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Mathematics and mechanics of granular materials

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The study of granular materials has always been a topic of considerable importance in engineering. Historically, the mathematical formulation of the subject dates back to the pioneering work of C.A. Coulomb in 1776 [1]. In his now famous memoir, Coulomb postulated the conditions that should be satisfied for failure to occur in a granular material. This postulate for failure still stands as a defining point in the mathematical study of mechanics of granular materials. Coulomb largely focused on a topic of importance to that time, namely the design of earth structures to avoid collapse. As a result, the study of the deformations that lead to failure received less emphasis [2]. Recently, however, several scientific disciplines, including geomechanics, mechanical, civil and chemical engineering, physics and applied mathematics, have shown renewed interest in accurately modelling granular materials to examine, concurrently, both failure and deformations. The study of how granular materials or bulk solids flow and deform is also of practical importance for a number of industries, including mining and minerals processing, agricultural materials processing, the construction industry, foodstuff production, pharmaceutical development and nanotechnology. In these applications the granular materials involved could be as diverse as crushed ore, cereal grains, sugar, flour, tablets and nano-particulates. In each case, granular materials frequently flow through devices such as bins, hoppers and chutes and a clear knowledge of how they behave under these circumstances is invaluable for the efficient design and application of related devices.

Granular materials form an important component in modern developments in geomechanics. For the most part, geotechnical engineers are less interested in fully developed granular flows, but the deformational aspects of granular materials are highly relevant in situations that require assessment of settlements of foundations on granular media. The development of mathematically correct and physically admissible theories to describe and predict the complex behaviour of granular materials or bulk solids is therefore a topic of fundamental importance to both the engineering sciences and applied mathematics.

Modelling the flow of granular materials has been extensively studied through the use of continuum mechanics. Using this approach, one formulates governing equations for the stress and velocity fields by coupling the equations of conservation of mass and linear momentum with appropriate constitutive laws that govern the initiation of failure and the rules applicable to the flow of the granular material subsequent to its failure. For rapid granular flows that accompany a reduction in the bulk density, the behaviour of each granular particle is determined primarily by inelastic collisions with neighbouring particles, in a way analogous to colliding molecules in dense gases. In contrast, for slow dense granular flows, the dominant mechanisms are quite different; here, the neighbouring particles continually slide and roll past each other, and friction between these particles becomes the dominant force.

The problem of modelling fully developed slow granular flows using continuum mechanics is, and continues to be, both complex and challenging. There is general agreement that stress fields within granular flows can be described by coupling the equations of linear momentum with the Coulomb–Mohr yield condition, or other forms of yield condition applicable to the myriad of granular materials that are encountered in engineering practice. However, there is little or no agreement as to how the equations for the velocity fields, that describe the deformations of fully developed flows, should be formulated, or even whether these equations should be mathematically well-posed or ill-posed. The constitutive assumption that is perhaps most widely employed by the engineering community is Saint-Venant's hypothesis, which is also referred to as the coaxiality condition. This condition states that the principal axes of the stress and strain-rate tensors should coincide. Drucker and Prager [3] were the first to formally adopt this hypothesis for the study of the mechanics of granular materials. They used the Coulomb–Mohr yield condition as a plastic potential to derive an associated flow rule. The condition of coaxiality must hold by virtue of material isotropy, and the rate-of-strain tensor depends only on the Cauchy stress tensor.

While the work of Drucker and Prager [3] marks the resurgence of the application of plasticity theories to mechanics of soils, these developments have limitations. Firstly, the theory predicts that all granular flows are accompanied by dilation or volume change, notably volume expansion, whereas in fact loose granular materials contract upon shearing, and others undergo isochoric or volume-preserving deformations. Even in situations for which dilation is appropriate, the predicted magnitude of volume increases is far in excess of those observed in most real materials. The second limitation is that for cohesionless materials; the theory predicts that the rate of specific mechanical energy dissipation is zero, which is clearly unrealistic. More sophisticated approaches attempt to overcome these difficulties by either including work-hardening/softening theories, similar to those proposed and developed by Drucker *et al.* [4], Jenike and Shield [5], Schofield and Wroth [6] or the incorporation of flow rules that are non-associated. In the former category of models, the yield condition varies with a state parameter, such as the density. For the work-hardening/softening models, the mathematical characteristics for the stress and velocity fields do not coincide, contrary to what is commonly observed experimentally; this leads to the adoption of non-associated flow rules. The subject matter in this area is extensive and no attempt will be made to provide an exhaustive review of non-associated plasticity. It is worth noting that Hill [7] proposed velocity equations for incompressible materials based on the Saint-Venant hypothesis, but, again, this theory has the undesirable property that the predicted stress and velocity characteristics do not coincide.

