An algebraic reconstruction technique (ART) for the synthesis of three-dimensional models
of particle aggregates from projective representations

by

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A Thesis Submitted to the
Graduate Faculty in Partial Fulfillment of the
Requirements for the Degree of
MASTER OF SCIENCE

Department: Electrical and Computer Engineering
Major: Engineering (Electrical Engineering)

Approved: Members of the Committee

_____________________________ ______________________________
In Charge of Major Work

_____________________________
For the Major Department

_____________________________
For the College

Rowan University
Glassboro, New Jersey
2005
ABSTRACT

There exists considerable evidence that the shear behavior and flow behavior of granular materials is significantly dependent on particle morphology. However, quantification of this dependence is a challenging task owing to a dearth of quantitative models for describing particle shape and the difficulty of modeling angular particle assemblies. The situation becomes more complex when discrete element analyses of realistic 3-D particle shapes are required. The thesis attempts to address this problem by adapting the algebraic reconstruction technique (ART) to synthesize composite 3-D granular particles from statistically obtained 3-D shape descriptors of the particles in an aggregate mixture. This thesis extends previous work where it was demonstrated that the 3-D shape characteristics of particles in an aggregate mixture can be numerically expressed by statistical models obtained from 2-D projective representations of multiple particles in the mixture.

In this thesis, attempts were made to validate the premise that multiple projective representations of multiple particles could be used to synthesize a composite 3-D particle that represents the entire mixture in terms of its 3-D shape descriptors. Also, single particles isolated from the aggregate mix were scanned using optical and X-ray tomography techniques to generate 2-D multiple projections and synthesize the 3-D particle shape. This research work proves useful for generating realistic shapes for discrete element applications or in obtaining more fundamental understanding of the micromechanics of granular solids.
ACKNOWLEDGEMENTS

I would like to thank Dr. Shreekanth Mandayam for the opportunity to work on this project, and for his patience while guiding and encouraging me toward the completion of this thesis. Although there were many times when I was not sure of my own abilities or lost sight of the bigger picture, he was always there to remind me of who I am and what I am capable of. I want to thank Dr. Sukumaran and Dr. Polikar for taking time out of their busy schedules to be a part of my committee, and also for providing memorable experiences for me during my studies at Rowan University.

I want to thank my family and friends for their support, for their pride in me and for their questions about my work. Their interest helped to bolster my confidence in my work and myself, and their understanding allowed me to devote the time necessary to complete my research. I want to give a special thank you to all of the members of my class who strove alongside of me to complete their own graduate studies: Justin, Nate, Rob, Don, Dave, Jon, Mike, Apostolis, Hussein, Hector (to name a few). I consider you all my brothers-in-arms; thank you all for your support and friendship during our time at Rowan together. I also want to thank Mike Kim, Pat Giordano, Phil Mease, Chuck Perri, and Kevin Kanauss for the work they did on this project for me; I couldn’t have done it without you guys! My thanks go to the National Science Foundation (Award #'s 0421000 and 0324437) for their support.

Finally, I want to thank God not only for the life He’s given to me, but also for all of the spectacular people He has allowed me to encounter during this particular chapter in it. Thank You for allowing me to finish this work and may it be a glory unto You.
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CHAPTER 1: INTRODUCTION

Shape characterization can be a very simple or very complex task, depending on the shape. With common shapes, such as circles, squares, and triangles, it is possible for someone to observe a shape and capture all of the relevant information needed to reproduce that shape by recording its name (i.e. circle) and one or more defining attributes (i.e. radius of 2cm). However, there are a limited number of names to describe shapes as they become more and more complex until the point is reached where a shape is so complex that it can only be described as an “n-sided polygon”. At this point, the name is inadequate to describe even the general shape, let alone define its specific characteristics. For total shape characterization of n-sided polygons (the ability to describe and reconstruct a shape from its description), all lengths and angles of the boundary must be recorded in some fashion.

