# Preface

The study of "granular" or "particulate" media is wide ranging. Classical examples include the study of natural materials, such as sand and gravel, associated with coastal erosion, landslides, and avalanches. A concise introduction is given by Duran [61]. Many manufactured materials also fall within this class of problems.[1] For general overviews of granular media, we refer the reader to Jaeger and Nagel [100], [101], Nagel [151], Liu et al. [139], Liu and Nagel [140], Jaeger and Nagel [102], Jaeger et al. [103]–[105], and Jaeger and Nagel [106]; the extensive works of Hutter and collaborators: Tai et al. [188]–[190], Gray et al. [80], Wieland et al. [201], Berezin et al. [28], Gray and Hutter [81], Gray [82], Hutter [96], Hutter et al. [97], Hutter and Rajagopal [98], Koch et al. [126], Greve and Hutter [85], and Hutter et al. [99]; the works of Behringer and collaborators: Behringer [22], Behringer and Baxter [21], Behringer and Miller [23], and Behringer et al. [24]; the works of Jenkins and collaborators: Jenkins and Strack [107], Jenkins and La Ragione [108], Jenkins and Koenders [109], and Jenkins et al. [110]; and the works of Torquato and collaborators: Torquato [194], Kansaal et al. [119], and Donev et al. [55]–[59]. In this monograph, we focus on a subset of the very large field of granular materials, namely, *fluidized (lower-density) particulate flows*.[2]

Recently, several modern applications, primarily driven by microtechnology, have emerged where a successful analysis requires the simulation of flowing particulate media involving simultaneous near-field interaction between charged particles and momentum exchange through mechanical contact.[3] For example, in many systems containing flowing particles below the one millimeter scale, the particles can acquire relatively large electrostatic charges, leading to significant interparticle near-field forces. In some cases, the

[1] Over half (by weight) of the raw materials handled in chemical industries appear in granulated or particulate form. The resulting structural properties of solid products which originate as granulated or particulate media, and which are transported and constructed using flow processes, are outside the scope of this monograph. For more details, see, for example, Aboudi [1], Hashin [90], Mura [150], Nemat-Nasser and Hori [152], Torquato [194], and Zohdi and Wriggers [216].

[2] It is worth noting that fast computational methods, in particular efficient contact search techniques, for the treatment of densely packed granular or particulate media, in the absence of near-field forces, can be found in the recent work of Pöschel and Schwager [167]. Such techniques are outside the scope of the present work, but they are relatively easy to implement.

[3] For example, industrial processes such as chemical mechanical planarization (CMP), which involves using chemically reacting particles embedded in fluid (gas or liquid) to ablate rough small-scale surfaces flat, have become important in the success of many micro- and nanotechnologies. For a review of CMP practice and applications, see Luo and Dornfeld [143]–[146].

near-field forces could be due to magnetic effects, or they could be purposely induced.[4] Charged material can lead to inconsistent "clean" manufacturing processes, for example, due to difficulties with dust control, although intentional charging of particulate material can be quite useful in some applications, for example, in electrostatic copiers, inkjet printers, and powder coating machines. The presence of near-field interaction forces can produce particulate flows that are significantly different from purely contact-driven scenarios. Determining the dynamics of such materials is important in accurately describing the flow of powders, which form the basis of microfabrication. Near-field forces can lead to particle clustering, resulting in inconsistent fabrication quality. Therefore, neglecting such near-field effects can lead to a gross miscalculation of the characteristics of such flows.[5] Thus, an issue of overriding importance to the successful characterization of such flows is the development of models and reliable computational techniques to simulate the dynamics of multibody particulate systems involving near-field interaction and contact simultaneously (including thermal effects). This is the primary focus of this monograph.

A central objective of this work is to provide basic models and numerical solution strategies for the direct simulation of flowing particulate media that can be achieved within a relatively standard desktop or laptop computing environment. A primary assumption is that the objects in the flow are considered to be small enough to be idealized as particles and that the effects of their rotation with respect to their mass centers is unimportant to their overall motion.[6] Our primary concern is with particulate media that are "fluidized," i.e., they are not densely packed together. Oftentimes, such media are referred to as "granular gases." In particular, the initial chapters of the monograph are dedicated to so-called dry particulate flows, where there is no significant interstitial fluid. *However, while this monograph focuses almost exclusively on the dry problem, Chapter* 8 *gives an introduction to strongly coupled (surrounding) fluid/particle interaction scenarios.* Also, an introduction to computational optical techniques for particulate media is provided. Simulations described in upcoming chapters can be found at `http://www.siam.org/books/cs04`.

Ideally, in an attempt to reduce laboratory expenses, one would like to make predictions of a complex particulate flow's behavior by numerical simulations, with the primary goal being to minimize time-consuming trial and error experiments. The recent dramatic increase in computational power available for mathematical modeling and simulation raises the possibility that modern numerical methods can play a significant role in the analysis of complex particulate flows. This fact has motivated the work presented in this monograph. This work can be viewed as a research monograph, suitable for use in a first-year graduate course for students in the applied sciences, engineering, and applied mathemat-

[4] For many engineering materials, some surface adhesion persists even when no explicit charging has occurred. For example, see Tabor [186] or Johnson [111].

[5] For example, on the atomic scale, forces of attraction can arise from a temporary dipole created by fluctuating electron distributions around an atom. This will induce a dipole on a neighboring atom, and if the induced dipole is directed in the same way as the first atom, the two molecules associated with these atoms will attract one another. Between two atoms, such a force acts over a nanometer; however, when two small-scale (1–100 microns) particles approach one another, the effect is greatly multiplied and the forces act over much larger distances. Also, for example, repulsion forces can arise due to ionization of the particle surfaces or due to the adsorption of ions onto the surfaces of particles. The combination of attraction and repulsion forces is called a near-field force. It is worth noting that near-field forces can be introduced into a model in order to mimic much smaller scale effects attributed to chemical potentials, interstitial fluid, etc., which do not necessarily have as their basis a "charge."

[6] However, even in the event that the particles are not extremely small, we assume that any "spin" of the particles is small enough to neglect lift forces that may arise from the interaction with the surrounding fluid.

ics with an interest in the computational analysis of complex particulate flows. Although it is tempting, a survey of all possible modeling and computational techniques will not be undertaken, since the field is growing at an extremely rapid rate. *This monograph is designed to provide a basic introduction, using models that are as simple as possible.* Finally, I am certain that, despite painstaking efforts, there remain errors of one sort or another. Therefore, if readers find such errata, I would appreciate if they would contact me at zohdi@newton.berkeley.edu.

T. I. Zohdi

Berkeley, CA
November 2006