By abandoning the assumption of coaxiality, an alternative family of models has been derived based on a kinematic hypothesis involving the concepts of shearing motion parallel to a surface, rotation of that surface, and dilation or contraction normal to the surface. One such model is the double-shearing theory, originally proposed by Spencer [8, 9] for incompressible flows, and extended to dilatant materials by Mehrabadi and Cowin [10] and Butterfield and Harkness [11]. In this theory, the characteristic curves for the stresses and velocities coincide, and every deformation is assumed to consist of simultaneous shears along the two families of stress characteristics. These ideas build upon those of the double sliding, free rotating model, developed by de Josselin de Jong [12–14], by fixing the rotation rate as the temporal rate of change of the stress angle. To reiterate, an important advantage of the double-shearing theory over the previous coaxial theories is that it retains the assumption of slip occurring along the stress characteristics, but does not give rise to unusually high levels of dilatancy. Spencer's [8, 9] original double-shearing theory is for incompressible materials, which in the context of fully developed granular flow is often a reasonable and a realistic assumption. Furthermore, when applied to gravity-driven flow problems [15, 16], the coaxial theory is shown to yield physically unacceptable predictions in the velocity field, whereas the double-shearing theory predicts results that are certainly reasonable. On the other hand, there are experiments, which are not consistent with predictions of Spencer's double-shearing theory, but tend to support the double-sliding, free-rotating model of de Josselin de Jong [12–14]. Research in this area must recognize the fact that there is little possibility for developing a mathematical theory of granular media for all eventualities: the materials are real and the circumstances diverse. A theory that shows promise for a given set of experimental conditions can fail for others. In any event, at this moment no single theory is clearly most applicable for describing the behaviour of fully developed flow of real granular materials. While the subject requires more reproducible non-conventional experiments to help resolve these issues, there is a serious need for in-depth mathematical and numerical analysis of the theories involved. This might include the solution of relevant boundary-value problems and initial-boundary-value problems that can allow the continuous transformation of a deformation-dominated process to a flow-dominated one, the exploration of exact and numerical solutions to the equations, and the comparison and contrasting of existing theories that will guide critical experiments of the future.

In addition to the issues raised above, a major unresolved question with Spencer's [8, 9] double-shearing theory, and most other plasticity-based theories for fully developed granular flow, is that the equations are linearly ill-posed in the sense that small perturbations to existing solutions may result in solutions that grow exponentially with time (see *e.g.* [17–19]). This characteristic places doubt on whether or not steady solutions to the governing equations actually describe real granular flows, and also leads to serious implications for numerical schemes, which do not converge in the limit as the size of a mesh discretization approaches zero. However, ill-posedness in itself is not necessarily an undesirable property for equations that describe granular deformations. In fact, it is well known that under certain circumstances granular materials exhibit unstable behaviour, in which case it is quite plausible that ill-posedness should be the norm. An example is the onset of shear-banding. Perhaps the ideal situation, as advocated by Harris [19], is a theory that contains a domain of well-posedness, in which solutions may be stable or unstable, and also a domain of ill-posedness, which corresponds to a definite physical instability. This motivation has led Harris [20, 21] to derive a single-slip model, which belongs to the class of models based upon the physical and kinematic considerations discussed above. This single-slip model is indeed well-posed under well-defined conditions and ill-posed when these conditions fail [19]. In this case the ill-posedness corresponds to the physical instability of grain separation, a process that invalidates the assumption that friction between particles is the dominant mode of momentum transfer, as opposed to inelastic collisions. There is much scope for further research in this complex and challenging field.

