TOY MODEL OF A BOLTZMANN-TYPE EQUATION FOR THE CONTACT FORCE DISTRIBUTION IN DISORDERED PACKINGS OF PARTICLES

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The packing of hard-core particles in contact with their neighbors is considered as the simplest model of disordered particulate media. We formulate the statically determinate problem that allows analytic investigation of the statistical distribution of the contact force magnitude. A toy model of the Boltzmann-type equation for the contact force distribution probability is formulated and studied. An experimentally observed exponential distribution is derived.

Keywords: contact force distribution, Boltzmann equation, packings of particles

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1. Introduction

Understanding rheological properties of packed particles at various spatial scales [1] requires the use of the apparatus of statistical mechanics. However, conventional statistical physics is inadequate in describing mechanical behavior of disordered packings of hard-core particles that can be static or driven by external forces [2]. There have been various attempts to develop the statistical-mechanics approach to such systems (see, e.g., recent review article [3]). Despite these advances, there still exists a certain degree of skepticism regarding the possibility of discovering new physical laws that govern mechanical behavior of particulate media. This can be linked to the structural complexity of such materials at different scales. However, experimental studies [4] and computer simulations [5] indicate the existence of phenomena that can and should be treated as physics problems. In order to discover physics laws, one should consider well-posed problems, whose solutions can be indicative of the laws. In this paper, we do not attempt to study the percolation geometry and mechanics of contact forces network [6]; we offer a very simple analytic model that produces a Boltzmann-type equation for the contact force distribution. This equation can be solved by using Fourier transformation, and the obtained solution agrees with an experimentally observed exponential distribution. We briefly discuss possible approaches to improve this simple model, which might allow explaining other phenomena observable in particulate media [4].

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2. The statically determinate problem

We consider a static array of hard-core particles in contact with their neighbors. The packing is assumed to be an assembly of discrete rigid particles whose interactions with their neighbors are localized at point-like contacts. Therefore, the description of the network of interparticle contacts is essential for understanding the force transmission. We assume that the set of contact points $C_{\alpha\beta}^i$ provides the complete geometrical specification for such static packing. We define the centroid of contacts of particle $\alpha$ as

$$ R_\alpha^i = \frac{1}{z_\alpha} \sum_\beta C_\alpha^\beta_i, $$

where $i = 1, \ldots, d$ is a Cartesian index and $z_\alpha$ is the coordination number of particle $\alpha$. The distance between particles $\alpha$ and $\beta$ is defined as the distance between their centroids of contacts

$$ R_{\alpha\beta}^i = R_\alpha^i - R_\beta^i = r_{\alpha\beta}^i - r_{\beta\alpha}^i, $$

where $r_{\alpha\beta}^i$ is the $i$th component of the vector joining the centroid of contact with the contact point:

$$ \sum_\beta r_{\alpha\beta}^i = 0. $$

In $d$ dimensions, Newton’s second law yields $N d(d + 1)/2$ equations for the interparticle forces $f_{\alpha\beta}^i$,

$$ \sum_\beta f_{\alpha\beta}^i + g_{\alpha}^i = 0, $$

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$$ \sum_\beta \epsilon_{ikl} f_{\alpha\beta}^{ikl} r_{\alpha\beta}^l + c_{\alpha}^i = 0, $$

where $g_{\alpha}^i$ is the external body force acting on grain $\alpha$ and $c_{\alpha}^i$ is the external body couple, which we set equal to zero without losing the generality. The counting of the number of equations and the number of unknowns allows formulating the simplest statically determinate problem of force transmission in a static packing. Particles are considered to be perfectly hard, perfectly rough, and each particle $\alpha$ is assigned a coordination number $z_\alpha = d + 1$ [7].

A theory that confirms these considerations has been proposed for periodic arrays of particles with perfect and zero friction [8]. What is the statistical distribution of contact forces in a packing of particles? Experimental [4] and computer simulation [5] studies have demonstrated that the probability of the normal contact force acting on a particle contact is

$$ P(f) \propto \begin{cases} 
\left( \frac{f}{\langle f \rangle} \right)^\gamma, & f < \langle f \rangle, \\
\exp(\delta(1 - f/\langle f \rangle)), & f > \langle f \rangle,
\end{cases} $$

where $\langle f \rangle$ is the average contact force, and $\gamma$ and $\delta$ are constants. The aim of this paper is to derive the statistical distribution of contact forces from “first principles.” We attempt such a derivation by constructing a Boltzmann-type equation, which can be solved if the packing of particles is assumed to be a statically determined, i.e., each particle $\alpha$ has a coordination number $z_\alpha = d + 1$. Some authors describe such system state as marginal [9].
3. An integral equation

When a static packing of incompressible particles in contact with each other is subjected to external forces at its boundaries, these forces are transmitted through the contact network. This network is determined by the set of contact points in our model. To develop a tractable theory, we assume our particles to be monodisperse spheres in multiple contact greater than or equal to three in two dimensions or four in three dimensions. Despite this simplification, the proposed theory is of interest because it admits an analytic solution.

