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Mathematical Models of Granular Matter

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Preface

The adjective 'granular' is attributed to materials when they are made of sets of unfastened discrete solid particles (granules) of a size larger than one micron, a length scale above which thermal agitation is negligible. In fact, the dominant energy scale in granular materials is the one of a single grain under gravity. Granular matter is common and we meet it everyday. Examples range from the dust settled on the books of our libraries, to the sand in the desert, to the meal used in cooking, itself obtained from grain, often stored in silos. Granular matter displays a variety of peculiarities that distinguish it from other substances studied by condensed matter physics and renders its overall mathematical modeling arduous. In a review paper of 1999 [dG] P.G. de Gennes writes: "granular matter is a new type of condensed matter, as fundamental as a liquid or a solid and showing in fact two states: one fluidlike, one solidlike. But there is as yet no consensus on the description of these two states!"

Almost all preconceptions on which the standard theory of continua is based seem to fail. The standard concept that the material element is well identified (even in the statistical conception common in gas dynamics) fails and, with it, the current mathematical picture assigning to it a precise placement. Even useful results of the standard kinetic theory of gases can be called upon confidently, in general. The populations of grains are far less profuse than the molecular ones in gases and far more crowded. The constraints imposed by grains on one another are generally too conspicuous to rigidify the lot. Also, boundary conditions are far from the simple classical scheme suggested by the divergence theorem and need separate critical modeling.

Heaps of granules do not sustain tension unless (at least a small) cohesion is present. They are, in general, in anisotropic metastable states. Such states last indefinitely unless external perturbations occur. Contrary to common solids and fluids, no thermal average among nearby states arises (see [JNB]). Interactions between granules are exerted through contacts occurring along graphs with topology depending on the way in which granules are packaged, on the distribution of the sizes of the granules themselves, on the boundary

conditions and, above all, on the sources of external disturbances. Subsets of granules may self-organize in order to sustain and distribute tensions along arcs: When granules are stored in a silo the pressure at the bottom of the silo does not increase indefinitely as the height of the stored material grows, rather it reaches a maximum value if the lateral walls of the silo are sufficiently tall. If the silo is shaken and grains with different sizes are stored within it, size segregation occurs instead of mixing. The phenomenon does not fit the entropic effects that one recognizes in standard liquids. Both traveling and standing waves accrue in the surface layer of grains, and slip appears along the walls of the silo. It is not clear yet how inelastic interactions and local disorder or segregation contribute to the acoustic propagation.

Layer dynamics is present also in 'avalanches'. The example is the addition of grains to a heap from the top: the surface layer moves, the core persists. The description of the connection between the surface flow and the core at rest forces one to account for the transition between two phases, if one wants to propose a global picture of the phenomenon. As for the contact stresses in granular materials at rest, even for rapid flows the stresses induced by the collisions depend on the local numerosity of granules, in other words on the 'degree of clustering'. Segregation in dense granular flows also has an influence. The overall mechanical behavior seems to be history-dependent.

Plastic effects may be prominent in the quasi-static regime: shear bands appear and inelastic deformations may be accumulated by cyclic loading processes. Inelastic collisions usually play a decisive role in dynamics, as in the fall of avalanches and in the walk of desert dunes. Chaotic agitation of granules leads them far from thermodynamic equilibrium, so fluctuations may be prominent. Microscopic slip friction between granules induces relaxation analogous to that of some solids with complex microstructure. Macroscopic friction is induced by earthquakes which may induce fluidization of granular matter.

Critical reviews such as [JNB], [dG], [K], and [AT] provide an adequate description of phenomena occurring in granular matter. They give a picture of the scenario.

A typical approach to the dynamics of polydisperse granular systems is based on the 'inelastic' Boltzmann equation which also provides the starting point for a plethora of hydrodynamic models. Assumptions on the types of contacts occurring must be chosen carefully: relative rotations may need to be accounted for, depending on the circumstances. Closures are obtained by assuming specific forms of the distribution function. A critical review of the results along these lines can be found in [V].

Even in a disperse state, a granular flow is dissipative as a consequence of the presence of inelastic collisions. Absence of equilibrium is the source of difficulties when one applies the Chapman-Enskog perturbative method to derive a (hydrodynamic) continuum picture from the kinetic description based on Boltzmann equation. Since collisions are inelastic, a double expansion in Knudsen number K and degree of inelasticity ϵ has to be used. Moreover, since

$\epsilon \propto K^3$ in the steady state, the expansion has to be extended up to Burnett or super-Burnett regimes to assure consistency, the latter regime being of degree $O\left(K^3\right)$. The appearance of unphysical instabilities under short-wave perturbations, typical of Burnett and super-Burnett regimes, requires viscosity regularizations of the field equations or the use of other possible techniques.

Attempts have been made to construct continuum models of granular matter from first principles, without resorting to kinetic justifications based on Boltzmann equation, especially in statics. Non-trivial difficulties arise, as already mentioned: at a gross scale some standard paradigms of traditional continuum mechanics need to be modified accurately. We have already mentioned for example the loss of the possibility of identifying perfectly a generic material element (i.e. even to define it). This difficulty is generated by the occurrence of segregation and also by the general lack of coherence due to the absence of cohesion between neighboring granules. Each material element must be then considered as an open system (as in [M]) from which granules may migrate from it to neighboring ones. Standard balances of interactions have to be then supplemented by an equation ruling the rate of local numerosity of granules. Such a rate, which is the rate of migration of granules, generates loss of information about the local texture of the granular matter, and increases the configurational entropy, although segregation is opposite to the entropic mixing (as mentioned above).

