Chapter 1

Introduction

1.1 General Overview

1.1.1 Characterization and modeling approaches

Most geomaterials used in field-scale applications are modeled using continuum mechanics [5; 6]. Continuum methods rely on constitutive models that are, by and large, developed phenomenologically [7–12]. These models have been shown to be predictive in many areas of science and engineering, but are unable to quantitatively answer more fundamental questions related to instability, shear banding, and failure in granular materials (e.g., avalanches and liquefaction), in which the changing micromechanical structure plays an important role.

On the experimental side, new technologies are enabling unprecedented access to information at lower scales that have not been considered possible several years ago. Progress has been made in unraveling much of the kinematic processes in granular matter mostly owing to X-ray computed tomography (CT) [13–16]. For example, it is now possible to obtain full field kinematics in sand particles as they are loaded macroscopically [17]. Using X-ray CT, it is thus possible to obtain all translational and rotational degrees of freedom in each particle for thousands of particles constituting a macroscopic assembly. In the area of interparticle forces, new developments using 3D X-ray diffraction [18] have shown that it is possible to measure average elastic strains in sand particles under macroscopic loading [19]. These experiments, however, do not furnish a means to measure interparticle forces. Photoelasticity was a tremendous contribution to the ability to infer interparticle contact forces, but it is limited to birefringent materials [20; 21] and hence cannot be applied to natural granular materials such as sands. The ability to measure interparticle forces in natural granular materials is the missing link to constructing better constitutive models for granular materials, especially with the advent of multiscale models capable of using these incredibly rich kinematics [22].

Given that the relationship between interparticle forces and macroscopic stresses has been known for decades [23], one natural proposal would be to use a discrete model in conjunction with grain shape measurements to reproduce the macroscopic response of an experiment and at the same time infer the interparticle forces. The discrete model would operate at the fundamental level, i.e., Newtonian mechanics for particles. One such discrete approach is offered by the Discrete Element Method [24] (DEM). DEM, introduced more than three decades ago, was predicated on the possibility of revealing micromechanical features that were simply not accessible to continuum models. This modeling paradigm has allowed tremendous access to quantities such as contact forces, enabling the understanding of most features of the micromechanical behavior of granular materials and link them to macroscopic response [23]. This link, however, remains qualitative and this is mostly due to the inability to capture grain morphology accurately.

1.1.2 The role of particle morphology

Particle morphology can be characterized, in general, by three properties: sphericity, roundness, and roughness [1] (see Figure 1.1). These properties are sometimes referred to by other

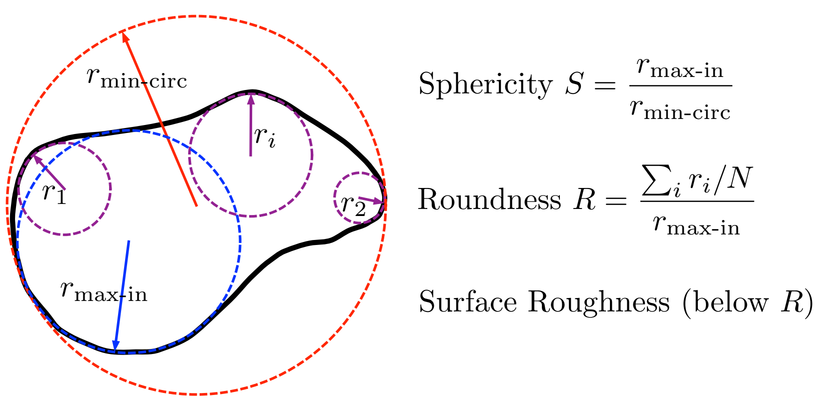

Figure 1.1: A definition of particle morphological features [1].

names, such as shape, angularity, and surface roughness, respectively [25]. These properties are scale dependent, as they measure morphological characteristics at different length scales, with increased spatial resolution needed to measure roughness, for example. Particle morphology has been shown to be crucially important for macroscopic properties in granular materials. Some of the most critical macroscopic properties used in granular materials are strength and permeability, and both of these are intimately affected by particle morphology (e.g. [1; 26]). In the case of macroscopic strength, it has been determined that lack of sphericity, sharper angularity, and increased roughness all lead to increased mobilized strength in granular materials [1]. This macroscopic effect is due to micromechanical effects such as an increased number of contact points. Therefore, the ability of discrete models for granular materials to accurately capture particle morphology is of paramount importance if they are to correctly predict the macroscopic strength in real granular materials such as sands.

