they include sliding friction, rolling friction, and cohesion to simulate ‘rough’ particles. For magnetic force, we use the model given by Sikka and Hartzell [99]. Their model is based on the inclusion model [1] and provides the most accurate calculation of magnetic forces. One reason for choosing LIGGGHTS software is that it is compatible with this magnetic force model.

5.2.2 Simulation Setup

We model an acrylic box similar to Sunday et al. [4] and Sikka and Hartzell [99], filling it with spherical particles on one side, then removing the middle wall to trigger an avalanche. The box is 300 mm long, 100 mm wide, and 180 mm deep, with a middle wall 150 mm thick as shown in figure 5.1. We fill the left side with particles of 10 mm diameter up to a height of 100 mm, as shown in blue in the figure. The gravity is in the downward direction ($-z$) while the magnetic field is applied

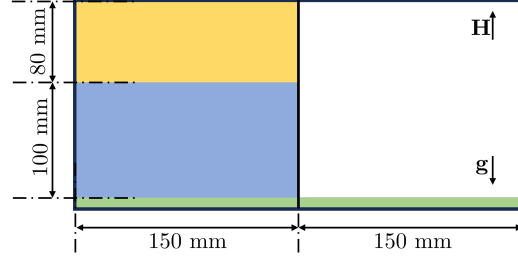


Figure 5.1: Simulation setup: the frozen floor particles in a hexagonal packing are shown in green, the blue depicts the section filled with the particles for avalanching, and the yellow shows the volume used to insert particles during the assembly preparation.

in the upward ($+z$) direction. We also model a coarse floor using a hexagonal particle packing. The assembly is prepared by inserting particles into an area above the 100 mm fill height, as shown in the figure 5.1. We use Earth's gravity (9.81 m s^{-2}) to assemble the system, as it significantly reduces the assembly time. Once particles are inserted, we set the gravity to Psyche gravity (0.13 m s^{-2}) and let the particles settle the minor force changes. To achieve the required packing fraction, we tap the assembly by inducing vibration in the floor, as done by both Frizzell et al. [50] and Sikka and Hartzell [99]. The packing fraction (ϕ) is the ratio of the volume occupied by the particles inserted to the total volume of the blue region in figure 5.1. We ensure that the packing fraction is chosen such that the bulk density ρ_b of the assembly is close to the bulk density of Psyche, which is around 4000 kg/m^3 [9]. In cases where the bulk density of 4000 kg/m^3 cannot be achieved, we use the highest possible packing fraction for that material mixture. Table 5.5 shows the packing fractions and bulk densities for different simulations. We use a higher vibration amplitude (2mm), scaled to our particle size (10mm), which is larger than that reported by Frizzell and Hartzell [29] (1mm). The extra particles above 100 mm height are then removed. We use this prepared particle assembly to simulate avalanching in different applied magnetic field environments.

5.2.3 Particle Properties

As discussed in section 5.1.2, the surface regolith on Psyche could be either metallic or non-metallic or a mixture of both. There could be iron-nickel ores, iron sulfide/oxide ores, or rocky regolith. We model three types of regolith, as described in the table 5.5. Kamacite is used to model Iron-Nickel ore with a high magnetic susceptibility ($\chi = 20$). Troilite is used as a representative of Iron oxides & sulfides with a lower magnetic susceptibility ($\chi = 5$), and finally, we use properties from Frizzell et al. [50] for rocky/non-magnetic regolith. The magnetic susceptibilities were chosen after reviewing the literature on the magnetic susceptibilities of different meteorites [19, 20, 21]. Terho et al. [19] measured the magnetic susceptibilities of multiple meteorites and showed that different classes of meteorite tend to cluster together on a plot of magnetic susceptibility vs. bulk density. The maximum magnetic susceptibility for iron meteorites is around 28, while for stony-iron meteorites, it is around 5. Kohout et al. [21] compiled a database and showed that the magnetic susceptibilities of iron meteorites can reach 100, while those of stony-iron meteorites can reach 40. We choose the values 20 and 5 to represent the magnetic susceptibilities of iron and stony-iron meteorites, respectively, to explore the effects of magnetic cohesion on regolith dynamics on Psyche.

The walls are modeled as an acrylic material, as in Sikka and Hartzell [99]. The inter-particle properties (table 5.2), such as friction, coefficient of restitution, and cohesion energy density, are kept constant across different materials as these properties dictate shape characteristics in a DEM simulation. The material properties are defined in the table 5.3. The densities of Kamacite and Troilite are based on Elkins-Tanton et al. [9] while the Young's modulus and Poisson ratio are based on Tang et al. [104]. A factor of 0.01-0.0001 for the Young's modulus does not affect the bulk behavior in a DEM simulation but significantly saves computational time [5, 50, 99]. Therefore, we utilize a factor

of 0.01 for the values mentioned in Tang et al. [104].

Table 5.2: Interaction Properties for Psyche Avalanching Simulations[49]

Quantity	Symbol	Units	
Coeff. of restitution	e	(-)	0.85
Friction coefficient	μ_s	(-)	1.0
Rolling friction coeff.	μ_r	(-)	0.7
Rolling visc. damping	$\gamma_{d,r}$	(-)	2.0
Cohesion energy density	k_c	(kPa)	1.0

5.2.4 Magnetic Field Strengths

Figure 5.2 shows the range of magnetic fields and particle sizes that could have significant magnetic cohesion, based on force comparisons for different particle sizes. We simulate this parameter space (shaded region) by scaling the magnetic field strength to a $10mm$ particle size. By maintaining a constant particle size, we can keep computational cost manageable while still exploring the effects of magnetic cohesion across a range of field strengths relevant to Psyche. The choice of $10mm$ particle size is based on the fact that a similar particle size was used in the experiments by Sunday et al. [4] and Sikka and Hartzell [99], allowing us to compare our results with theirs. Sánchez et al. [23] used the van der Waals cohesion bond number to scale particle size with varying gravitational strength. We

Table 5.3: Material Properties for Kamacite, Troilite and Rocky Regolith [9, 50, 99, 104]

Quantity	Symbol	Units	Kamacite	Troilite	Rocky Regolith	Acrylic (Walls)
Density	ρ	(kg/m ³)	7870	4900	2500	1250
Young’s modulus	E	(MPa)	1509.6	6000	5	30
Poisson ratio	ν	(-)	0.17	0.375	0.2	0.4
Magnetic Susceptibility	χ	(-)	20.0	5.0	0	0

