Dilatancy Transition in a Granular Model

by

David Aristoff and Charles Radin *

Mathematics Department, University of Texas, Austin, TX 78712

Abstract

We introduce a model of granular matter and use a stress ensemble to analyze shearing. Monte Carlo simulation shows the model to exhibit a second order phase transition, associated with the onset of dilatancy.

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1. Introduction.

Static granular matter, such as a sand pile, can exist in a range of densities. In its densely packed state, the more common form, it expands under shear, while when its grains are loosely packed it contracts under shear [RN]. We introduce a model within which the transition between these qualitative behaviors is singular in the precise traditional sense of a second order phase transition. (For two dimensional treatments see [AS, PLR], and for an interpretation as a glass transition see [CH].)

Our "granular hard cubes" model is a granular variant of the classical hard cubes model of equilibrium statistical mechanics [HHB], the latter being a simplification of the classical hard sphere model in which the spheres are replaced by nonoverlapping, parallel unit cubes. In our granular version, following Edwards [EO], we only allow configurations in which the parallel cubes are mechanically stable under gravity, where gravity is acting parallel to edges of the cubes. We require that the centers of our cubes be approximately at the vertices of an fcc lattice, which we orient so that gravity acts along the 001 axis, so the fcc lattice is thought of as parallel 2-dimensional square lattice layers. We enforce this approximate structure by requiring that each cube sit on exactly four cubes in the layer below it; see Fig. 1.

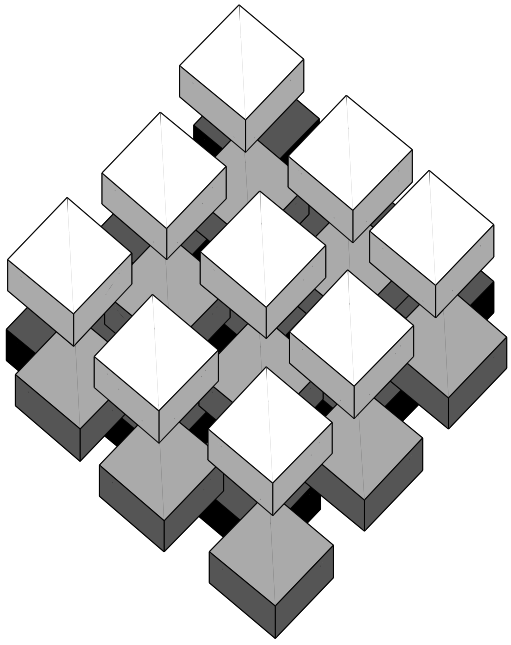

Figure 1. Layers of parallel cubes.

We want to model the reaction of a sandpile to shear and in particular we need a model which exhibits a critical state density, a density separating a high density regime of states, in which the material expands under shear, from a low density regime in which it contracts under shear [RN]. As we show, this is easy to arrange. The more interesting question is whether the model predicts that the transition through that critical state density is smooth, or is singular.

To understand why it is natural for a granular model to have a critical state density it is useful to use the following "stress" ensemble. Instead of constant density we introduce a pressure parameter, and in place of constant strain we introduce a shear stress parameter. In other words the states of the model, which, in the general approach of Edwards [EO] are probability densities of configurations of grains, optimize the free energy

$$F(p, f) := S - pV + f\alpha V, \tag{1}$$

where $S = \ln(Z_{p,f})$ is the entropy, V is the volume in physical space, and α is the shear strain. The parameter p is pressure, f is shear stress, and

$$Z_{p,f} = \int \int \exp(-pV + f\alpha V)\, dV d\alpha. \tag{2}$$

This is equivalent to saying that a configuration C has an unnormalized probability density:

$$Pr(C) = \exp(-pV + f\alpha V). \tag{3}$$

It follows from this probability density that, in the absence of shear, the state of lowest possible particle density, called random loose packing, occurs at zero pressure [AR1] and some shear strain $\alpha = \alpha_0$. Therefore at sufficiently low pressure if one shears the system from α_0, the density has no way to change except to increase. So at sufficiently low density there is a regime in which the system contracts.

On the other hand, at least since Reynolds [Re] one understands the expansion of (dense) granular matter under shear, which he termed dilatancy, in geometric terms, as the need for parallel layers of spheres to get out of each others' way under a strain deforming the layers, either by separating and/or by thinning within the layers. So we adjust the model to arrange for this (thinning) phenomenon, as follows.

