

**A Hybrid Continuum and Discrete Element Method for
Granular Media Modeling**

by

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Submitted to the Department of Mechanical Engineering
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Abstract

In this thesis, I designed and implemented a compiler which performs optimizations that reduce the number of low-level floating point operations necessary for a specific task; this involves the optimization of chains of floating point operations as well as the implementation of a “fixed” point data type that allows some floating point operations to be simulated with integer arithmetic. The source language of the compiler is a subset of C, and the destination language is assembly language for a micro-floating point CPU. An instruction-level simulator of the CPU was written to allow testing of the code. A series of test pieces of codes were compiled, both with and without optimization, to determine how effective these optimizations were.

Thesis Supervisor: Kenneth Kamrin
Title: Associate Professor

Acknowledgments

This is the acknowledgements section. You should replace this with your own acknowledgements.

Contents

1	Introduction	13
1.1	Granular Media Modeling	14
1.1.1	Discrete Methods	15
1.1.2	Continuum Models	17
1.1.3	Related Hybridization Work	19
2	Discrete Element Method	21
2.1	DEM Model	22
2.2	DEM Algorithm	23
3	Continuum Model	27
3.1	Hyperelastic-Plastic Model	27
3.2	Hypoelastic-Plastic Model	27
3.2.1	Material Point Method	28
A	Tables	29
B	Figures	31

List of Figures

1-1	Flowing hourglass displaying three distinct phases, with entire hourglass (a) and closeup of bottom region (b)	15
1-2	Aftermath of a landslide in La Conchita California.	17
2-1	Two disks in contact with relevant properties labeled for DEM.	22
B-1	Armadillo slaying lawyer.	32
B-2	Armadillo eradicating national debt.	33

List of Tables

A.1 Armadillos	29
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Chapter 1

Introduction

Modeling is a game of balance. Tractability and reasonable solution times fight against the physical realities of vast length and time scales. The assumptions one makes when formulating a model directly impact the solution methods that can be brought to bear to the problem at hand. There is almost always guaranteed trade-offs between the level of simplification of a model and the amount of time needed to solve that model.

Granular media present an interesting intermediary between the world of the discrete and continuum. While often times they are studied in contexts where continuum approximations are appropriate (i.e. geological), their behavior at much smaller length scales (a bucket of sand at the beach or flow through an hour glass) are still of great interest. However at those more everyday scales, the length scale of a single grain of sand is a relatively large proportion of the scale of the entire problem, and thus cannot be ignored. And even at the larger aforementioned geological scales, the initiation of an earthquake, for example, still relies on individual grains of sand slipping and deforming against each other.

The great challenge, then, is to formulate a model that can capture length scale effects but still have enough simplifying assumptions to make the problem solvable with efficient methods. This however seems to fly in the face of the modeling trade-off previously discussed; it is nearly impossible to have a single model that allows for fine-scale resolution and yet ignores those small length scales to become efficiently solvable. The solution proposed in this work addresses this issue by ignoring the "single" part of the "single model" clause, and instead hybridizes two distinct models to yield the two distinct attributes desired: resolution of length scale while maintaining efficient solvability. It is noted that the current work

focuses on cohesionless granular systems, and thus approximate dry granular systems with no sources of attraction, like liquid bridges or electrostatic charges.

The work is structured as follows. The remainder of chapter 1 puts the current work in the greater academic context and discusses prior work on the modeling of granular media. Hybridization models in and out of granular media contexts are also discussed.

Chapter 2 discusses the discrete element method used and some details of its algorithmic solution. While the level of detail presented may seem overly exhaustive, it provides important context for where the hybridization technique interfaces with the discrete element method.

Chapter 3 discusses the continuum models used. The method used to solve these models, the Material Point Method, is also discussed in detail.

Chapter 4 introduces the hybridization technique. Its goal, formulation, and solution are discussed.

Chapter 5 shows examples of the hybridization technique at work, with comparisons to the discrete and continuum model solutions, as well as to literature.

Finally chapter 6 concludes the thesis and discusses future work.