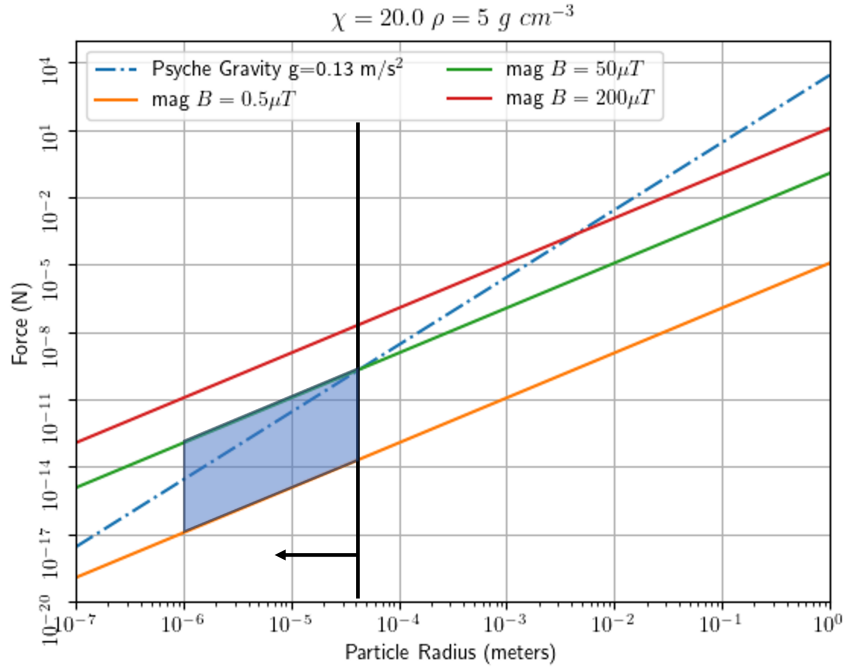


Figure 5.2: Comparison of magnetic force for different field strengths ($0.5 \mu T$, $50 \mu T$ & $200 \mu T$) with Psyche gravitational force for different particle sizes. We assume a particle density of 5000 kg/m^3 and a magnetic susceptibility of 20, which is the value for kamacite. The black vertical line shows the particle size where the gravitational force is equal to the magnetic force for a $50 \mu T$ field. Particle sizes smaller than this line are more susceptible to magnetic cohesion. We simulate the parameter space shown in the shaded region by scaling the magnetic field strength for a fixed particle size of 10 mm.

Table 5.4: Magnetic bond numbers (assuming Psyche gravity $g = 0.13 \text{ m/s}^2$, particle density $\rho = 5000 \text{ kg/m}^3$, and particle susceptibility $\chi = 20.0$) used for scaling of the parameter space shown in figure 5.2 to 10 mm particle size. We also show the corresponding particle sizes for the different field strengths ($0.5\mu T$ and $50\mu T$) at Psyche, which are calculated by using the corresponding magnetic bond number for a 10 mm particle size.

Simulated Fields for 10 mm particles	Magnetic Bond Number (B_{mag})	Particle sizes(mm) at Psyche Fields	
		$0.5 \mu T$	$50 \mu T$
10	0.000186	0.025	250
100	0.018583	0.00025	2.5
500	0.464585	0.00001	0.1
1000	1.858340	0.0000025	0.025

utilize the same principle by first defining the magnetic bond number:

$$B_{mag} = \frac{F_{mag}}{F_g}, \quad (5.1)$$

where F_g is the gravitational force on a particle and F_{mag} force between two particles placed in a uniform magnetic field B . [81] gave an empirical model for F_{mag} . We use the maximum force case (both the particles are touching, and the magnetic field is parallel to the line joining the particles) to calculate the magnetic Bond number:

$$B_{mag} = \frac{a^2 B^2 (q_3 \chi^3 + q_2 \chi^2 + q_1 \chi + q_0)}{\rho \frac{4}{3} \pi a^3 g}, \quad (5.2)$$

where ρ is particle density, a is particle radius, B is the applied magnetic field strength, χ is particle magnetic susceptibility and q_i are the constants.

Studies have shown that magnetic cohesion affects bulk parameters, as measured by the magnetic bond number [4, 59, 60], irrespective of particle size and magnetic field strength. Therefore, we can scale the magnetic field strength for a fixed particle size to simulate the parameter space shown in

Table 5.5: Simulation Properties for each case. N is the total number of particles inserted, ρ_b is the bulk density of the assembly, ϕ is the packing fraction, $\bar{\theta}_0$ is the mean angle of repose for the no magnetic force ($B = 0 \mu T$) case.

Name	Material	N	$\rho_b (kg/m^3)$	ϕ	$\bar{\theta}_0$
RR	Rocky Regolith	1533	1337.78	0.54	35.70 ± 2.89
TL	Troilite	1513	2587.86	0.53	33.56 ± 2.36
KC-RR 1:3	25% Kamacite, 75% Rocky	1491	1987.20	0.52	31.19 ± 1.81
KC-RR 1:1	50% Kamacite, 50% Rocky	1470	2651.19	0.51	34.63 ± 2.62
KC-RR 3:1	75% Kamacite, 25% Rocky	1500	3400.92	0.52	34.40 ± 3.21
KC	Kamacite	1480	4065.78	0.52	35.30 ± 3.76

Figure 5.2. The magnetic fields $0.5 \mu T$ - $50 \mu T$ and particle sizes $1 \mu m$ - $0.04 mm$ scale to $0.71 \mu T$ - $5000 \mu T$ for $10 mm$ sized particles. We simulate $0 \mu T$ $10 \mu T$, $100 \mu T$, $500 \mu T$ and $1000 \mu T$ among the scaled magnetic fields. The table 5.4 shows the magnetic bond numbers for the simulated field strengths for a $10 mm$ particle size. It links them to different particle size-field strength combinations within the parameter space shown in figure 5.2.

5.2.5 Simulation Characteristics

We simulate six different material cases: 25%, 50%, 75%, and 100% kamacite, 100% troilite, and rocky regolith. The percentage of kamacite is defined as the number of kamacite particles divided by the total number of particles inserted in the system. The remaining particles are rocky regolith in the mixture cases. The floor particles are rocky for the rocky regolith case, troilite for the troilite case, and kamacite for the kamacite case. For each material case apart from rocky regolith, we simulate five different magnetic field strengths: $0 \mu T$, $10 \mu T$, $100 \mu T$, $500 \mu T$, and $1000 \mu T$. Table 5.5 lists all the simulations and their parameters. Table 5.6 shows the different timesteps used in the simulations. The simulation timestep (dt) is chosen to be $2 \mu s$, which is less than 2% of hertzian time for all simulations [29]. The neighbor timestep is the time interval at which the neighbor list is updated, and

Table 5.6: Timesteps used in the simulations.

Quantity	Symbol	Units	Value
Timestep	dt	μs	2
Magnetic timestep	mag_t	ms	4
Neighbor timestep	(-)	ms	10

the magnetic timestep is the time interval at which the magnetic forces are calculated. We check the magnetic timestep for a force change of 0.5% to ensure that the magnetic forces are calculated at the right intervals, which is important for computational efficiency.

5.2.6 Data Analysis

The objective of this study is to investigate whether the regolith on Psyche is likely to be influenced by magnetic cohesion. We use the same data analysis techniques as [4] and [99] to compare mass-wasting with no magnetic cohesion ($B = 0 \mu T$) to the different applied field strengths for each of our simulation scenarios. We use Ovito [97] to visualize our simulations, along with Python libraries such as numpy, scipy, and pandas, to analyze the angle of repose and surface roughness. The visualization helps us understand the flow characteristics, while the angle of repose and surface roughness analysis help us quantify the effect of magnetic cohesion on the mass-wasting process.