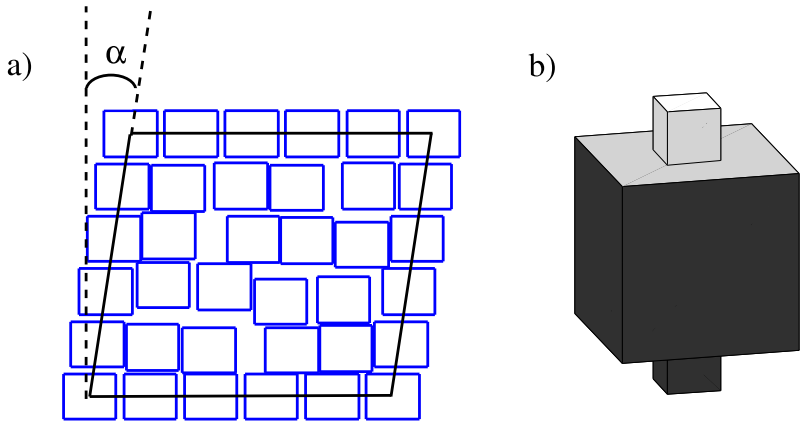

Figure 2. a) A view from above of a layer in a configuration, with a definition of the angle α; b) A cubic grain, with bumps on top and bottom faces.

To react to the strain (see Fig. 2a) we mimic the spherical caps that grains in one layer present to grains in neighboring layers by adding "bumps" to the top and

bottom of our cubes; see Fig. 2b. Such cubes will, when we strain a sufficiently dense configuration in response to the shear, feel the bumps in the layers above and below it, and this will produce a dilatancy effect by thinning the layers. By considering optimally symmetric configurations one quickly finds $\phi_d := (1+w)^{-1}$, where w is the width of a bump, as an estimate of the density required for dilatancy; see Fig. 3. In our simulations we use $w = 0.15$, and so $\phi_d \approx 0.59$. The qualitative dilatancy effect is not sensitive to the precise value of w, though the value ϕ_d is.

So the bumps, together with the universal behavior at low pressure or density, explain the existence of a critical state density. The main question then is: as density is varied, does the transition through the critical state density proceed in a smooth or in a singular manner? We will show there is an unambiguous second order phase transition at dilatancy onset, at density near ϕ_d. This suggests, by analogy with matter in thermal equilibrium, that the material in the two regimes differs in other characteristics as well, for instance it would be expected that the yield force behave differently in the two regimes. In [SNRS] the yield force is measured as a function of density, and a second order phase transition is found at a density roughly 0.598. The critical state density was not carefully measured because of the experimental setup, but approximately coincided. Our result suggests the two phenomena are simply different manifestations of the same transition.

We also note that the behavior of granular matter at the random close packing density, about 0.64, has been interpreted in [Ra, AR2] as a first order phase transition in which the high density regime is an ordered phase. Together with our results here, this means that the usual freezing transition of equilibrium fluids, at which the material acquires the solid features of an ordered (typically crystalline) internal structure as well as a strong resistance to shear, seems to be split into two stages in granular materials, with the resistance to shear occuring at dilatancy onset at density about 0.6 and the ordered internal structure occuring at the random close packing density of about 0.64.

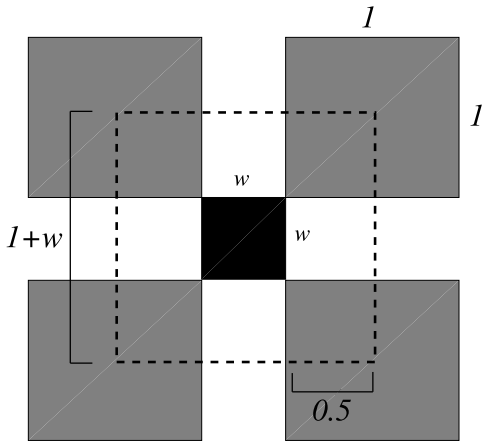

Figure 3. A regular arrangement of grains at maximum density, from above. The configuration can be partitioned into unit cells defined by the dotted lines.