1.1 Granular Media Modeling

The ubiquity of granular media in everyday life cannot be understated. We walk on it on trails, drive over it on roads [23], ingest it in our pharmaceuticals, and eat it in our meals. Slightly less directly, granular media is second only to water for the type of material most commonly handled in industry [17]. Despite this ubiquity however, a comprehensive model that can capture the behavior of granular media remains elusive.

While much of the difficulty stems from the length and time scale problems mentioned before, granular media is also unique from many other materials in its ability to transition between different states. This is clearly evident in a flowing hourglass, as shown in Figure 1-1. At the bottom of the hourglass, settled sand acts as a solid, able to support compressive stress without flowing. At the top of the static pile is a region of grains flowing over the static region, acting like a liquid. In between the top and bottom of the hourglass the grains flow much like a dilute gas, with no cohesive structure and interacting via collisions.

Different models and solution techniques are able to capture granular behavior in a given



(a) data a



(b) data b

Figure 1-1: Flowing hourglass displaying three distinct phases, with entire hourglass (a) and closeup of bottom region (b)

state, though of course with trade-offs in accurately capturing behavior in other states. A summary of different methods are thusly discussed.

1.1.1 Discrete Methods

Perhaps the most straightforward way one could model a system of granular material is to model the grains themselves. Methods that model individual grains and the interactions between them fall under the umbrella of discrete methods. While this can be expensive for very large systems (greater than approximately 50,000 particles per core given current CPU capabilities), the one-to-one correspondence of a single simulated grain to a physical grain can produce accurate results. Discrete element methods can largely be broken down into two classes: penalty based methods and contact dynamics.

Penalty methods, as their names suggest, penalize the overlap of particles with some type of force that is a function of that overlap. The discrete element method (note that in some literature the term "discrete element method" is used to denote the larger class of what is here termed "discrete methods"), first formulated by Cundall and Strack, still enjoys much use due to its simplicity and accuracy [2]. Even within the confines of the simplicity of the proposed method though, great generalizability can be realized by having a free choice of the penalty function. The advantages of course come at some cost. For example, a major drawback is that, depending on the choice of penalty function, multiple material parameters may need to be fit to experiment. The material parameters themselves may then

put constraints on the computational solve time. To concretely demonstrate this point, many penalty models have some notion of an elastic parameter that must be tuned. However, most individual grains of sand are fairly stiff, with **FINDREFERENCE** bulk moduli on the order of $49 GPa$ and densities on the order of $2000 kg/m^3$. These properties, combined with the small size of many grains (0.1 mm in diameter), result in a large wave speed through the material that travels a small distance, and this must be resolved within a given time step. Implicit methods of course exist to alleviate this issue somewhat, but those come with the usual drawbacks of additional computational overhead elsewhere.

Contact dynamics on the other hand treats grains as completely rigid and allow no overlaps. They are then formulated as optimization problems, and more specifically, mixed linear complementarity formulations, minimizing some potential with a no overlap constraint. While the question of material properties is then largely avoided in these methods, the introduction of friction and other properties is much less straightforward than in the formulation of discrete element methods. The lack of material properties is also a double-edged sword of sorts, as while infinitely stiff grains are often a better approximation of a system of grains than computational grains that are extremely soft, the reality is that grains do have a finite, though large, stiffness. Capturing that finite stiffness and its consequences, such as a finite wave speed and non-negligible grain deformation, can be crucial in some applications. These properties are in fact important for the hybrid scheme, and will be discussed later.

A key characteristic of both classes of discrete methods is that they can easily capture all phases of discrete matter. If compressed by exterior forces or boundaries, they act like a solid, able to support load through the creation of force chains, much like physical granular media. The removal of these forces and boundaries, and/or the introduction of shear forces, causes grains to flow over other grains in a liquid-like fashion. Pouring a system of discrete grains will see the grains separate, capturing a granular gas.

