Preface

Granular materials cover a broad area of research at the intersection of different scientific fields including soft matter physics, soil mechanics, powder technology, agronomic transformations, and geological processes. Despite the wide variety of physicochemical and morphological grain properties, the discrete granular structure of these materials leads to a rich generic phenomenology, which has motivated federative research for its fundamental understanding. The grain-scale description of granular systems has therefore been a vital lead for research for 30 years with the goal of enriching macro-scale variables that happen to be too poor to account for the rheology.

In this context, although model experiments and modern measurement techniques have been used for probing local granular variables (particle positions and velocities, contact forces, and so on), the *discrete* approach developed in parallel for particle-scale numerical modeling of granular materials has now become a powerful and reliable research tool. This approach is simply based on the integration of the equations of motion simultaneously for all particles, described as rigid elements, by considering the contact forces and the external forces acting on the particles. Given the boundary conditions, the mechanical response of a collection of particles to external loading leads to relative particle motions constrained by steric exclusions in a dense state and/or by inelastic collisions in a loose or dilute state.

Technically, the discrete approach requires a time-discretized form of the equations of motion governing particle displacements and rotations, on the one hand, and a force law or a force-displacement relation describing particle interactions, on the other hand. When P. Cundall applied this method nearly 30 years ago to granular geomaterials, he called it the *distinct element method* (DEM) in contrast to the *finite element method* used in continuum mechanics. The attribute "distinct" refers to the degrees of freedom carried by individual particles, but it was later replaced by "discrete" as a way to underline the discrete nature of the system. A similar method called molecular dynamics (MD) was used at that time for the simulation of molecular systems with classical schemes that could be directly applied to granular media. For this reason, many authors keep using indiscriminately the acronyms MD and DEM for the discrete simulation methods of granular materials.

However, in spite of this formal analogy (particles and force law) between granular and molecular systems, the physics is fundamentally different. The interactions between particles in a granular material are governed by the unilateral character of contact and energy dissipation by friction and inelastic collisions. Moreover, granular materials involve a variety of particle shapes and size distributions, cohesion forces, and interstitial solid or fluid phases that require appropriate numerical treatment. It is also important to remark that in the absence of thermal agitation, a granular material can be found in various states of packing and flow with a strong memory effect so that the initial state cannot be specified without a preparation protocol. Therefore, even in a minimalistic model with spherical particles of the same size interacting via frictional contacts, the discrete numerical simulation of granular media involves subtle aspects that require proper solutions. Nevertheless, such details are rarely published, and many useful and vital "tricks" are still in the realm of "simulator's art."

It is also noteworthy that the contact interactions in a mechanical system can be treated without resorting to a force law and using the overlap between particles as a displacement variable for the calculation of repulsive forces. An alternative method, known as contact dynamics (CD), was introduced by J. J. Moreau and M. Jean 20 years ago. This method allows for an exact treatment of frictional contacts between solid bodies. We thus distinguish the MD-DEM from the CD-DEM. In the same way, in the limit of dense systems, the dynamics can be replaced by a quasi-static (QS) treatment in which the evolution of the system is described by consecutive states of mechanical equilibrium. This is an interesting numerical approach which can be applied to a broad class of problems and to which we refer as QS-DEM. Finally, dilute systems (granular gases) are governed by an event-driven (ED) dynamics in which the state evolves by consecutive binary collisions between particles. This method, to which we refer as ED-DEM, has been technically refined for fast simulations of collisional dilute systems.

The goal of this book is to provide the reader with a self-contained introduction to various methods and skills for discrete numerical simulation of granular materials. The authors are known for their rich experience with DEM or innovating numerical developments. The book brings together pedagogical presentations to various aspects of discrete numerical modeling with many technical details often omitted from regular research papers. It also includes most recent developments such as fluid–particle interactions where the state of the art is presented with abundant bibliography.

The chapters follow a rational and progressive order while reflecting the cultural diversity of the research community interested in granular materials. A numerical methodology requires not only a simulation method but also a "toolbox" of different methods for the construction of granular packings, the management of boundary conditions, and the choice of parameters. All these topics are covered in the first part of this book basically in the framework of a minimalistic model. The second part is devoted to more advanced developments dealing with complex particle shapes, cohesion forces, hydrodynamic and thermal interactions, and modeling of complex granular systems. A multitude of cross references is included for transversal reading, and the index list contains most familiar jargon of the field of granular simulations.

Let us finally underline here that the material presented in this book cannot be comprehensive as the field of numerical simulations is constantly enriched by new developments. But the editors hope that this book contributes as a first "forum" bringing together different methods and skills for discrete-element modeling of granular materials.

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