2. Simulating the Model.

As noted above, our model consists of hard, parallel, oriented unit cubic grains, with two small cubic bumps of width $w \ll 1$ attached to the middle of their upper and lower faces. We use $w = 0.15$. Each grain must sit on exactly four other grains (except grains on the outside of the configuration), but not on the bumps, and grains cannot overlap. Thus, the grains appear on discrete vertical levels, so the distance in the vertical or z-direction between the centers of grains on adjacent levels is equal to 1; see Fig. 4.

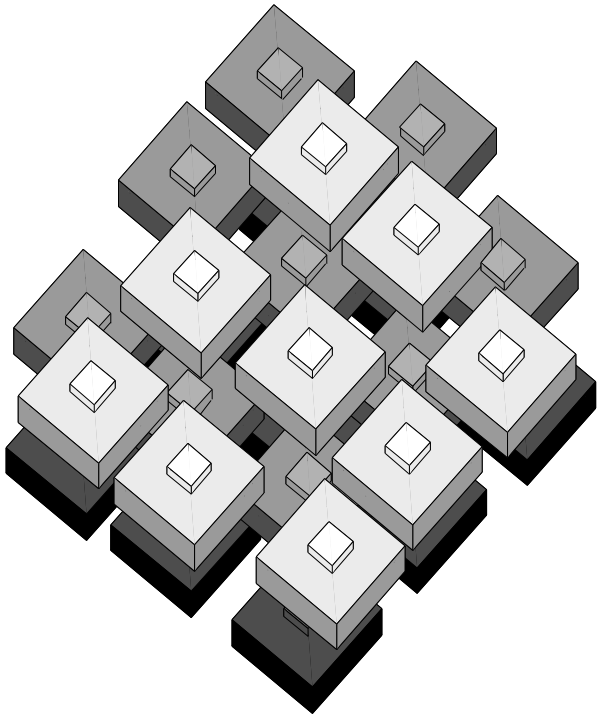

Figure 4. An arrangement of grains, viewed from above.

Each simulation begins with a perfectly regular arrangement of $N = n^3$ grains in a large cubic structure, so that there are n^2 grains in each level, with n in each row and each column of a level, and n total levels. (For ease in notation we associate a row with the x-direction and a column with the y-direction; note that the model has a well-defined row and column structure.) The grains on the side boundaries of the cubic structure are allowed to make coordinated moves corresponding to changes in configuration volume and shape, but they are not allowed to move singly.

We allow three types of Monte Carlo steps. With probability $1 - 1/N$ we choose a random grain inside the boundary to move in either the x- or y-direction; and with probability $1/N$ we allow a configuration to change shape or volume. When a configuration changes volume, the x- and y-coordinates of each grain, on each level, are scaled by the same factor λ. When it changes shape, the x-coordinate of each grain

in the kth column of each level is scaled, for some α, by the factor αk.

To prevent grains from getting stuck between the boundary grains, we impose top-bottom periodic boundary conditions, and we remove the bumps from the grains nearest to the boundary and on the boundary.

As is standard in Monte Carlo, to simulate the distribution (3) we choose steps with relative acceptance probabilities given by $V^N \exp(-pV + f\alpha V)$. (The factor V^N arises from the necessity of rescaling position coordinates to live in a fixed-size box [Mc]). Here α is the angle of deformation of a configuration (see Fig. 2b), where from symmetry we can assume $\alpha \geq 0$ without loss of generality. The volume V of a configuration is the volume of the convex hull of the set of centers of all the grains. The volume can be computed directly from the scale factor λ described above.

3. Results of the Simulations.

We ran Markov chain Monte Carlo simulations on the model, with the Monte Carlo steps designed so that the stationary distribution of the Markov chain has the probability density

$$m_{p,f}(C) = \frac{\exp(-pV + f\alpha V)}{Z_{p,f}} \tag{4}$$

described above. We want to measure how the (average) density $\phi = N/V$ changes as shear stress f varies near $f = 0$. (For convenience we do not include the bumps in the calculation of ϕ, but since particle number N is fixed in our simulation, the "true" volume fraction is just a constant multiple of ϕ.) That is, we want to estimate the derivative

$$D := \left.\frac{\partial \langle\phi\rangle}{\partial f}\right|_{f=0} \tag{5}$$

of the average of ϕ as a function of p. From the definition of $m_{p,f}$ it is easy to see that

$$D = D(p) = N\langle\alpha\rangle_{p,0} - \Big[\langle\phi\rangle_{p,0}\Big]\Big[\langle V\alpha\rangle_{p,0}\Big], \tag{6}$$