Another property of discrete element methods is that they are able to elucidate particle level properties and dynamics that are difficult to gather from experiment. Photoelastic disks can be used to investigate force chains, such as in the pioneering work of Behringer et al and continued by the likes of Daniels et al **FINDREFERENCE**. However these photoelastic disks are made of relatively soft polymers and are mostly used to investigate 2D arrangements of disks, and not 3D arrangements of spheres. On the other hand, discrete element methods calculate inter-particle forces out of necessity and can thus report quantitative data for these

contacts. Expanding from 2D to 3D is also a straightforward process, and every contact in a 3D system can be easily obtained. The dynamics of every single grain in a system modeled with discrete methods can also be tracked and studied, which can be done in experiment, but only with much difficulty and cost, i.e. methods such as X-ray tomography and CT scans [FINDREFERENCE](#). While computational expenses can limit the size of simulated systems, physical limitations of scanning equipment can limit the size of an experimental system that can be studied, greatly hampering one of the key advantages of experiments over simulations in granular media: scale.

Thus despite the drawbacks of discrete element methods, they are still popular and widely used in congruence with, and sometimes in the place of, physical experiment. The ability to accurately capture grain-scale level dynamics, and to obtain quantitative data for every grain and contact, means that they can effectively be treated as computational "ground truth" for simulated granular systems. When accuracy in a simulation is needed, discrete element methods can be used with confidence, at least compared with other methods.

1.1.2 Continuum Models



Figure 1-2: Aftermath of a landslide in La Conchita California.

As stated before, for large (what constitutes "large" varies from system to system, though 20 grain diameters per continuum element dimension is used as a rule of thumb [FINDREFERENCE](#)) granular systems, one can ignore the fact that there are individual grains of sand, treat the system as a continuous granular medium, and retain many physical properties of the system. A classic example of this can be seen in Figure 1-2, which shows the aftermath

of a landslide. A useful feature of the shown landslide is that a road can be seen that cuts through the hill, and acts as a deformation marker. The deformed shape is reminiscent of Poiseuille flow, suggesting that the moving bulk is well represented by a continuum.

Continuum theory applied to granular media in fact goes back more than 50 years, with the pioneering work of Coulomb who proposed a relation between shear stress, pressure, and a coefficient of friction in a granular continua, very similar in form to Coulomb friction [FINDREFERENCE](#). Since that initial proposal, granular continuum theory has been greatly expanded upon. The incorporation of additional complexity displayed in physical granular systems into the continuum theory have resulted in models that capture behavior such as critical-state, and anisotropy [19][3].

Much work on granular continuum theory has been conducted in the fields of civil engineering and soil mechanics, where understanding the behavior of granular systems under load is crucial [FINDREFERENCE](#). There is thus a large body of work on granular media in a solid phase, and continuum modeling of grains in this state is well understood. Granular gases too have been well investigated, with kinetic theory being effectively used to understand granular systems in this state.

The "liquid" flowing phase of granular materials has been much more difficult to model. It was only recently that a seminal study conducted by GDR MiDi suggested a possible model for flowing granular systems [6]. The rheological model posited, commonly referred to as the $\mu(I)$ relation (μ of I), suggests a yield condition similar to that suggested by Coulomb nearly half a century ago, but with a friction coefficient dependent on a nondimensional inertial number, I , which describes the ratio of inertia to confining pressures in a granular system. Further work by Jop and De Cruz provided empirical relations between the friction coefficient μ and I [10][FINDREFERENCE](#). Further extensions of this model have since been proposed, and work continues to this day on clarifying the high and low inertia number bounds of the $\mu(I)$ relation.

All of the previously described models, while increasingly complex, still retain some simplicity in the sense that they are all local models. No length-scale is introduced, and thus no non-local effects are captured. This deficiency has been recently addressed by the work of Kamrin et al, who have proposed a non-local continuum model and thus introduce a notion of a length scale back into the continuum model [12]. At first glance this seems provides a possible solution to the beginning stated problem of capturing length-scale effects

while retaining the ability of efficient continuum equation solving methods. However, much additional work must be done to completely characterize these non-local models, and thus for now cannot be relied upon to have the fidelity of discrete methods which capture length-scale effects by their very nature.