The best way to describe arbitrarily complex shapes then would be to use a set of numbers that describe the boundary of the shape. These numbers may be either the lengths and angles or a more complicated method that relates many features of the shape in a relatively small set of numbers. Either way, these numbers provide a quantitative way of describing a shape, which can be utilized by computer algorithms to determine trends of values. These trends could then be used to relate the values obtained from the shape characterization to physical or geometric properties of the object in question. An example of this would be a smooth, round shape vs. an angular one. The values for the round shape would lie in a separate part of the descriptor domain than those of the angular shape. This fact could be used by algorithms to identify shapes that are similar (because the values used to characterize them are similar) as well as those shapes which are dissimilar.
1.1 Application Areas of Shape Characterization

Shape characterization has many applications ranging from robotic vision to fingerprint matching to character recognition to iris scans and face recognition. Figure 1.1 shows a face recognition application.

Figure 1.1: Example of a face recognition application

In most cases of complex shape comparison (such as Figure 1.1), it is highly probable that direct image comparison will be impractical. With a large database of images, it would be costly in terms of the hardware necessary to store the images, and would increase the comparison algorithm’s execution time tremendously. This can be remedied by using descriptors to characterize shapes with a much smaller set of numbers, such as Hu’s invariant moments [2]. Figure 1.2 illustrates a database containing the letters ‘a’ and ‘b’, with their corresponding descriptors and how one would compare an unknown character’s descriptors with the ones in the database.
1.2 Motivation

The necessity for automated shape description is typically found in imaging applications related to computer vision. There has not been a great need for numerical means of shape characterization in three dimensions, and the standard two dimensional descriptors are not readily translated into compact representations in three dimensions. The situation is exacerbated when attempting to characterize a mixture of three dimensional objects.

The application that is the focus of this thesis (and of great importance to civil engineers), is describing the three dimensional shapes of particle aggregates in a sand mix. The geotechnical properties of a particular soil are affected by the shape characteristics of sand grains that constitute that soil. The size, shape, and way the sand particles interlock with each other are all factors that determine the soil’s behavior under load. There are three major categories that affect the stress-strain behavior of soils; inherent particle characteristics, geology history and the environmental or external factors [4]. This is shown in Figure 1.3.
The majority of these factors can be quantified for further analysis by the use of standard techniques. For example, a sieve analysis can be used to calculate particle size and size distribution. This is when a sample of the soil is placed on a mesh screen and then is sifted down into another screen with a smaller mesh. This process then continues and the mass retained in each sieve is recorded. Specific gravity distribution can also be measured using the displacement of water. The shape and angularity of a particle is the only inherent particle characteristic that still needs an effective algorithm to quantify. The standard techniques that are in use, such as radius expansion or spherical harmonics, are useful only for characterizing 2-D boundaries or comparing 3-D shapes to spheres.

The particle to particle interaction (known as the friction angle) in the mix is affected by the shape of the sand particles. Friction angles are important in understanding the properties of natural soils because they determine the strength of a sand. Compaction of the soil with its minimum and maximum void ratios (measurement of the space between the particles in a mix) are also greatly dependent on the shape of the particles [4]. For instance, more jagged sands will
typically have higher shear strength and higher yield strength than a mix of soil with more rounded particles. These examples illustrate how shape information can be more important than other inherent particle characteristics, and despite this a definitive method does not exist for calculating this feature.

Although a qualitative understanding of the relationship between shear strength and shape already exists, a quantification of shape parameters would allow for a more quantitative relationship to be obtained. Once the reconstruction of particles is made possible, more realistic models using the discrete element method can be developed. These models can then be used to observe microstructure effects on shear strength and particle contact forces, which will in turn allow for more accurate constitutive models to be developed.

However, the limitation with these methods is that finding valid data that provide a three dimensional-description of aggregates in a mix is very difficult. While two-dimensional models have been developed using optical microscopy observations, they are not very accurate and can only be used reliably for charting behavior trends [5]. A three-dimensional model is essential for developing a more realistic model that can closely replicate actual tests. Development of three-dimensional models is difficult due to the expensive equipment and large amounts of computational resources required by the majority of existing methods to obtain the necessary information. Figure 1.4 shows an X-ray tomographic reconstruction of a single Melt Sand particle – the digitization and reconstruction process for this experiment took approximately 2 hours.
Figure 1.4: X-ray tomographic reconstruction of a Melt Sand particle.