where $\langle\cdot\rangle_{p,f}$ denotes average with respect to $m_{p,f}$. Thus, to estimate $D(p)$ from our simulations we set $f = 0$ and calculate the sample averages of $N\alpha$, ϕ, and $V\alpha$. With the free energy $F(p, f) = S - pV + f\alpha V$, which is the quantity minimized by the state $m_{p,f}$, one can see from a direct calculation that

$$D(p) = -\langle\phi\rangle_{p,0}^2 \frac{\partial}{\partial f}\left(\frac{\partial F}{\partial p}\right)\Bigg|_{f=0}, \tag{7}$$

which shows that the function $D(p)$ is a quantity for which a discontinuity might reasonably be described as a second order phase transition.

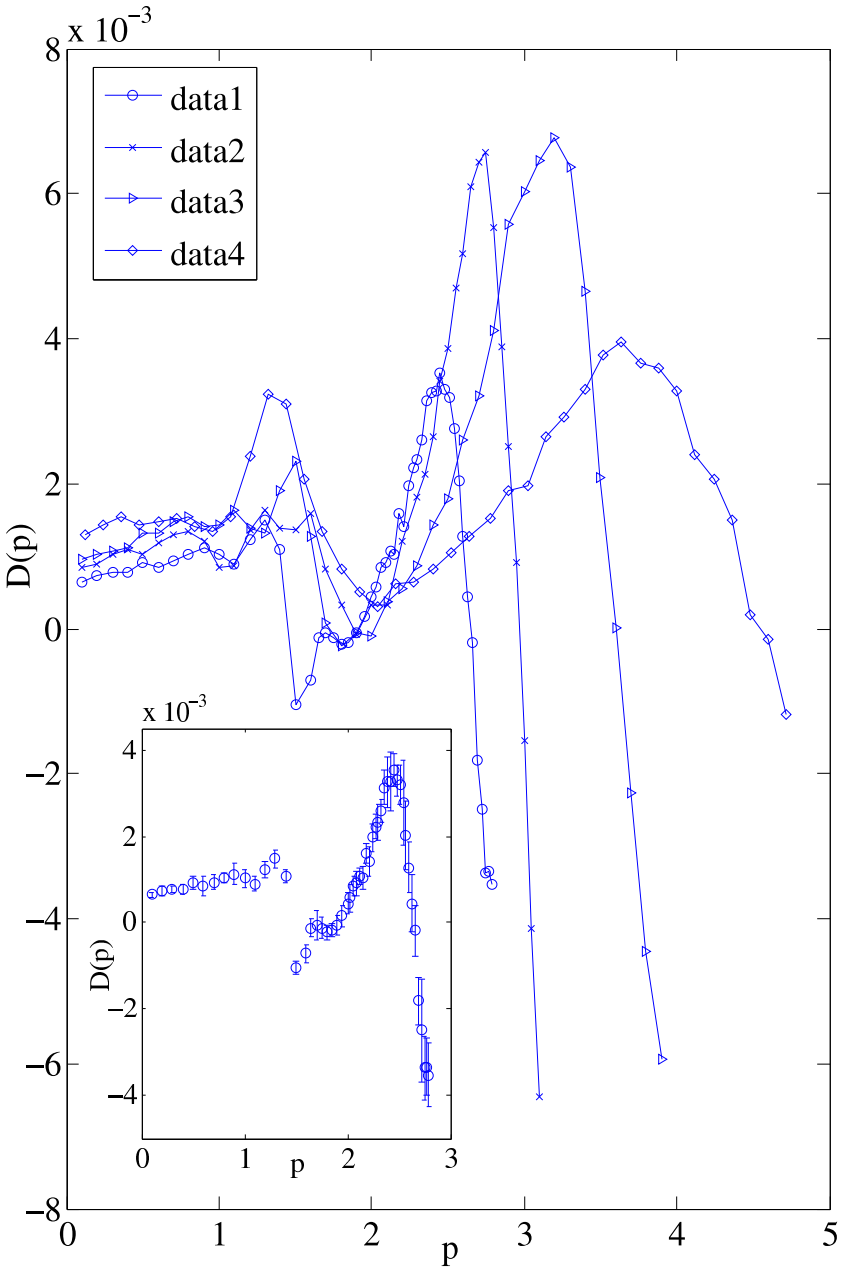

Figure 5. The graph of $D(p) = \left.\dfrac{\partial\langle\phi\rangle_{p,f}}{\partial f}\right|_{f=0}$, for systems of $14^3 = 2744$, $12^3 = 1728$, $10^3 = 100$, and $8^3 = 512$ grains (data1-data4, resp.). The insert gives error bars on the system with 14^3 grains.