1.1.3 Related Hybridization Work

Quasi-Continuum and Arlequin-type methods have been explored primarily for crystalline solids, to expedite otherwise lengthy atomistic simulations by hybridizing with a crystal plasticity continuum model in zones where atomistic refinement is not needed [24, 21, 20, 27, 4]. The idea of hybridizing discrete-particle and continuum approaches to simulate granular media is in its infancy, with only initial work done to show the validity of communicating mechanics between discrete grains and finite-element facets [26]. Recent work has explored when continuum and discrete treatments are simultaneously accurate [18, 11, 13], including an Arlequin-type method that couples statically-defined regions of a discrete element (DEM) simulation to the interior of a continuum FEM-based simulation to enrich stress fields around drill tips, for instance [25]. We build on and extend these ideas to target regimes in which enriched degrees of freedom are required at surfaces, and where the boundary between continuum and discrete regimes evolves dynamically.

In the granular physics and graphics literature, lower-level ideas have been tried where instead of implementing a general continuum model, the user imposes kinematic constraints to the particle motion in certain regions, often chosen based on experience with the problem at hand. The graphics literature has explored freezing rigid bodies that are sufficiently stationary [22]. Similar techniques have been proposed to accelerate the generation of granular packings for industrial applications [15]. In common granular setups such as rotating tumblers and growing sand piles, semi-empirical models can be used to guess zones of rigid material, and grains in these zones can be removed from the discrete update [14, 9, 28, 1]. Holladay et al.[8] carve out interior regions of granular materials moving at constant velocities and replace these groups of grains with meshes, but this method does not homogenize over rigidly rotating regions or over shear flows, and as the paper notes, can lead to volume loss. These ideas have been developed further in follow-up work [7, 16]. These methods make no claims as to the accuracy of the techniques for science and engineering applications, and have not yet demonstrated stable granular flows.

Chapter 2

Discrete Element Method

As described generally in Chapter 1, the discrete element method (DEM) models a system of grains by modeling each grain as a separate entity and calculates the dynamics of each grain by integrating what essentially amounts to $\Sigma \mathbf{f} = m\mathbf{a}$ through time. In 2D, each grain is modeled as a disk with a radius r , parameterized by three degrees of freedom: two for the center of mass position of the disk (held by a position vector $\mathbf{x}_d \subset \mathbb{R}^2$), and a third for the rotation of the disk relative to some rest state. The dynamics are captured by another three parameters: two for the center of mass velocity and a third for the angular velocity about the center of mass. In 3D this representation is generalized to a sphere, again with radius r and six degrees of freedom: three for the center of mass ($\mathbf{x}_d \subset \mathbb{R}^3$) position and three for the angles that describe grain orientation. The dynamics analogously generalize to six parameters, with three for center of mass velocity and three for angular velocities. For a system of K particles, the degrees of freedom of all particles can be concatenated into a single degree of freedom list, the generalized coordinate vector \mathbf{q}_d . In 2D, $\mathbf{q}_d \subset \mathbb{R}^{3K}$ and in 3D, $\mathbf{q}_d \subset \mathbb{R}^{6K}$. A generalized velocity vector, v_d can be similarly defined, with $\mathbf{v}_d \subset \mathbb{R}^{3K}$ in 2D and $\mathbf{v}_d \subset \mathbb{R}^{6K}$ in 3D. Momentum balance for the whole granular system can then be summarized with

$$M_d \mathbf{a}_d = \mathbf{f}_d(\mathbf{q}_d, \mathbf{v}_d, t)$$

where $M_d \subset \mathbb{R}^{3K \times 3K}$ (2D) and $M_d \subset \mathbb{R}^{6K \times 6K}$ (3D) is the mass matrix, $\mathbf{a}_d \subset \mathbb{R}^{3K}$ (2D) and $\mathbf{a}_d \subset \mathbb{R}^{6K}$ (3D) is the generalized acceleration vector, and \mathbf{f}_d is the force vector that encapsulates all internal and external forces of the system. The evolution of the system

configuration can then be described with

$$\dot{\mathbf{q}}_d = \hat{\mathbf{q}}_d(\mathbf{q}_d, \mathbf{v}_d, \mathbf{a}_d)$$

where $\hat{\mathbf{q}}_d$ is a function that encapsulates configuration updates.