3.1. The 2D model. We consider a packing in two dimensions, where forces $f_1$ and $f_2$ act on a particle, which then exerts a force $f$ on its neighbor. The average position of the forces is symmetric. We let $f$ be in the $x$ direction and use the symbols $f_1$ and $f_2$ for the $x$ components of the vector forces. The forces can only push but not pull, and the simplest representation of the problem is as follows:

$$P(f) = \int_0^\infty df_1 \int_0^\infty df_2 \delta(f - f_1 - f_2) P(f_1) P(f_2).$$  \hspace{1cm} (6)

After projecting the contact force vectors, we have

$$P(f) = \int_0^\infty df_1 \int_0^\infty df_2 \int_0^1 d\mu \int_0^1 d\lambda \delta(f - \lambda f_1 - \mu f_2) P(f_1) P(f_2).$$  \hspace{1cm} (7)

which can be transformed into

$$P(f) = \int_0^\infty df_1 \int_0^\infty df_2 \int_0^1 d\mu \int_0^1 d\lambda P(\lambda f_1) P(\mu f_2).$$  \hspace{1cm} (8)

This equation has a solution in the form

$$P(f) = \frac{f}{p^2} e^{-f/p},$$  \hspace{1cm} (9)

which has been normalized and where $p = \bar{f}/2$, $\bar{f}$ corresponds to the mean force. The distribution $P(f)$ is exponential for large values of $f$ and tends to zero at small $f$.

3.2. The 3D model. In three dimensions, the coordination number of particles is greater than or equal to four. Using the same framework of simplifications, the three-dimensional model can be written as

$$f = \frac{1}{3} f_1 + \frac{1}{3} f_2 + \frac{1}{3} f_3.$$  \hspace{1cm} (10)

After applying the Fourier transformation

$$P(f) = \frac{1}{(2\pi)^3} \int d^3 k \mathcal{P}(k) e^{ikf},$$  \hspace{1cm} (11)

we obtain

$$\mathcal{P}(k) = \mathcal{P}^3 \left( \frac{k}{3} \right),$$  \hspace{1cm} (12)

and then

$$\mathcal{P}(k) = e^{ik/p}.$$  \hspace{1cm} (13)
After applying the inverse Fourier transformation

\[ P(k) = \int d^3f \, P(f) e^{-ikf}, \quad (14) \]

we obtain

\[ P(f) = \delta(f - p). \quad (15) \]

A blurring process is always used in the form of a “toy model.” In this case, the angular effects can be represented by three “direction cosines” \( \lambda_i \), such that the force balance equation in the form

\[ f = \lambda_1^2 f_1 + \lambda_2^2 f_2 + \lambda_3^2 f_3 \quad (16) \]

has the analytic solution

\[ P(f) = \left( \int_{-\infty}^{\infty} \int_{0}^{1} P(\lambda^2 k) \, dk \, d\lambda \right)^3. \quad (17) \]

Using \( \lambda^2 k = \mu \), we obtain

\[ P(f) = \left( \int_{0}^{K} P(\mu) \frac{d\mu}{2\mu^{1/2} k^{3/2}} \right)^3. \quad (18) \]

Applying the Fourier transformation to this expression, we obtain

\[ P(k) = \frac{4p^{3/2}}{(k - ip)^{3/2}}. \quad (19) \]

whence

\[ P(f) = \int \frac{4p^{3/2} e^{ikf}}{(k - ip)^{3/2}} \, dk = \frac{4p^{3/2}}{k^{3/2}} \int \frac{e^{ikf}}{f^{3/2}} \, dJ. \quad (20) \]

Integrating this expression gives the normalized distribution

\[ P(f) = \frac{\sqrt{\pi}}{2} f^{1/2} p^{3/2} e^{-f/p}, \quad (21) \]

where \( p \propto \bar{f} \) and the proportionality constant depends on the behavior of the power-law exponents for small forces. Certainly, a number of improvements must to be made in order to derive this expression with experimentally observed coefficients. However, as a starting point, the use of this simple model appears to be justified.

4. Discussion

We proposed the simplest Boltzmann-type equation for the probability distribution of contact forces in two and three dimensions. This equation can be solved under some approximations and an experimentally observed exponential distribution of contact forces can be obtained. Other proposed approaches [10]–[12] employ entropy maximization or functional minimization concepts. These models produce elements of the empirically observed probability distribution function. However, but they are not derived from first principles but are developed by analogy with other entropic systems. We hope that our approach to studying the Boltzmann-type equation for the probability distribution of contact forces can serve as the foundation for future research. In particular, one can develop it further to account for the presence of structural disorder at various spatial scales and obtain the statistics of the so-called “force chains” observed in experiment [4].

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