We investigate systems of $8^3 = 512$, $10^3 = 100$, $12^3 = 1728$ and $14^3 = 2744$ grains at pressures $p_1 < ... < p_k$, where the pressures chosen are different for each size system. In the simulations we begin at low pressure p_1, and then slowly increase p until just after the derivative $D(p)$ falls sharply below zero, roughly corresponding to pressure p_k. The last configuration in the simulation of p_i is used as the starting configuration

of the simulation of p_{i+1}. We use the standard biased autocorrelation function to determine a "mixing time", measured as the number of Monte Carlo steps required before the autocorrelation first crosses zero. We run our simulations long enough so that the simulation of each p_i contains, on average, at least 20 mixing times, and we run 200 independent copies of each simulation to obtain the averages $\langle N\alpha\rangle_{p,0}$, $\langle\phi\rangle_{p,0}$, and $\langle V\alpha\rangle_{p,0}$. From these averages we compute $D(p)$ from (6). (We also ran some of our simulations much longer, with fewer copies and pressures, and noted agreement with the already-obtained data on $D(p)$.) Then, for error bars on $D(p)$, we repeat the entire experiment 8 times and use the Student's t-distribution.

Our simulations suggest that $D(p)$ develops a discontinuity as the system size increases (see Fig. 5). Changing variables we note that D, as a function of $\langle\phi\rangle_{p,0}$, develops a discontinuity near the (average) volume fraction $\phi_d \approx 0.59$ discussed in the introduction; we plot $\langle\phi\rangle_{p,0}$ against p in Fig. 6b and D against $\langle\phi\rangle_{p,0}$ in Fig. 6a.

Note that for $p \leq 1$, $D(p)$ exhibits regular behavior in which $D(p)$ is roughly constant, $D(p) = \eta \approx 0.001$. Then for $1 < p < 2$, $D(p)$ has some oscillation which is characteristic to the system size. Then for $p \geq 2$, $D(p)$ steadily increases to a peak, then sharply decreases through zero. We believe that $D(p)$ is discontinuous in the limit of infinite system size, but the rate of change of $D(p)$ is so large it is difficult to measure its variation with system size. Instead we consider two measures of the interval R in which the discontinuity is developing, and then note that R gets smaller and smaller as system size increases.

We expect that the oscillation observed in $D(p)$ in the interval $1 < p < 2$ is caused by finite-size effects, so that it disappears in the limit $N \to \infty$. Furthermore we expect the critical pressure p_c to fall at either the end or the beginning of the oscillation region. These two possibilities underlie, respectively, our measurements R_1 and R_2, defined below. Let η be the average value of $D(p)$ over $p \leq 1$. The left endpoint of R_1 is the smallest value of p where $p > 2$ and $D(p) \approx \eta$, and the right endpoint of R_1 is the value of p where $p > 2$ and $D(p) \approx 0$. The widths of R_1 are approximately 1.75 ± 0.05, 1.15 ± 0.05, 0.75 ± 0.05, and 0.50 ± 0.05 for systems of $N = 8^3$, 10^3, 12^3 and 14^3 grains, respectively. On the other hand, the left endpoint of R_2 is defined as the smallest value of p such that $D(p)$ differs significantly from η, while the right endpoint of R_2 is the same as the right endpoint of R_1. We estimate that the widths of R_2 are approximately 3.55 ± 0.05, 1.55 ± 0.05, 1.25 ± 0.15, and 1.15 ± 0.05 for systems of $N = 8^3$, 10^3, 12^3 and 14^3 grains, respectively.

In either case, based on the decreasing sizes of the intervals R_1 and R_2, we believe that the jump from $D(p) \approx \nu$ to $D(p) \ll 0$ occurs over an interval which is vanishing in the infinite volume limit, which, given the relation between $D(p)$ and the free energy $F(p, f)$ in (7), is reasonably termed a second order phase transition. And as noted in the introduction, there is experimental evidence for this interpretation in [SNRS].