2.1 DEM Model

The construction of \mathbf{f}_d , and specifically the contact model that goes into \mathbf{f}_d , has been the source of much work. Popular contact models include Hertzian contact and linear spring-dashpot systems, the latter of which we use [FINDREFERENCE](#). While Hertzian contact in theory accounts for a nonlinear penalty force with respect to penetration depth due to geometric considerations not present in the simple Hookean spring model, the simplicity of the Hookean spring model along with its acceptable accuracy from literature motivate the latter's use in the current study [FINDREFERENCE](#).



Figure 2-1: Two disks in contact with relevant properties labeled for DEM.

In the current work, the contact force, \mathbf{f}_c , is a linear combination of a normal contact force \mathbf{f}_n and tangential contact force \mathbf{f}_t , such that simply $\mathbf{f}_c = \mathbf{f}_n + \mu\mathbf{f}_t$, where μ is the coefficient of friction. \mathbf{f}_d more concretely is

$$\mathbf{f}_n = k_n d \mathbf{n} - \gamma_n \mathbf{v}_n$$

where k_n is the Hookean spring constant in the normal direction, d is the penetration depth

between the two disks, \mathbf{n} is the contact normal unit vector, γ_n is the normal damping coefficient, and \mathbf{v}_n is the normal component of the relative velocity between the two disks. Similarly, the tangential contact force is given by

$$\mathbf{f}_n \mathbf{t} = k_t \Delta s - \gamma_t \mathbf{v}_t$$

where k_t is the spring constant in the tangential direction, γ_t is the tangential damping coefficient, and \mathbf{v}_t is the tangential component of the relative velocity. Friction is captured in this model by requiring that

$$\mathbf{f}_t \leq \mu \mathbf{f}_n$$

which is accomplished by adjusting Δs . For a given enduring contact over time, Δs for that contact is the time integral of the tangential relative velocity during that contact. Δs is then rescaled so that it \mathbf{f}_t falls within the friction cone determined by $\mu \mathbf{f}_n$.

With the given spring-dashpot system, a coefficient of restitution (COR) e can be tuned as a function of the model parameters. Given a desired e and a normal spring coefficient k_n , γ_n is determined as

$$\gamma_n = \sqrt{mk_n}(-2 \log e) / \sqrt{2(\pi^2 + \log e^2)}$$

where m is the mean mass of a grain [13]. Note that the use of a "mean" mass is due to the fact that in all of the simulations conducted in this study, a slight polydispersity in granular radii is used with a single density for all particles, resulting in a mass distribution. This is done to better match real shape distributions in a granular system, and to avoid crystallization that commonly arises in monodisperse systems. The choice of k_n and other material parameters is further explained for specific simulations later in the study, but in general is chosen to be as stiff as possible while still retaining a reasonable cost per time step, with a timestep usually on the order of 10^{-6} seconds.

2.2 DEM Algorithm

The DEM code used in this study was built completely in house, though is similar in general algorithmic structure to many DEM codes that exist, such as LAMMPS or LIGHTS [FINDREFERENCE](#). Thus for transparency as well as necessity when later explaining the hybrid algorithm, the structure of the used DEM code is discussed.

Algorithm 1 Overall_DEM_Algorithm

```
1: Broad_Phase_Collision_Detection
2: for  $i = 0 \dots num\_possible\_collisions$  do
3:   Narrow_Phase_Collision_Detection
4: end for
5: Collision_Update
6: for each_collision_type do
7:   Update_Properties
8:   Integrate_Δs
9: end for
10: Force_Update
11: for each_collision do
12:   Calculate_Penalty_Force
13:   Correct_Δs
14:   Add_Force_To_Contact_Grains
15: end for
16: Time_Integration
```

The *Broad_Phase_Collision_Detection* creates an axis-aligned bounding box (AABB) around each grain, and checks the intersection of those AABBs with a background grid. Each grid cell then has a vector of AABBs that intersect it, with each combination of AABB in that vector constituting a possible collision. All possible collisions are then looped over for an actual collision detection (*Narrow_Phase_Collision_Detection*) and any real collisions are added to a vector of actual collisions for a given type. Collision types include, for example, circle_circle collisions for grains in contact, or circle_plane collisions for grains in contact with a rigid plane. The list of all collisions for every collision type are then looped over, and properties such as penetration depth and Δs are updated. With this information, a penalty force is calculated at every contact according to the model presented in 2.1. With these forces, an explicit Forward Euler update is used to numerically integrate the velocity of the grains, which is then used to integrate the position of the grains.