5.2.6.1 Angle of Repose

Angle of Repose (θ_B) is the angle between the horizontal and the slope of the surface of the particles after the avalanche has settled for a given magnetic field strength B . We collapse the y-dimension and fit a line to the centers of the top-most particles to calculate the angle of repose. Particles that did not move during the avalanche are excluded from the analysis to ensure we are examining only

the avalanche surface. To ensure the best fit, we calculate the angle of repose by truncating particles from the right end of the box toward the left and keeping the x -range that maximizes R^2 . We also look at the dynamic angle of repose over time to understand the flow characteristics of the mass-wasting process. The dynamic angle of repose is calculated using the same method as above, but at multiple time step intervals.

5.2.6.2 Surface Roughness

Surface roughness is a measure of the irregularity of the surface of the particles after the avalanche has settled for a given magnetic field strength B . We calculate the RMS height (ξ) and the RMS slope (θ_{rms}) of the surface to quantify the surface roughness. We do not truncate any particles in the surface roughness analysis, as we are interested in the overall roughness of the avalanche surface. RMS height is calculated as the standard deviation of the heights of the particles above the mean height. In contrast, the RMS slope is calculated as the standard deviation of the avalanche surface slope with respect to the horizontal. The following are the equations for RMS height and RMS slope:

$$\xi = \left[\frac{1}{n-1} \sum_{i=1}^n (z_i - \bar{z})^2 \right]^{1/2}, \quad (5.3)$$

where n is the number of particles considered, z_i is the height of the i^{th} particle and $\bar{z}$ is the mean height of the n particles.

$$\theta_{rms} = \tan^{-1} \left(\frac{v(\Delta x)}{\Delta x} \right), \quad (5.4)$$

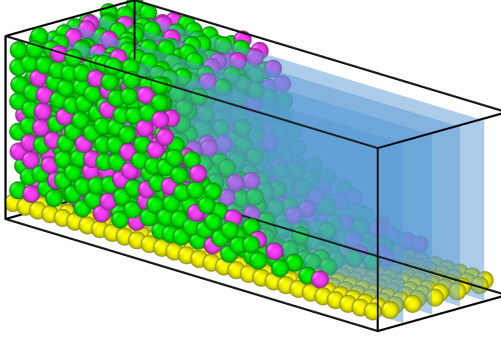


Figure 5.3: Different slices to analyze the angle of repose, RMS height, and RMS slope. The simulation box is divided into five equal slices in the y-dimension, depicted by translucent blue planes. The angle of repose and surface roughness are calculated for each slice to understand the spatial variation of these properties across the box.

where Δx is the difference in x -coordinate of consecutive particles and $v(\Delta x)$ is the RMS height of the surface calculated over a window of Δx ,

$$v(\Delta x) = \left[\frac{1}{n} \sum_{i=1}^{n-1} [z_i - z_{i+1}]^2 \right]^{1/2}. \quad (5.5)$$

We divide the simulation box into 5 slices in the y-dimension (as shown in Figure 5.3) and analyze the angle of repose and surface roughness for each slice to understand the spatial variation of these properties across the box. We then calculate the average angle of repose and surface roughness parameters by taking a weighted average of the R^2 values across the slices and a single value for the entire box, to understand the overall effect of magnetic cohesion on the mass-wasting process. The error bars are similarly calculated as a weighted average of the standard errors for each parameter. The mean parameters are denoted by $\bar{\theta}_B$, $\bar{\xi}$, and $\bar{\theta}_{rms}$ for angle of repose, RMS height, and RMS slope, respectively.

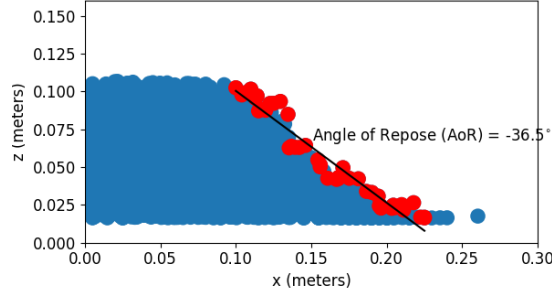


Figure 5.4: Final frame of avalanching of rocky regolith with no magnetic field. Red particles are considered for the angle of repose analysis. The black line shows the best-fit line.

5.3 Results

We present the results of our simulations in this section, starting with rocky regolith and then magnetic results. Figure 5.4 shows the final settled configuration of rocky regolith after avalanching, which serves as a baseline for understanding the effect of magnetic cohesion on the mass-wasting process. Figure 5.5 shows the final settled configuration of the various material configurations for different magnetic field strengths. The particles considered for angle of repose calculation are shown in red, while the black line shows the best-fit line through the centers of the considered particles. We have labeled the overall angle of repose for the simulation box in these figures. Table 5.7 and figure 5.6 show the trends of mean angle of repose, RMS height, and RMS slope parameters with the increasing magnetic field strength.

Based on these plots, we can see that magnetic cohesion plays no significant role up to a field strength of $500 \mu T$. Still, at $500 \mu T$ field strength, we start to see differences in the cases with a higher percentage of kamacite, as expected, since they have higher magnetic susceptibility. KC 1:1

Table 5.7: Mean angles of repose for different magnetic field strengths and the corresponding bond numbers. $\bar{\theta}_0$, $\bar{\theta}_{10}$, $\bar{\theta}_{100}$ and $\bar{\theta}_{1000}$ are the mean angles of repose for 0 μT , 10 μT , 100 μT , 500 μT and 1000 μT magnetic fields respectively.

Angle of Repose Bond Number	$\bar{\theta}_0$ (deg) 0	$\bar{\theta}_{10}$ (deg) 0.000186	$\bar{\theta}_{100}$ (deg) 0.018583	$\bar{\theta}_{500}$ (deg) 0.464585	$\bar{\theta}_{1000}$ (deg) 1.858340
TL	33.56 ± 2.36	33.36 ± 2.44	34.09 ± 2.33	33.29 ± 2.96	33.40 ± 4.18
KC-RR 1:3	31.19 ± 1.81	32.46 ± 2.25	31.26 ± 1.97	32.36 ± 2.24	31.78 ± 1.90
KC-RR 1:1	34.63 ± 2.62	35.01 ± 2.66	32.33 ± 2.73	37.36 ± 3.14	N/A
KC-RR 3:1	34.40 ± 3.21	34.97 ± 3.50	35.12 ± 3.45	36.94 ± 5.03	N/A
KC	35.30 ± 3.76	36.91 ± 3.54	35.86 ± 3.44	N/A	N/A