1.1.3 Current shape representation techniques in discrete models

In the past, researchers have attempted to incorporate the effects of particle shape or non-sphericity through rolling resistance. The prototypical rolling resistance model appears to originate from the work of Iwashita and Oda [27], who recognized that rotational resistance arises not only from contact behavior, but also from particle shape. In particular, they observed large voids and rotational gradients in shear band experiments, which were never reproduced by conventional DEM (at the time disks and spheres) since rolling would occur without any resistance at the contacts. To minimize the discrepancy between DEM simulations and experiments, they modified the classic DEM to include rolling resistance at the contacts. Their model treated the rolling resistance with a combination of an elastic rotational spring, a dashpot, a non-tension joint and a slider. The rolling resistance was provided through a pair of torque couples calculated as the product of the relative particle rotation and rotational spring stiffness, with the dashpot providing viscous damping for numerical stability. Using this model, they were able to predict shear band behavior that was similar to that seen in natural granular soils.

The work of Iwashita and Oda attracted wide interest and their rolling resistance model was subsequently adopted and extended in other studies (e.g., [28–33]). There can be, however, marked differences between the various proposed rolling resistance models, which may be attributed to the different assumptions on the physical sources contributing to rolling resistance [34]. As a result, the effectiveness of rolling resistance models can be problem dependent. In addition, these models contain artificial parameters, which are usually chosen independently by trial and error. Despite these limitations, the introduction of rolling resistance models marked a defining moment in discrete modeling, when particle shape was recognized as an importance source of rolling resistance affecting the macroscopic strength of granular media.

More recent discrete simulation approaches include techniques to represent complex particle morphology or shape, beyond disks/spheres and ellipses/ellipsoids, which are based mostly on the clustering or clumping technique [35; 36] and polyhedra approach [37–41]. Through these techniques, rolling resistance would directly emanate from the geometry representation without relying on artificial rolling resistance models.

In the clustering technique, a group of spheres or circles are arranged and overlapped so that the outer curves or surfaces combine to approximate the shape of the grain. Then, the same disk-disk or sphere-sphere contact algorithm is reused over all potentially contacting pairs. The use of spheres in clustering techniques, while computationally inexpensive and easily implemented, is unappealing because of the lack of continuity in the curvatures and tangents. For example, the grains appear 'clumpy' at locations where spheres overlap or clump, and the curvature at any point in spherical-based discrete element is always positive. These anomalies prevent spherical-based discrete elements from higher fidelity contact mechanics calculations without further numerical treatment.

The polyhedra is essentially a rigid finite element. In 2D, the boundaries are represented as line segments while in 3D, the surfaces are represented using triangles or quads, similar to finite elements. In principle, polyhedra-based discrete elements can be refined as much as needed for an arbitrarily accurate grain shape representation. In practice, however, this resolution increase makes computational cost associated with narrow-phase contact detection and force calculations prohibitively expensive. As such, polyhedra-based discrete elements tend to appear 'blocky' and their shape representation capabilities not fully realized. In addition, the contact algorithms available for these geometrical entities are rather complex as they introduce the need to deal with face-to-node, node-to-node, and face-to-face contact. All development work on polyhedra techniques to date have focused almost exclusively on the treatment of convex particles (e.g., [42]).