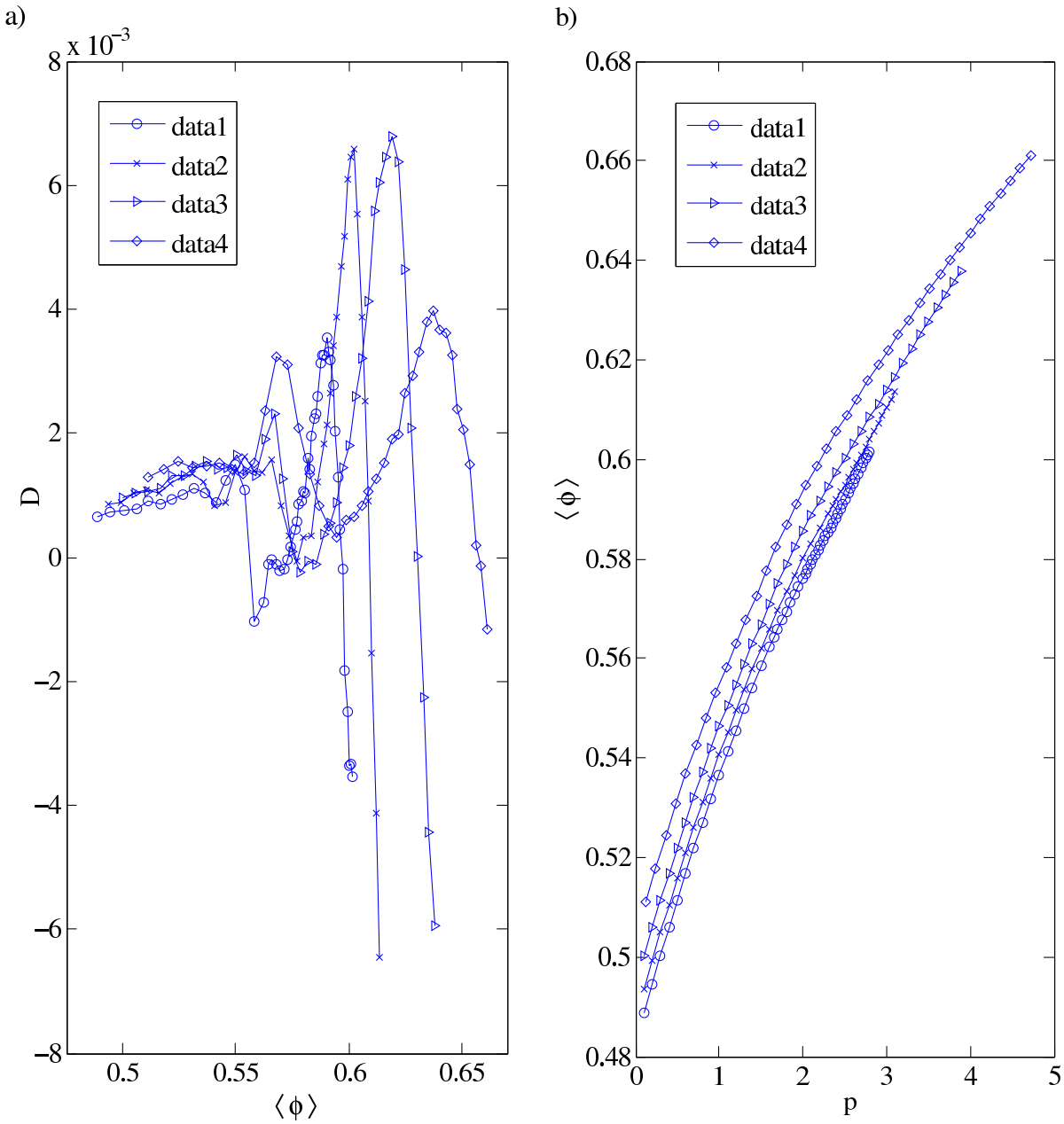

Figure 6. a) $D(p)$ as a function of $\langle\phi\rangle_{p,0}$; b) $\langle\phi\rangle_{p,0}$ as a function of p. In both plots, data1-data4 represent systems of $14^3 = 2744$, $12^3 = 1728$, $10^3 = 100$, and $8^3 = 512$ grains, respectively.

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