Though dry, cohesionless grains are the focus of the current work, it is noted that the DEM framework allows for a simple extension for cohesive grains. A new collision type can be defined that allows for tracking of grain interactions at a distance. As will be explained later, some initial work has in fact been done on this, by tracking liquid bridges that provide a source of cohesion in the system, in order to extend the hybrid method for cohesive systems.

As a final note, the DEM code is an extension and modification of the SCISIM code developed by Smith for contact dynamics [FINDREFERENCE](#). In fact, as will be later

discussed, that contact dynamics code was first used as the discrete method of choice for the hybrid project. However, the explicit penalty method was determined to better suit the needs of hybridization.

Chapter 3

Continuum Model

3.1 Hyperelastic-Plastic Model

3.2 Hypoelastic-Plastic Model

In general, hypoelastic models differ from hyperelastic models in that the stress is not obtained from a gradient of a strain energy density function with respect to deformation. The specific hypoelastic granular continuum model used in this study was developed by Dunatunga and Kamrin [5]. To start one again begins with momentum balance and mass balance

$$\rho \frac{D\mathbf{v}}{Dt} = \nabla \cdot \boldsymbol{\sigma} + \rho \mathbf{b}$$

$$\frac{D\rho}{Dt} + \rho \nabla \cdot \mathbf{v} = 0$$

with all terms similarly defined as in the hyperelastic model. A useful quantity, the spatial velocity gradient \mathbf{L} , is defined as

$$\mathbf{L} = \nabla \mathbf{v}$$

\mathbf{L} can be decomposed into a symmetric part (known as the strain rate tensor) and skew part (known as the spin tensor), \mathbf{D} and \mathbf{W} respectively, such that

$$\mathbf{L} = \mathbf{D} + \mathbf{W}$$

$$\mathbf{D} = \frac{1}{2}(\mathbf{L} - \mathbf{L}^T)$$

$$\mathbf{W} = \frac{1}{2}(\mathbf{L} + \mathbf{L}^T)$$

In contrast to the hyperelastic model, the used hypoelastic model takes an additive split of the strain and strain rate-like terms into an elastic and plastic part. For example,

$$\mathbf{L} = \mathbf{L}^e + \mathbf{L}^p$$

The elastic and plastic spatial velocity gradients can then be decomposed into spin and strain rate tensors

$$\mathbf{L}^e = \mathbf{D}^e + \mathbf{W}^e$$

$$\mathbf{L}^p = \mathbf{D}^p + \mathbf{W}^p$$

A commonly taken assumption that is also taken here is one of spin-less plastic flow, so that $\mathbf{W}^p = \mathbf{0}$ and $\mathbf{L}^p = \mathbf{D}^p$. Plastic flow codirectionality with the stress deviator and isochoric plastic flow are also taken as assumptions, leading to an plastic flow rate of

$$\mathbf{L}^p = \hat{\mathbf{D}}^p(\boldsymbol{\sigma}) = \frac{1}{\sqrt{2}}\dot{\gamma}^p(\boldsymbol{\sigma})\frac{\boldsymbol{\sigma}_0}{\|\boldsymbol{\sigma}_0\|}$$

where $\dot{\gamma}^p$ is the equivalent plastic shear strain rate.

Due to the fact that a hypoelastic-plastic model is used and there is no tracking of the deformation gradient, an objective rate must be used to update the stress. While many exist, the Jaumann rate is used here as suggested by Dunatunga and Kamrin, and is defined as

$$\overset{\triangle}{\boldsymbol{\sigma}} = \dot{\boldsymbol{\sigma}} - \mathbf{W} \cdot \boldsymbol{\sigma} + \boldsymbol{\sigma} \cdot \mathbf{W}$$

3.2.1 Material Point Method

Appendix A

Tables

Table A.1: Armadillos

Armadillos	are
our	friends

Appendix B

Figures

Figure B-1: Armadillo slaying lawyer.

Figure B-2: Armadillo eradicating national debt.

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