and KC 3:1 transitioned into a correlated regime at 500 μT field strength before becoming nearly plastic at 1000 μT , as seen in figure 5.5. KC case shows a transition to a plastic regime directly at a 500 μT field strength, as seen in figure 5.5. The angle of repose for the nearly plastic cases is not calculated, as there is no substantial grain motion. RMS height, on the other hand, shows an increase from 12.55 ± 8.16 mm to 18.94 ± 4.78 mm and 13.14 ± 8.18 mm to 20.72 ± 6.29 mm for KC 1:1 and KC 3:1 cases, respectively, which is expected as the surface becomes more irregular with increasing magnetic cohesion. The KC case shows a decrease in RMS height from 14.05 ± 8.62 mm to 10.38 ± 8.13 mm, indicative of a plastic regime in which the surface remains flat, with no avalanches. RMS slope also shows the opposite trends. KC 1:1 and KC 3:1 cases show a decrease in RMS slope from 61.08 ± 13.71 deg to 50.04 ± 17.23 deg and 59.89 ± 5.25 deg to 55.23 ± 19.59 deg, respectively, which is expected as the surface becomes more irregular with increasing magnetic cohesion. All these trends indicate a transition from a granular to a plastic regime, with increasing magnetic cohesion, as the particles become more magnetically cohesive and less likely to flow during the avalanche.

Note that the error bars for RMS height and RMS slope are quite large, which is expected as there is a lot of uncertainty in the surface roughness parameters for each slice. This is because we have only a two-particle-diameter resolution per slice, which yields very few particles to estimate the

surface roughness parameters, leading to substantial uncertainty in these parameters. Simulating more particles by increasing the box width or decreasing the particle size can help reduce this uncertainty, but it is computationally expensive. Another possible way to reduce this uncertainty is to simulate more seeds per scenario to obtain more data points for each parameter. Both approaches significantly increase computational cost, which is why we have not implemented them in this study.

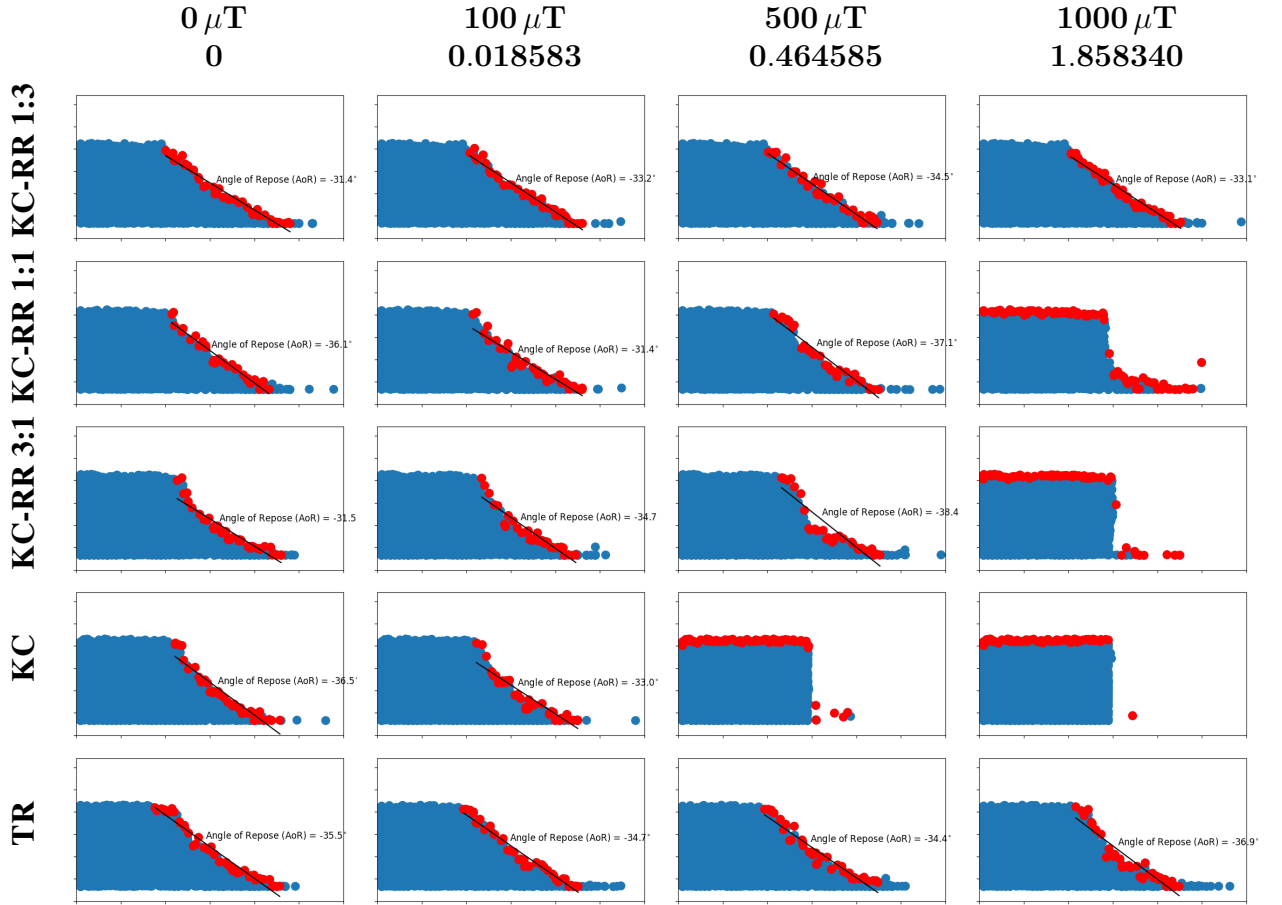


Figure 5.5: Final frames of avalanching simulations for all the material compositions, magnetic field strengths, and corresponding bond numbers. The first three rows show the mixture cases with varying percentages of kamacite, while the last two rows show the single material cases of 100% kamacite and 100% troilite. The columns show the different magnetic field strengths applied in the simulations. The particles considered for angle of repose calculation are shown in red, while the black line shows the best-fit line through the centers of the considered particles. The angle of repose for the entire box is labeled in each frame. Bond numbers of 0.45 or higher show a significant effect of magnetic cohesion. This bond number translates to particle sizes of $< 0.1 \text{ mm}$ for Psyche, assuming a maximum surface magnetic field of $50 \mu T$.