Alternatives, which are essentially combinations of the aforementioned techniques, include spheropolyhedra [43; 44] and potential particles [45; 46]. Spheropolyhedra are defined by the Minkowski sum of a simplex (either a point, a line segment, a triangle, or a tetrahedron) with a sphere with radius r centered at the origin. The simplex serves as a skeleton for the particle and the radius r defines the distance of the particle surface from the skeleton. Potential particles are based on polyhedra with slightly rounded corners, edges, and faces. They are described by a smooth function that provides an analytical inside-outside check determined by the sign of the potential function, and the level sets of the function are strictly convex. In [46], a different potential function that enables the representation of spheres truncated with flats is proposed. These alternatives are still limited in terms of shape representation because their underlying formulations are based primarily on primitive geometries such as spheres, planes, and simple analytical functions.

In the several decades following the inception of DEM [24], there were tremendous efforts in the development of shape representation capabilities and associated contact algorithms (e.g., [35–37; 40]). Currently, however, it appears that progress has hit a plateau with shape representations, largely belonging to either the polyhedra or clustering approach, still too crude for real grain-scale calculations.

1.1.4 Connection between experiments and discrete modeling

While the influence of particle morphology on properties such as strength, permeability, etc. is well established [1; 26], it appears that grain-scale modeling and characterization efforts have remained compartmentalized, as exemplified by a relative lack of connection between real experiments and discrete modeling. In cases where discrete modeling of real granular materials with non-trivial geometries were attempted, crude discrete models with large geometrical biases and significantly calibrated parameters have been widely employed. Interestingly, the effects of geometrical bias on grain-scale response from use of simplified geometries are largely not discussed or quantified in the literature. It appears that the current gap between grain-scale modeling and characterization technologies is quite large. While imaging techniques are becoming increasingly sophisticated [13–17], there continues to be a lack of effort to bring discrete granular simulation technology closer to the engineering application level. To our knowledge, there is currently no work on discrete modeling of real granular materials at the grain scale.

1.2 Motivation

A discrete model that can directly incorporate particle morphological features (to within imaging resolution), and that can predict the response of real granular assemblies would eliminate the current bottleneck preventing the application of discrete models on real granular materials. More generally, a morphologically representative discrete model would allow computational discrete mechanics to catch up with and probe into the wealth of information offered by experimental techniques such as X-ray CT and X-ray diffraction, and probe the micromechanical response of a wide array of granular materials available in nature. At the same time, these advances would enable the development of new and more physics-based continuum constitutive models, relying less on phenomenology, as well as improve the predictive capabilities of multiscale methods that incorporate an underlying granular discrete model.

1.3 Research Objective

We look at the research objective in relation to the recent development of a tomography-to-simulation framework for studying granular materials [4], as illustrated in Figure 1.2. In support of this framework, computational techniques have been developed to extract and transition from binary image data of grains to the grain-scale quantities such as particle morphological features, kinematics, and contact spatial topologies. In particular, the very challenging region of grain-to-grain contact and particle morphology can now be accurately resolved (to within imaging resolution) using the level set method [47]. The transition from this information to discrete models and computations is the next logical step.

The research objective is therefore to devise a new DEM that can account for particle morphological features that have already been captured in the image data and that are necessary to make discrete computations predictive. Below, we list the components required to meet this research objective.

1. **Geometry basis**. The development of a new DEM requires the choice of a basis for representing particle geometries. Based on promising results from the realm of isogeometric analysis [48], Non-Uniform Rational Basis-Splines (NURBS) was experimented with. In the context of granular simulations, NURBS provides great flexi-