The definition of measures of deformation and stresses in terms of granular geometries and grain-to-grain interactions may be non-trivial. As regards the standard stress tensor, for example, a typical definition is made by the sum of the tensor product between the intergranular force and the vector indicating in a local frame the contact point between neighboring granules, a sum extended to all granules in contact with a given granule. However, although such a definition has a physical meaning, one does not know point by point (or better, element by element) the local distribution of granules, their geometry and the type of contact which may be inelastic and not even punctual. All these information characterize each model that can be constructed and have also constitutive nature.

By looking at deeper details, it is natural to consider a granular material as a complex body (in the sense of a body in which the material texture influences strongly the gross behavior). So, multifield descriptions of granular matter need to be called upon, as explained in some chapters of this book.

In any case, no accepted general consensus about the overall description of granular bodies exists. Such an absence of a unified description of the mechanics of the granular matter and the lack of preference for one or another approach, for aesthetic or experimental reasons, has pushed us to collect advances in the various prominent directions of research. Our aim is to furnish a panorama clarifying the state of current researches, solving problems, discussing critically points of view and opening new questions. Contributions range, in fact, from the kinetic approaches to granular flows to the continuum description of static and quasi-static behaviors. A non-trivial tentative of a

connection between the kinetic approach and a continuum modeling based on first principles is also present (see Chap. 4).

At the present state of knowledge and in the absence of a unitary point of view, one can only say that the variety and the peculiarities of behavior of granular matter render arduous the task of its overall mathematical modeling. Mathematical and physical questions of an intricate nature appear and tools additional to the traditional ones are needed. Some of these questions and tools are discussed in the subsequent chapters.

Motivated by experimental results on shear bands due to (unstable) plastic behavior of granular bodies, in Chap. 1, *Joe D. Goddard* discusses critically various techniques for the homogenization of granular media in a quasi-static regime, media that are seen here as multipolar continua in the sense of the mechanics of complex bodies. An energy-based method of homogenization is proposed as an improvement on previous approaches.

If one describes granular flows from the point of view of the kinetic theory, inelastic collisions play a role as mentioned above. The Maxwell model of binary collisions is a typical scheme adopted and is based on the assumption that the collision frequency is independent of the velocity of colliding particles. Such a model can be translated from rarefied gases to the description of granular flows. In Chap. 2, *Alexander V. Bobylev*, *Carlo Cercignani* and *Irene Martinez Gamba* discuss, from a general point of view, variants of the Maxwell model of pairwise interactions and establish their key properties that lead to self-similar asymptotics. Existence and uniqueness issues are also analyzed.

The approach based on the dissipative Boltzmann equation is further analyzed in Chap. 3 by *Giuseppe Toscani*. Two paths toward the hydrodynamic limit are discussed. They account for two different methodologies for the closure of macroscopic equations: (i) low inelasticity in the system, namely a perturbation in a precise sense that allows the local resort to Maxwellian functions, (ii) small spatial variations implying the use of a homogeneous cooling state.

One of the editors (**GC**) proposes in Chap. 4 (a chapter already mentioned above) further results on an earlier proposal for fast sparse flows. Complex bodies with kinetic substructure are considered. They are bodies in which each material element is a system in continuous agitation and are called *pseudofluids*. Granular flows fall naturally in this framework. The maelstrom within each material element and its influence on the neighboring fellows is governed by peculiar hydrodynamic balances: they are offspring of the microscopic interactions between granules.

The recursive analysis of higher momenta of the distribution function, even beyond Grad's 13 moments, has been the basic source of Extended Thermodynamics. The results on monoatomic gases provided by such an approach suggest its use in modeling granular flows. After summarizing the main modeling issues of Extended Thermodynamics, in Chap. 5 *Tommaso Ruggeri* analyzes the resulting hyperbolic system and discusses global existence questions and stability of constant state on the basis of Kawashima condition.

The construction of hydrodynamic models from first principles can find appropriate suggestions from detailed numerical simulations performed by looking directly at single granules and their contact interactions. The molecular dynamic approach is pursued in Chap. 6 by *Ramon García-Rojo*, *Sean McNamara* and *Hans J. Herrmann* who analyze (amid possible choices) the persistent elastic–plastic strain accumulation in compacted granular soils under cyclic stress conditions.

Since driven sets of granules (for example confined in a box) are in essence systems very far from thermodynamic equilibrium, as mentioned above, the effects of fluctuations are in general significant. Analysis of the injected power fluctuations is presented by *Alain Barrat*, *Andrea Puglisi*, *Emmanuel Trizac*, *Paolo Visco* and *Frederic van Wijland* in Chap. 7, a chapter divided into two parts: The first part deals with the way in which the probability density function of the fluctuations of the total energy is related to the characterization of energy correlations for both boundary and homogeneous driving. The second part contains an interpretation of some numerical and experimental results that seem to invalidate Gallavotti–Cohen symmetry [GC]. Such results appear contradictory to common analyses that seem to satisfy Gallavotti–Cohen fluctuation relation. By means of Lebowitz–Spohn approach to Markov processes, an approach applied to the inelastic Boltzmann equation, a functional satisfying a fluctuation relation is also introduced.

The last two editors collect their contributions in Chaps. 8 and 9. In particular, in Chap. 8 **PG** analyzes in the continuum limit the thermodynamics of a granular material modeled as a complex body endowed with a microstructure which is constrained and/or latent in the sense introduced by Capriz [C]. The consequences of grain rotations are described together with effects like dilatancy.

Finally, in Chap. 9, **PMM** considers granular matter in slow motion and describes it as a two-scale complex body for which each material element is considered as a grand-canonical ensemble of granules. The evolution equation of the numerosity of grains in each material element is derived in terms of grain-to-grain interactions.

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