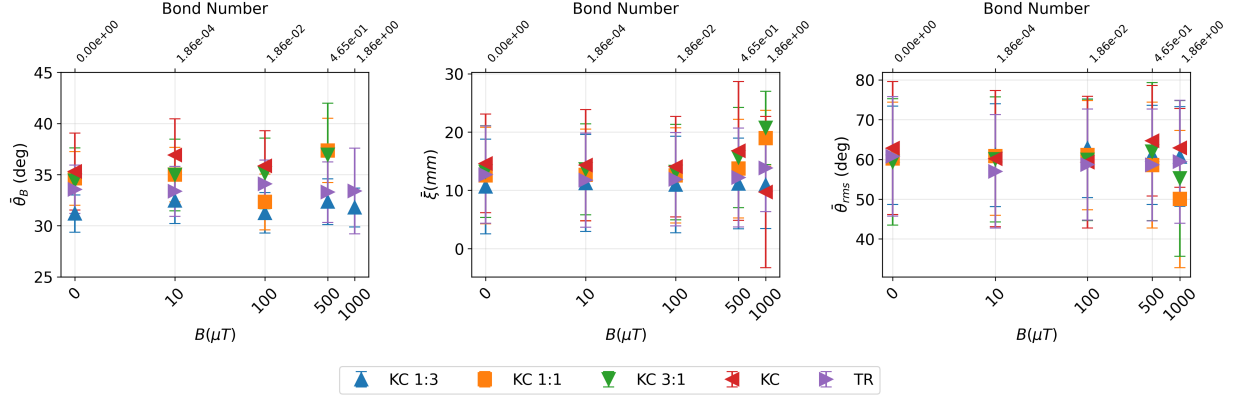


Figure 5.6: Trends of mean angle of repose ($\bar{\theta}_B$), RMS height ($\bar{\xi}$), and RMS slope ($\bar{\theta}_{rms}$), with the increasing magnetic field strength (B) and the magnetic bond numbers for different material compositions. The mean values are calculated as weighted averages, with R^2 values as weights. The error bars are calculated as a weighted average of the standard errors for each parameter. The effects of magnetic cohesion are evident in the RMS height and RMS slope plots for the 500 and 1000 μT field strength and bond numbers > 0.45 , where the values are higher than those for the other field strengths in cases with a higher percentage of kamacite. All other cases remain similar across field strengths, as suggested by the angle-of-repose plot.

Some key characteristics can be seen in the final settled avalanches as shown in Figure 5.7. Particle colors are based on material type: magenta for rocky regolith and green for kamacite. The yellow color is used for the floor particles, which are the same material as the particles in the box for each case. For the KC 3:1 case, we can see that a few particles from the top-right corner (Red circle in figure 5.7a) of the assembly fall while the rest of the particles stay plastic. This is because, in the top-right corner, a few magnetic kamacite particles (green) are surrounded by more non-magnetic rocky particles (magenta), which lowers the net cohesion in this region. The fall of these particles also lowers the magnetic cohesion below them, which leads the particles below to bulge out but remain plastic (Red circle in figure 5.7b). For the KC case (figure 5.7c-d), we can see that only a couple of particles from the top-right corner (marked in red) move. The higher particle falls, while the lower particle bulges out but remains plastic, similar to the behavior seen in the KC 3:1 case.

We performed a simulation at 1000 μT with a hypothetical material with all the same properties

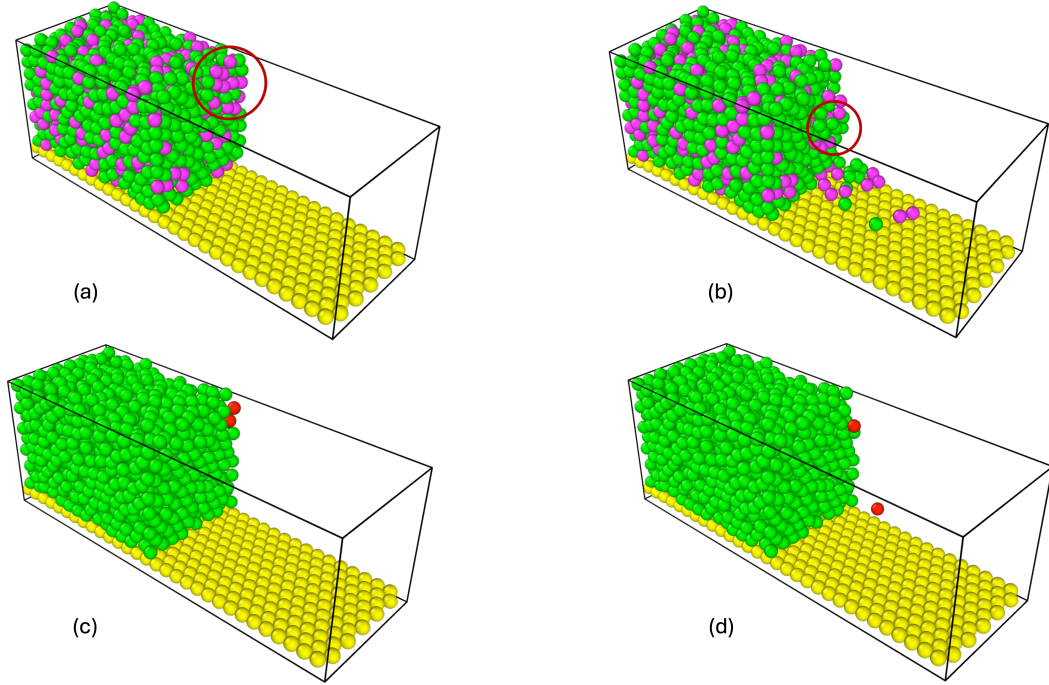


Figure 5.7: Perspective views of the final settled avalanches for $1000 \mu T$ field strength in KC-RR 3:1 case (a) before avalanche, and (b) after avalanche, and KC case (c) before avalanche, and (d) after avalanche. Particle colors are based on material type: magenta for rocky regolith and green for kamacite. Yellow color is used for the floor particles, which are the kamacite in this case. Red circles show key characteristics discussed in the text. Red particles in (c-d) show the particles that moved during the avalanche. Both cases show some particles bulging out, but the bulk remains plastic. This behavior could lead to the formation of hanging boulders and overhangs on Psyche's surface.

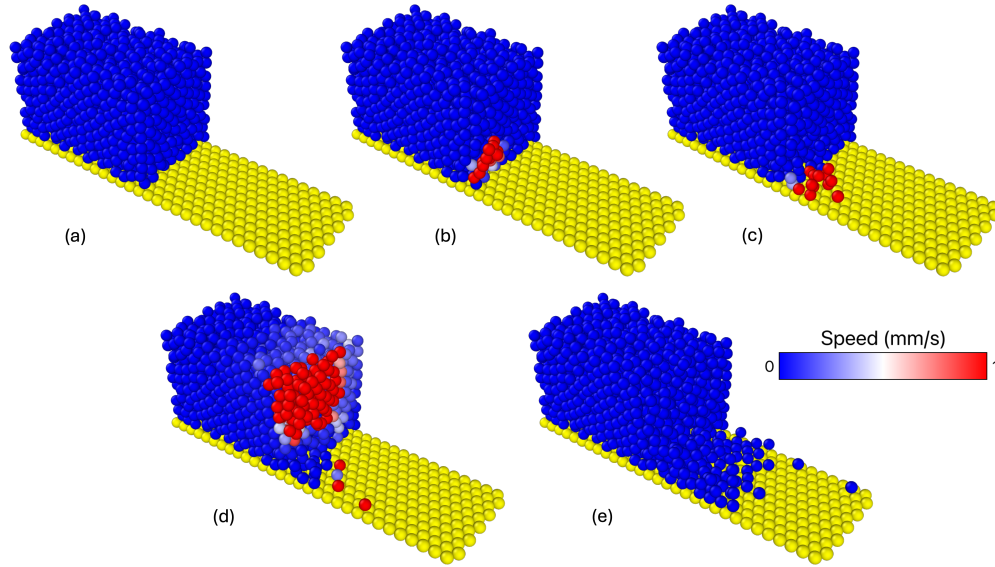


Figure 5.8: Frames at different time intervals during the avalanche for a simulation with a hypothetical material with all the same properties as troilite but with the density of rocky regolith at $1000 \mu T$ field strength. The colors of particles are based on the velocity of particles, as shown in the included legend. Floor particles are shown in yellow for better visibility. The lower density results in a more cohesive material, leading to an unstable plastic regime in which, earlier, only a few particles fall from the bottom of the assembly, leaving an overhang. As one of these particles strikes the assembly, it triggers a chain reaction in which more particles fall, indicating an unstable plastic regime.