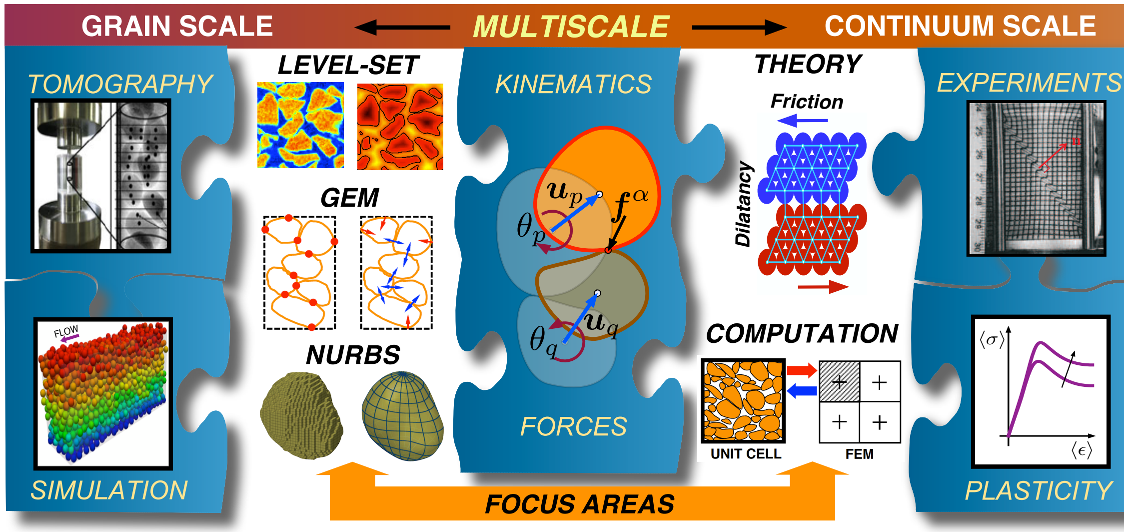

Figure 1.2: Schematic showing unified tomography-to-simulation framework across scales (left to right) and integration of characterization and simulation (top to bottom). Areas of relatively established understanding (shown in solid puzzle pieces), such as grain-scale tomography and simulation, are contrasted with focus areas that are in active development. Level sets, GEM [2; 3], and NURBS are key computational ingredients to enabling grain-scale characterization and simulations, which yield particle kinematics and forces. Using such quantities, multiscale methods provide the link between experiments and continuum plasticity models to complete the proposed framework (after [4]).

bility in representing arbitrary and complex geometries with much less information than conventional faceted or polygonal counterparts. The idea of using NURBS for representing grain geometry is shown in Figure 1.3, which shows an example of a sand particle imaged with 3D X-ray CT, with thousands of voxels used to render morphology (roundness and angularity) accurately, as well as the concept of seamlessly transitioning from binary image data in (a) to a smooth functional representation using NURBS in (c). The intermediate figure in (b) shows the control mesh furnished by the so-called NURBS control points.

2. **Contact algorithm**. The contact algorithm is one of the major components of DEM. Here, the quantity that needs to be determined is the signed gap or penetration, which is subsequently used in the calculation of the normal contact force. The major difficulty in using NURBS is that there is a separation between the control points and actual curve or surface. Therefore, there are no vertices or facets to simplify the determination of the signed gap. In addition, the process is necessarily iterative

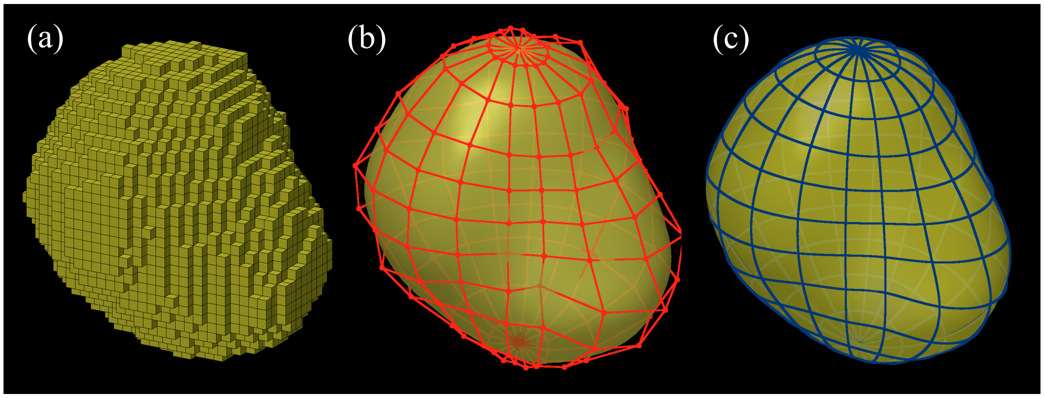

Figure 1.3: Using NURBS as a representation for grain morphology.