We note that there have been several recent attempts to model the transitional region between dense, slow granular flows and rapid, collisional flows (see, for example, [22–25]. These models combine traditional plasticity ideas with notions borrowed from the kinetic theory of gases [26]. In general, the condition of coaxiality is enforced, and again it is not entirely clear whether these theories are well-posed or ill-posed. Often in fully developed slow granular flow, there are narrow layers, referred to as shear layers, in which the material experiences intense shearing. While the models mentioned previously capture many features of fully developed flow to varying degrees, none have the ability to accurately predict the thickness of the layers over which such intense shearing materializes. A reason for this limitation has been attributed to the fact that classical continuum models have no intrinsic length scale built into the constitutive equations. Attempts to rectify this deficiency probably date back to the work of Voigt [27] and later expanded by Cosserat and Cosserat [28] who introduced the concept of couple stresses for examining the mechanics of deformable media (see *e.g.* [29]). Here, the Cauchy stress tensor is no longer symmetric, and the conservation of angular momentum is no longer automatically satisfied but becomes a set of field equations that need to be satisfied explicitly. There are two extra field variables for Cosserat materials, namely the angular velocity and the couple-stress tensor. As a consequence of the notion of couple stresses, a length parameter or an intrinsic length scale naturally arises in the definition of constitutive relationships. The work on both micromorphic and couple-stress theories was an active area of research from the mid-1960s to the mid-1970s and the developments are summarized in [30]. A number of authors have applied these concepts to the examination of problems associated with granular media and references to recent works are given by Vardoulakis and Sulem [31]. The investigations by Mühlhaus [32], Tejchman and Wu [33], Bauer [34], Tejchman and Bauer [35], Tejchman and Gudehus [36] and others also deal with the application of higher-order formulations in elastoplasticity, in the context of the theory of hypoplasticity, which is described below, and by Mohan *et al.* [37, 38] who use more traditional ideas from plasticity. In each case, this improvement is achieved by modelling the granular material as a Cosserat (or micropolar) continuum. Mohan *et al.* [37, 38] apply an extended-associated flow rule, with the yield condition depending on the bulk density, and apply the equations to model flow through vertical channels and cylindrical Couette flow. These studies are successful in that they predict the main qualitative features of the shear layers; however, the yield condition and flow rule were chosen purely for illustrating the effectiveness of this approach.

In many civil and geotechnical engineering applications the constrained response of a granular material, such as a soil or sand, under loading is most important [29]. Examples of such situations occur with the analysis of foundations, excavations and underground structures, or simply in elemental tests. Here, the deformation of the material is contained by a surrounding material, which prevents the development of a state of plastic flow or collapse. Traditionally, a variety of elastoplastic models have been applied to problems of this nature. The history of development of theories of geomaterial behaviour that account for contained deformations of granular materials is quite extensive, and no attempt will be made here to provide an all-encompassing review. More recently, however, the constitutive theory of hypoplasticity has been developed, and has proven to be an attractive alternative to the elastoplastic models. Hypoplasticity is a natural extension of the theories of hypoelasticity developed by Truesdell [40] and the connection between the theories of hypoelasticity and theories of plasticity and of elastic-plastic flow has been discussed and investigated by Green [41, 42], Truesdell and Noll [43] and Jaunzemis [44]. Hypoplasticity in a formal sense was extensively investigated by Kolymbas [45] and many co-workers (see [46–48]). The characterizing feature of all hypoplastic theories is that the constitutive law can be written in a single nonlinear tensorial equation for the stress-rate as a function of the stress and the rate-of-deformation tensor, without reference to a yield condition or a flow rule. With hypoplasticity there is no need to decompose deformations into elastic and plastic regimes *a priori*, or to distinguish between loading and unloading; all these notions are automatically built into the theory, and arise as a consequence. Excellent reviews of hypoplasticity and its development are contained in Kolymbas [49] and Wu and Kolymbas [50].

The popularity of hypoplasticity among researchers and practitioners can be attributed to its elegance and the fact that the theory is deeply rooted in experimental observations. It is, nonetheless, a sophisticated constitutive theory, which involves complicated nonlinear constitutive relationships. When combined with the governing equations of continuum mechanics, there are little prospects for the analytical solution of real-life boundary-value problems, and progress is usually made via numerical schemes. As a result, it is often difficult to grasp the underlying mathematical structure of the equations (see [51–54]).