as troilite but with the density of rocky regolith to understand the effect of density on the mass-wasting process. At lower density, the magnetic bond number increases proportionally, resulting in a more cohesive material. We see interesting behavior in this simulation. Figure 5.8 shows various frames at different time intervals during the avalanche. At first, only a few particles from the bottom of the assembly fall, which leads to an overhang (figure 5.8b-c). As one of these particles strikes the assembly, it triggers a chain reaction in which more particles fall (figure 5.8c-d), indicative of an unstable plastic regime. This behavior underscores the importance of density, magnetic susceptibility, and magnetic field strength in determining the magnetic bond number and, consequently, the mass-wasting process on Psyche’s surface.

5.4 Implications and Future Work

Our results suggest that the probable conditions on Psyche would be susceptible to magnetic cohesion, leading to granular, correlated, and plastic flow regimes as magnetic cohesion increases. The simulations showed that magnetic fields below $500\mu T$ don't produce significant magnetic cohesion for a particle size of 10 mm . When the field strength is increased to $1000\mu T$, we observe a transition from a correlated to a plastic regime in the cases with a higher percentage of kamacite, as the particles become more magnetically cohesive and less likely to flow during the avalanche.

We can interpret these results in terms of the Bond number for more general applicability. The Bond number helps us understand the relative importance of magnetic cohesion compared to gravitational forces for different particle sizes, magnetic susceptibilities, and magnetic field strengths. The transition from a granular to a plastic regime occurs at a Bond number of around 0.464585 to 1.858340 for our simulations, which corresponds to the $500\mu T$ to $1000\mu T$ field strength range for our particle size and magnetic susceptibility. For the conditions on Psyche, with magnetic fields of lower than $50\mu T$, the 0.464585 bond number corresponds to a particle size of around 0.1 mm for a particle density of 5000 kg/m^3 and a magnetic susceptibility of 20, which are reasonable estimates for the conditions on Psyche. If the probable conditions on Psyche differ, we can use a Bond number of around 0.45 as a reference for the given surface magnetic field strength, gravity, grain density, and magnetic susceptibility to understand the effect of magnetic cohesion on mass wasting on Psyche's surface.

For these conditions, the surface of Psyche could be more irregular and have a higher angle of repose than expected from a non-magnetic perspective, with implications for our understanding of surface processes on Psyche. While the troilite case did not show a significant effect of magnetic cohesion, the hypothetical case with the same properties as troilite but with lower density showed a

significant effect of magnetic cohesion, which suggests that the density of the material on Psyche could also play a significant role in the mass-wasting process on the surface of Psyche. If smaller particles with higher magnetic susceptibility dominate Psyche's surface, magnetic cohesion could significantly influence mass wasting, leading to steeper slopes, hanging boulders, and overhangs.

Future work should focus on simulations at higher resolution within the $500 \mu T$ and $1000 \mu T$ field-strength range, which scale to bond numbers of 0.464585 to 1.858340, to quantify better the increase in angle of repose and surface roughness parameters. The transitions from a granular to a correlated regime and from a correlated to a plastic regime are not well defined in our simulations, and more simulations with finer resolution in the magnetic field strength can help us better understand these transitions. These simulations should also use more seeds or increase the box width to reduce uncertainty in the surface roughness parameters.

Our simulations assume uniform particle size, shape, and magnetic susceptibility, along with a constant magnetic field strength, which do not reflect the actual conditions on Psyche. Future work should focus on understanding the effect of these factors on the mass-wasting process on the surface of Psyche. For example, we can examine the effects of particle shape by varying the particles' rolling friction. We also look at a non-uniform magnetic field by applying a gradient magnetic field in our simulations. Future work should also focus on understanding the avalanche process by examining the force chains and flow characteristics during avalanches, which can help us understand the conditions under which hanging boulders and overhangs can form on Psyche's surface. A hypothetical case with the same properties as troilite but lower density exhibited an unstable plastic regime, suggesting that Psyche's surface could be unstable under some conditions. We can examine this unstable regime in more detail to understand the conditions under which it can occur and its implications for Psyche's surface.

5.5 Conclusions

We performed discrete element method simulations of avalanching in a granular assembly with magnetic cohesion to understand its effect on mass wasting on the surface of Psyche. A bond number of around 0.45 was found to be the threshold for the transition from a granular to a plastic regime in our simulations, corresponding to magnetic field strengths of around $500 \mu T$ to $1000 \mu T$ for our particle size and magnetic susceptibility. The bond number can serve as a reference for understanding the effect of magnetic cohesion on mass wasting on Psyche and other metallic bodies across different particle sizes, densities, magnetic susceptibilities, magnetic field strengths, and gravitational fields. For Psyche, this bond number corresponds to a particle size of around 0.1 mm for a particle density of 5000 kg/m^3 and a magnetic susceptibility of 20, which are reasonable estimates for the conditions on Psyche. Therefore, we can expect the magnetic cohesion to play a significant role in the mass-wasting process on the surface of Psyche for particles of size lower than 0.1 mm and magnetic fields of lower than $50 \mu T$. With increasing magnetic cohesion, we observe a transition from a granular to a plastic regime in samples with a higher kamacite content, as the particles become more magnetically cohesive and less likely to flow during avalanches. The surface of Psyche could be more irregular and have a higher angle of repose than expected from a non-magnetic perspective, with implications for the morphological features observed by the Psyche spacecraft and for our understanding of surface processes on Psyche. The surface magnetic field strength, particle size, magnetic susceptibility, and material density on Psyche could all play a significant role in the mass-wasting process, and these factors should be further investigated in future work to better understand surface processes on Psyche.