The concept of describing three-dimensional shapes by finding shape numbers is not a trivial task. As the object to be discretized is not a flat, continuous shape (which would require only an x and y coordinate), a z coordinate is necessary. This need for the z coordinate implies that the object would be described in layers, where a set of x and y coordinates would be required for every unique value of z. In turn, the number of points needed to analyze the boundary of an object would be increased dramatically. As a very large number of particles from a mix with varying three-dimensional coordinates would need to be observed, this technique of direct three-dimensional characterization is not efficient. However, finding a two-dimensional approach for characterizing shapes of three-dimensional particles will be rapid, computationally efficient, and parsimonious, as will be discussed in this thesis. The necessary imaging equipment will be inexpensive (optical microscope and digital camera) and the required techniques will draw upon the vast amount of work done already in the area of two-dimensional shape description.

The technique must be able to find descriptors in order to characterize different shapes of sand, as well as be able to reconstruct a three-dimensional object from this data for use in the
discrete element model. The reconstruction procedure must be able to estimate a three-dimensional particle by combining a set of two-dimensional projections. The work of soil analysis would be greatly advanced by the development of a method as easy to implement as a two-dimensional characterization algorithm, but with the accuracy of a three-dimensional model.

1.3 Objectives, Scope, and Organization of Thesis

The goal of this thesis is the design and development of an automated 3D tomographic reconstruction algorithm applied to the shape characterization of particle aggregates. The specific research objectives are:

1. Design and development of an automated 3D tomographic reconstruction algorithm applied to the shape characterization of particle aggregates.

2. Demonstrate the ability of this algorithm to accurately and repeatably reconstruct composite 3D objects from 2D projections of multiple particles and their corresponding 2D shape descriptors.

3. Numerical validation of the reconstruction method by comparing with 3D reconstructions obtained from multiple projections of a single particle generated using optical and X-ray methods.

4. Develop experimental protocols and a database of results obtained by optical and X-ray tomography of a varying set of particle aggregate mixtures.

5. Demonstrate the consistency, separability and uniqueness of the 3D shape descriptor algorithm by exercising the method on a varying set of particle aggregate mixtures.
The tomographic reconstruction algorithm premise of the research was validated using 4 aggregate mixes, which were scanned using both the X-ray CT scanner and the experimental optical tomography system. The available database contains 200-300 digital images (single projections) from each of the four mixes, and 2-3 three-dimensional models of single particles from each of the four mixes, for which 300+ digital images were available for each.

This thesis is organized as follows. Chapter 1 describes the problems associated with 3-D shape description and the specific application for geomaterial aggregates. Chapter 2 discusses the method used for sand particle characterization and common tomographic reconstruction techniques for 3-D objects. Chapter 3 describes the use of the chosen tomographic reconstruction method to validate the shape characterization method, synthesis of 3-D sand particle models using descriptors selected randomly from the distributions of descriptors generated for the different aggregates. Chapter 4 contains the results of the validation and synthesis of models using the 3-D characterization and reconstruction algorithms. The experimental setup is also described in this chapter. Chapter 5 has a summary of accomplishments and recommendations for future work and is the conclusion of this thesis.

1.4 Expected Contributions

This thesis expects to demonstrate that a set of randomly generated 2-D projective representations may be used to form a composite model possessing shape characteristics that are representative of the shape properties found in an aggregate mix. This composite model will be generated by using tomographic reconstruction techniques to combine the projections. Projection generation is done according to the premise found in the shape characterization using multiple projective representations work [2]. This thesis also expects to demonstrate that optical
tomography techniques may be used in lieu of X-ray CT techniques for the purpose of generating particle aggregate models for use in a discrete element modeling system.
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