As mentioned previously, for each particular hypoplastic law there is a yield surface and a flow rule, but rather than being assigned in advance, they are consequences of the original constitutive relationships. Thus hypoplasticity as a theory can, in principle, be used to model fully developed granular flow. The explicit equations describing the yield condition and the flow rule can be derived from the given hypoplastic law, as illustrated by Wu and Niemunis [55] and von Wolffersdorff [56]. Von Wolffersdorff [56] has derived particular hypoplastic models that give the yield surfaces of Drucker and Prager [3] and Matsuoka and Nakai [57] as limiting cases. It is not immediately clear whether a similar derivation can be made to link hypoplasticity with other plasticity theories such as the double-shearing theory [8–10] described above. This possibility is of considerable interest, especially in light of the recent work of Spencer [58], who shows that in a strict sense, the double-shearing theory can be regarded as a special form of hypoplasticity. There is an absence of understanding of the strict connection between hypoplasticity and theories of plasticity that describe granular flow.

Shear layers often occur in the vicinity of solid boundaries, but this is not generally the case. An important property of granular materials is that shear-banding or shear layers can also occur within the bulk of the material. Shear bands are usually accompanied by localised strains, spanning several grain diameters in thickness, and as discussed above, classical continuum approaches fail to account for the dimensions of the shear bands due to the absence of an intrinsic length-scale. Furthermore, although the onset of shear-banding can be predicted [59], the ill-posedness of the governing equations prevents a complete analysis. As discussed previously, the subject of layers with intense shearing or shear-banding has received much attention by investigators who have developed approaches that incorporate Cosserat-type effects, and this is most prominent in hypoplasticity (see *e.g.* [34–36, 60]). Various hypoplastic theories have been developed and validated using finite-element techniques. The topic of mechanics and mathematics of granular materials has a rich history of involvement of researchers in the engineering sciences as well as those in the mechanics and applied-mathematics communities. These contributions are too numerous to cite as a comprehensive and complete review; readers are referred to the following Edited volumes of Symposia and Conference Proceedings for more in-depth reviews of the historical developments and the current state of advanced mathematical and mechanics approaches to the study of granular materials [61–78].

This Special Issue on the Mathematics and Mechanics of Granular Materials presents a mix of mathematical and engineering contributions to the discipline. Some of the papers, but not all, originate from four Mini-Symposia held at the 2003 ICIAM (International Congress of Industrial and Applied Mathematics) in Sydney, Australia, June 7–11, 2003. This meeting was jointly organised by the Guest Editors together with Drs. Claudio Tamagnini and Antoinette Tordesillas. The papers presented in this Special Issue cover the full range of current research activity in the area, and include general, analytical, hypoplastic, numerical and engineering contributions, but appear as follows according to the alphabetical listing of the first-named author:

1. F. Alonso-Marroquin and H.J. Herrmann, Investigation of the incremental response of soils using a discrete element model.
2. E. Bauer, Initial response of a micro-polar hypoplastic material under plane shearing.
3. R. Chambon, Some general results about second order work, uniqueness, existence and controllability.
4. G.M. Cox, S.W. McCue, N. Thamwattana and J. M. Hill, Perturbation solutions for flow through symmetrical hoppers with inserts and asymmetrical wedge hoppers.
5. B.S. Gardiner and A. Tordesillas, Micromechanical constitutive modelling of granular media: evolution and loss of contact in particle clusters.
6. D. Harris and E.F. Grekova, A hyperbolic well-posed model for the flow of granular materials.
7. S.C. Hendy, Towards a theory of granular plasticity.
8. M. Hjiaj, W. Huang, K. Krabbenhoft and S.W. Sloan, Formulation of non-standard dissipative behaviour of geomaterials.
9. W. Huang, M. Hjiaj and S.W. Sloan, Bifurcation analysis for shear localization in non-polar and micro-polar hypoplastic continua.
10. V.A. Osinov, Large-strain dynamic cavity expansion in a granular material.
11. E. Pasternak and H.-B. Muhlhaus, Generalised homogenisation procedures for granular materials.
12. J.F. Peters, Some fundamental aspects of the continuumization problem in granular media.
13. A.J.M. Spencer, Compression and shear of a layer of granular material.
14. C. Tamagnini, F. Calvetti and G. Viggiani, An assessment of plasticity theories for modelling the incrementally non–linear behavior of granular soils.
15. G.J. Weir, Incompressible granular flow from wedge-shaped hoppers.
16. H.P. Zhu and A.B. Yu, Micromechanics modeling and analysis of unsteady state granular flow in a cylindrical hopper.

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