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MAXIMUM-ENTROPY ESTIMATES AND VIRTUAL THERMOMECHANICS FOR GRANULAR ASSEMBLIES

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Summary This is an extension of previous work by others, dating back some thirty years on more (1), on maximum-entropy estimates of the statistical distribution of quasi-static contact forces in granular assemblies.

The precise form of the probability density is shown to depend on the statistical weight assigned to elements in the state space of contact forces or displacements. A brief review is given of comparisons with experiment and computer simulations. The formal methods of statistical thermodynamics are employed to establish a virtual thermomechanics. without reference to a granular temperature. This leads to an elastoplastic work function, of the type appearing in various phenomenological models of complex solids and fluids. The possibility of non-convexity, leading to continuum- and meso-scale material instability, is discussed.

EXTENDED SUMMARY

A major challenge in granular mechanics is to establish reliable connections between continuum-level phenomenological models and micromechanical models, which is essentially a problem in statistical mechanics. This accounts in part for the long-standing efforts to apply the maximum-entropy principle, not only to granular dynamics with large kinetic energy, but also to granular statics (11; 1). In systems devoid of a classical thermodynamic structure, the entropy can be taken as information-theoretic Shannon entropy, and the maximum-entropy principle provides one type of maximum-liklihood estimate for the statistics of systems with prescribed macroscopic averages as global constraints . The purpose of the present article is to establish certain qualifications and ramifications anticipated in previous articles by this author (4; 2).

Bagi's (1) maximum-entropy estimates for the interparticle contact-force distribution exhibit the exponential behavior at large force observed in numerous experiments and numerical simulations (10; 9). Hence, the exponential distribution may be a robust statistical feature of static granular packings, independently of the precise details of force transmission, in which case it cannot be taken as an unequivocal confirmation of various load-diffusion models proposed in the soil-mechanics and physics literature. This conclusion is further supported by the maximum-entropy estimates of (7) on contact forces in granular assemblies subject to the Coulomb condition ($\mu f_n \geq |f_t|$) at particle contacts. It can be shown that local mechanical constraints of this type can be treated as a restriction on state-space weight, without jeopardy to the exponential distribution of large forces (2)

Maximum Entropy with Constant Stress

With the standard expression for (Cauchy) stress (1; 7; 4)

$$\mathbf{T} = n_c \langle \mathbf{M}(\mathbf{f}, \mathbf{l}) \rangle, \text{ with } \mathbf{M}(\mathbf{f}, \mathbf{l}) := -\mathbf{f} \otimes \mathbf{l}, \tag{1}$$

where n_c denotes contact number density, $\mathbf{f}$ the vectorial contact force, $\mathbf{l}$ the branch vector connecting centroids of adjacent grains, and $\mathbf{M}$ the associated force dipole.

The maximization of entropy:

$$S[P] = -\langle \log P \rangle = -\int_\Omega P \log P d\Omega \tag{2}$$

based on a state-space measure $d\Omega$ and subject to stationarity of Eq. (1) yields the canonical distribution

$$P(\mathbf{f}, \mathbf{l}) = Z^{-1} \exp\{\mathbf{\Lambda} : \mathbf{M}\} = Z^{-1} \exp\{-\mathbf{f} \cdot \mathbf{\Lambda} \cdot \mathbf{l}\}, \tag{3}$$

where the colon denotes contracton of a tensor product and Z the *partition function*

$$Z(\mathbf{\Lambda}) = \int_\Omega \exp\{-\mathbf{f} \cdot \mathbf{\Lambda} \cdot \mathbf{l}\} d\Omega(\mathbf{f}, \mathbf{l}), \tag{4}$$

a function of the Lagrange multiplier (tensor) $\mathbf{\Lambda} = (\lambda_{ij})$.

As discussed by the present author (4; 2), the actual probability distribution in $\mathbf{f}, \mathbf{l}$ depends on the statistical weight factor J connecting $d\Omega$ and the cartesian volume element $d\mathbf{f}d\mathbf{l}$. Employing an argument based on conservation of power-law elastic contact energy $d\Omega \propto f^{\nu-1} df$, one finds a Poisson distribution of force magnitude f for frictionless spheres (4; 2):

$$\rho(F) = \nu \frac{(\nu F)^{\nu-1}}{\Gamma(\nu)} e^{-\nu F}, \text{ where } F = \frac{f}{\langle f \rangle}, \tag{5}$$

previously obtained by Bagi (1). Figure 1 of (4) shows a favorable comparison of Eq. (5) to experiment and numerical simulation, except for a troubling discrepancy arising from "dead" contacts with zero force in experiment and simulation.

Virtual Thermodynamics

The standard thermodynamic approach (6), according to which all macroscopic properties are derivable from Z, gives

$$\mathbf{T} = \partial_{\mathbf{\Lambda}}\psi, \quad \text{with} \quad \psi(\mathbf{\Lambda}) = -n_c \log Z, \tag{6}$$

with ψ and $\mathbf{\Lambda}$ assuming the respective roles of free energy and (infinitesimal) displacement or velocity gradient.
Eq. (6) represents a "virtual" thermodynamics involving no explicit reference to temperature. In the limit of perfectly rigid particles the energy ψ must be regarded as purely extrinsic, arising from external work done by particle rearrangement.
For frictional sphere assemblies, the real (as opposed virtual) thermodynamic validity of Eq. (6) appears to hinge on some type of elastic-plastic decomposition analogous to that employed in well-known incremental plasticity theories. For example, if we assume that the contact force can be written as a linear combination $\mathbf{f} = \mathbf{f}^E + \mathbf{f}^D$ of elastic and dissipative forces and that the state space measure factors as

$$d\Omega(\mathbf{f}^E, \mathbf{f}^D, \ldots) = d\Omega(\mathbf{f}^E, \ldots) d\Omega(\mathbf{f}^D, \ldots) \tag{7}$$

then Eq. (6) decomposes linearly into an elastic strain energy and a dissipation function, of the form assumed in certain phenomenological treatments of inelasticity (3; 5). However, the standard elastic-plastic version requires a treatment of kinematics like that given in (1), which results in a complimentary energy function (2) resembling that employed for plastic flow rules. Given the highly nonlinear nature of frictional-elastic contacts, it is not clear that the necessary statistical decoupling of force or displacement is realized in the typical granular medium.
There is a further interesting interesting question as to the possible non-convexity of relations such as Eq. (6). In particular, he associated bifurcations might serve to describe strain localization, in the form of shear bands, or stress localization in the form of force chains (4; 2), as a kind of virtual-thermodynamic phase transition.
Given the success of the maximum-entropy method in describing certain aspects of the force distribution in granular assemblies, further investigation of the validity of the above thermodynamic formalism would seem to warranted.

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