Chapter 6: Conclusions

In this work, we developed tools to simulate magnetic cohesion and used them to investigate its effect on mass wasting on the surface of Psyche, a metallic asteroid. First, we developed an empirical model for the magnetic force between two paramagnetic particles based on the Spherical Harmonic Approximation (SHA), providing a more accurate representation than the commonly used dipole-dipole approximation. Second, we developed a framework in LIGGGHTS, an open-source DEM software, to simulate magnetic cohesion in a granular assembly, and we validated it against trends and flow regimes observed in experiments of avalanching of metallic granular materials. Finally, we performed discrete element method simulations of avalanching in a granular assembly with magnetic cohesion to understand its effect on mass wasting on the surface of Psyche. These simulations showed that magnetic cohesion can significantly affect the net cohesion on metallic bodies, with implications for the morphological features observed by the Psyche spacecraft and for our understanding of surface processes on Psyche. We review the main findings of this work in more detail below.

First, we compared various methods for calculating the magnetic force between two paramagnetic particles, including the commonly used dipole-dipole approximation, the Spherical Harmonic Approximation (SHA) method, and a Finite Volume Method (FVM). The comparisons showed that the dipole-dipole approximation can significantly underestimate or overestimate the magnetic force between two particles, especially when the particles are close to each other or have high magnetic

susceptibility. As the dipolar approximation is commonly used to define bond number and other characteristic properties of magnetic cohesion, this can lead to significant errors in our understanding. We used the SHA method to develop an empirical model of the magnetic force between two paramagnetic particles, providing a more accurate representation than the commonly used dipole-dipole approximation. Using this model, we compared different forces in the context of avalanching of metallic granular materials on the asteroid Psyche. We found that the magnetic force can be significant for particles $< 1m$ in size, depending on the magnetic field strength. Therefore, we established that magnetic cohesion could play a significant role in regolith processes on metallic bodies, and that the commonly used dipole-dipole approximation can lead to significant errors in our understanding of these processes.

Next, we developed a framework in LIGGGHTS, an open-source DEM software, to simulate magnetic cohesion in a granular assembly, and we validated it against trends and flow regimes observed in experiments of avalanching of metallic granular materials. We used the inclusion method in our model, combining dipolar interactions for far-field effects and correcting near-field interactions using the SHA method, which provides a more accurate representation of the magnetic force between particles than the commonly used dipole-dipole approximation. To mitigate the computational cost of the inclusion method, we formulated a characteristic magnetic timestep for magnetic interactions, allowing us to update magnetic forces at a lower frequency than mechanical forces while maintaining simulation accuracy. We validated this model against experimental data in the literature and showed that it can replicate the granular, correlated, and plastic flow regimes. The model also reproduced the observed trends in the angle of repose and surface roughness parameters with increasing magnetic cohesion, making this model the first experimentally validated DEM model for magnetic cohesion in granular materials.

Finally, we used our magnetic force model to perform DEM simulations of avalanching in a

granular assembly with magnetic cohesion to understand its effect on mass wasting on the surface of Psyche. We modeled granular assemblies with varying percentages of kamacite, an iron-nickel alloy commonly found in meteorites and expected to be present on Psyche, along with troilite, an iron sulfide mineral, and rocky particles, to represent the regolith on Psyche. Different magnetic field strengths were simulated, which correspond to different bond numbers. We showed that, with increasing magnetic cohesion, there is a transition from a granular to a plastic regime in cases with a higher kamacite percentage, as particles become more magnetically cohesive and less likely to flow during avalanches. A bond number of around 0.45 was found to be the threshold for this transition, corresponding to a magnetic field strength of around $500 \mu T$ to $1000 \mu T$ for our particle size and magnetic susceptibility. Using this bond number as a reference, we can understand the effect of magnetic cohesion on mass wasting on Psyche and other metallic bodies across different particle sizes, densities, magnetic susceptibilities, magnetic field strengths, and gravitational fields. For Psyche, this bond number corresponds to a particle size of around 0.1 mm for a particle density of 5000 kg/m^3 and a magnetic susceptibility of 20, which are reasonable estimates for the conditions on Psyche. Therefore, we can expect the magnetic cohesion to play a significant role in the mass-wasting process on the surface of Psyche for particles of size lower than 0.1 mm and magnetic fields of lower than $50 \mu T$. The surface of Psyche could be more irregular and have a higher angle of repose than expected from a non-magnetic perspective, with implications for the morphological features observed by the Psyche spacecraft and for our understanding of surface processes on Psyche.

This work has limitations that should be addressed in future research. First, our simulations were limited to a small number of particles and a narrow range of particle sizes, which may not fully capture the complexity of the regolith on Psyche. Future work should explore a larger simulation box to accommodate more particles and improve the resolution of surface roughness. Second, our simulations

established transition limits in bond number for the transition from a granular to a plastic regime. Still, future work should explore higher-resolution bond-number data around this transition to quantify the increases in angle of repose and surface roughness parameters with increasing magnetic cohesion. We also did not explore the effects of other factors, such as particle shape, particle size polydispersion, porosity, and the presence of electrostatic forces, to name a few, which could affect the mass-wasting process on Psyche and should be investigated in future work. Finally, our simulations were limited to the mass-wasting process on Psyche's surface. Still, future work should explore the effect of magnetic cohesion on other surface processes, such as impact cratering, landslides, and seismic shaking, to better understand the overall surface evolution of Psyche and other metallic bodies.

In conclusion, this work sets the stage for understanding the effect of magnetic cohesion on mass wasting on the surface of Psyche and other metallic bodies. It provides a framework for future research in this area. We have shown that magnetic cohesion can significantly affect the net cohesion on metallic bodies, with implications for the morphological features observed by the Psyche spacecraft and for our understanding of surface processes on Psyche. With NASA's Psyche mission set to arrive at the asteroid in August of 2029, we have an exciting opportunity to test our predictions and further our understanding of the surface processes on Psyche and other metallic bodies in our solar system.

Appendix A: Spherical Harmonics Approximation

We present a brief overview of the spherical harmonics approximation [1] used in the inclusion model.

Consider a system of two particles separated by a center-to-center distance c in an applied uniform magnetic field $\mathbf{H}_0 = H_0(h_\perp \hat{x} + h_\parallel \hat{z})$. The magnetic scalar potential ϕ satisfies the Laplace equation as described in equations 4.3-4.4. This problem was solved by Keaveny and Maxey [1] using a sum of spherical harmonics.

$$\phi_{in}^{(n)} = \sum_{l=0}^{\infty} \sum_{m=0}^1 \alpha_{lm}^{(n)} r_n^l P_l^m(\cos \theta_n) \cos m\phi \quad (\text{A.1})$$

$$\phi_{out} = -H_0(h_\perp x + h_\parallel z) + \sum_{n=1}^2 \sum_{l=0}^{\infty} \sum_{m=0}^1 \beta_{lm}^{(n)} \frac{P_l^m(\cos \theta_n)}{r_n^{(l+1)}} \cos m\phi \quad (\text{A.2})$$

where (x, y, z) are the Cartesian coordinates of the system and (r_n, θ_n, ϕ_n) are the spherical coordinates of a system with the origin at the center of sphere n . The associated Legendre function is defined as

$$P_l^m(\cos \theta) = (-1)^m (1 - \cos^2 \theta)^{\frac{m}{2}} \frac{d^m P_l(\cos \theta)}{d(\cos \theta)} \quad (\text{A.3})$$