because of the generally nonlinear nature of parametric curves and surfaces. The challenge here is to devise a methodology that can take advantage of the parametric nature of NURBS to compute the signed gap or penetration between two non-convex NURBS surfaces.

3. **Time integration**. While this component is not related to particle morphology, it needs to be improved for practical reasons. It is well known that explicit algorithms used in classic DEM lead to very small time steps when nearly rigid particles (e.g., sand) are modeled. Here, a contact dynamics (CD) approach is desirable since the equations of motions and constraints are considered implicitly, allowing the use of larger time steps. Current CD approaches, however, are fairly difficult to implement and here, we seek a simpler CD formulation that would remedy this difficulty.

4. **Application with real particle geometries**. As a new DEM that aims to bring grain-scale characterization and modeling to a real application level, it needs to be assessed experimentally. In the past, we have characterized internal variables such as dilatancy and residual strength in shear bands using experimental data. As a first grain-scale application of our new DEM, we will attempt to numerically reproduce these experimentally-inferred internal variables. For this work, X-ray CT experimental data can be obtained from our collaborators at the University of Grenoble, France.

1.4 Contribution

The contribution of the work described in this thesis is the development of a new DEM that has enabled the seamless transition from X-ray CT image data to discrete computations, and in this process has allowed for the capturing sphericity and roundness, the two morphological measures that are used in characterizing real particle geometries. We have applied the new DEM to characterize and model the shear band response in a real triaxial specimen in which we have obtained a consistent set of internal variables — dilatancy and residual strength — between experiment and discrete simulation, providing the first complete link between grain-scale experiment and modeling in the tomography-to-simulation framework.

1.5 Overview of Thesis

This thesis is organized as follows: Chapter 2 covers some fundamental background concerning discrete methods, namely, their governing equations, time integration approaches, shape representation techniques and the current state of affairs of these methods in terms of granular materials modeling.

In Chapter 3, the details of our NURBS-based DEM is presented. In particular, the basics of NURBS are explained and the solution of the closest-point projection of a point on a NURBS surface through the Lipschitzian *di*viding *rect*angle (DIRECT) global optimization algorithm is described. The latter development is crucial to enabling the contact treatment of arbitrary-shaped non-convex particles, as well as making the implementation of the new DEM simple and robust.

In Chapter 4, a CD approach to our NURBS-based discrete method is presented. By combining particle shape flexibility, properties of implicit time integration (e.g., larger time steps) and non-penetrating constraints, as well as a reduction to a static formulation in the limit of an infinite time step), we target applications in which the classical DEM either performs poorly or simply fails, i.e., in granular systems comprising rigid or highly stiff angular particles and subjected to quasi-static or dynamic flow conditions.

Chapter 5 presents an application of the new DEM within a computational mechanics avatar framework in which a quantitative comparison of microscopic quantities from discrete simulation and experiment is made. This is the first attempt at using a discrete model inferred from real grain-level XRCT data to study the response of a real macroscopic triaxial specimen.

Finally, Chapter 6 summarizes some key developments of this dissertation. Limitations of the current work are also discussed and future directions of research are outlined.

This thesis is based on a number of papers [4; 49–52]. To make this thesis flow better, content repetition is minimized as much as possible. In certain chapters (e.g., Chapter 5), however, there will be some repetition of concepts, equations, and ideas, as these chapters are in the process of being published as individual journal articles.