The coefficients $\alpha_{lm}^{(n)}$ and $\beta_{lm}^{(n)}$ are found by satisfying the boundary conditions. We need the Hobson formula to describe the general solution in a single coordinate system for a pair of spheres separated

by a distance c :

$$\frac{P_l^m(\cos \theta_1)}{r_1^{l+1}} = \sum_{s=m}^{\infty} (-1)^{s+m} (-1)^{l+s} \binom{l+a}{s+m} \frac{r_2^s}{c^{l+s+1}} P_s^m(\cos \theta_2) \quad (\text{A.4})$$

$$\frac{P_l^m(\cos \theta_2)}{r_2^{l+1}} = \sum_{s=m}^{\infty} (-1)^{s+m} \binom{l+a}{s+m} \frac{r_1^s}{c^{l+s+1}} P_s^m(\cos \theta_1) \quad (\text{A.5})$$

On substituting the general solution into the boundary conditions, using the Hobson formula and eliminating $\alpha_{lm}^{(n)}$, we find for each $m = 0, 1$

$$((\chi + 2)l + 1)\beta_{lm}^{(1)} + \sum_{s=1}^{\infty} \beta_{sm}^{(2)} (-1)^{l+m} \chi l \binom{l+s}{s-m} \frac{a^{2l+1}}{c^{l+s+1}} = \delta_{1j} a^3 \chi H_0 (\delta_{0m} h_{\parallel} - \delta_{1m} h_{\perp}) \quad (\text{A.6})$$

$$((\chi + 2)l + 1)\beta_{lm}^{(2)} + \sum_{s=1}^{\infty} \beta_{sm}^{(1)} (-1)^{l+s} (-1)^{l+m} \chi l \binom{l+s}{s-m} \frac{a^{2l+1}}{c^{l+s+1}} = \delta_{1j} a^3 \chi H_0 (\delta_{0m} h_{\parallel} - \delta_{1m} h_{\perp}) \quad (\text{A.7})$$

Considering only a finite number of multipoles, $l = 0, \dots, L$, we arrive at $2L \times 2L$ linear systems of equations. For each $m = 0, 1$

$$\begin{pmatrix} \mathbf{X} & \mathbf{\Delta}_m \\ \mathbf{\Gamma}_m & \mathbf{X} \end{pmatrix} \begin{pmatrix} \beta_m^{(1)} \\ \beta_m^{(2)} \end{pmatrix} = \begin{pmatrix} \mathbf{q}_m \\ \mathbf{q}_m \end{pmatrix} \quad (\text{A.8})$$

where

$$\begin{aligned}\beta_m^{(1)} &= \left(\beta_{1m}^{(1)}, \beta_{2m}^{(1)}, \dots, \beta_{Lm}^{(1)} \right)^T, \\ \beta_m^{(2)} &= \left(\beta_{1m}^{(2)}, \beta_{2m}^{(2)}, \dots, \beta_{Lm}^{(2)} \right)^T,\end{aligned}\tag{A.9}$$

$$\begin{aligned}\mathbf{q}_0 &= \left(H_0 h_{\parallel} a^3 \chi, 0, \dots, 0 \right)^T, \\ \mathbf{q}_1 &= \left(-H_0 h_{\perp} a^3 \chi, 0, \dots, 0 \right)^T\end{aligned}\tag{A.10}$$

and the $L \times L$ matrices are

$$X_{ij} = \delta_{ij} ((\chi + 2) i + 1),\tag{A.11}$$

$$\Delta_{ij;m} = (-1)^{i+m} \chi i \binom{i+j}{j-m} \frac{a^{2i+1}}{c^{i+j+1}},\tag{A.12}$$

$$\Gamma_{ij;m} = (-1)^{i+j} \delta_{ij;m}\tag{A.13}$$

After solving the system of equations, with $\beta_{lm}^{(n)}$ known, the contribution of the magnetic field from the particles is found by taking the gradient of the scalar potential ϕ_{out} :

$$H_r = \sum_{l=0}^L \sum_{m=0}^1 \left[(l+1) \beta_{lm}^{(1)} \frac{P_l^m(\cos \theta_1)}{r_1^{l+2}} - \beta_{lm}^{(2)} \sum_{s=m}^L (-1)^{s+m} \binom{l+s}{s+m} s \frac{r_1^{s-1}}{c^{l+s+1}} P_s^m(\cos \theta_1) \right] \cos m\phi\tag{A.14}$$

$$H_{\theta} = - \sum_{l=0}^L \sum_{m=0}^1 \left[\beta_{lm}^{(1)} \frac{dP_l^m(\cos \theta_1)}{r_1^{l+2} d\theta_1} + \beta_{lm}^{(2)} \sum_{s=m}^L (-1)^{s+m} \binom{l+s}{s+m} \frac{r_1^{s-1}}{c^{l+s+1}} \frac{dP_s^m(\cos \theta_1)}{d\theta_1} \right] \cos m\phi\tag{A.15}$$

$$H_{\phi} = \sum_{l=0}^L \left[\beta_{l1}^{(1)} \frac{P_l^1(\cos \theta_1)}{r_1^{l+2} \sin \theta_1} + \beta_{l1}^{(2)} \sum_{s=1}^L (-1)^{s+1} \binom{l+s}{s+1} \frac{r_1^{s-1}}{c^{l+s+1} \sin \theta_1} P_s^1(\cos \theta_1) \right] \sin \phi\tag{A.16}$$

The magnetic force on particle 1 is then calculated as

$$F_x = \int_{r_1=a} T_{xr} dS \quad (\text{A.17})$$

$$F_y = 0 \quad (\text{A.18})$$

$$F_z = \int_{r_1=a} T_{zr} dS \quad (\text{A.19})$$

where the stress tensor components are given by $T_{ij} = \mu_0 H_i H_j - \delta_{ij} \frac{\mu_0}{2} H_k H_k$.

We solved the dependence on ϕ analytically using Mathematica to reduce the surface integrals to polynomials in θ . First, we add the uniform magnetic field contribution and rewrite the magnetic field components as

$$H_r = P + A \cos \phi \quad (\text{A.20})$$

$$H_\theta = Q + B \cos \phi \quad (\text{A.21})$$

$$H_\phi = 0 + C \sin \phi \quad (\text{A.22})$$

where P , Q , A , B , and C are functions of θ only. After substituting these expressions into the stress tensor components, we find the x and z force integrals reduced to:

$$F_x = \int_0^\pi \pi \left[-CP + (BP + AQ) \cos \theta + (AP - BQ) \sin \theta \right] d\theta \quad (\text{A.23})$$

$$F_z = \int_0^\pi \frac{\pi}{2} \left[(A^2 - B^2 - C^2 + 2P^2 - 2Q^2) \cos \theta - 2(AB + 2PQ) \sin \theta \right] d\theta \quad (\text{A.24})$$

Finally, we used Gaussian quadrature to evaluate the integrals over θ .

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