Random Loose Packing in Granular Matter

by

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Abstract

We introduce and simulate a two dimensional probabilistic model of granular matter at vanishing pressure. The model exhibits a perfectly sharp random loose packing density, a phenomenon that should be verifiable for real granular matter.

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1. Introduction

We introduce and analyze a crude model for the random loose packings of granular matter. These packings, as well as random close packings, were carefully prepared by Scott et al in the 1960’s [S,SK], mainly in samples of steel ball bearings. Gently pouring samples of 20,000 to 80,000 spheres into a container, the lowest possible volume fraction obtainable – the so-called random loose packing density – was determined to be $0.608 \pm 0.006$.

The above refers to monodisperse steel spheres immersed in air; similar experiments were performed with spheres of other materials immersed in other fluids; variations in the coefficient of friction and in the effective gravitational force lead to somewhat different values for the random loose packing density [SK].

Matter is generally described as “granular” if it is composed of a large number of noncohesive subunits each of which is sufficiently massive that its gravitational energy is much larger than its thermal energy. A common example is sand.

There are several classic phenomena characteristic of static granular matter, in particular dilatancy, random close packing, and random loose packing, none of which can yet be considered well-understood; see [dG] for a good review. A basic question about these phenomena is whether they are sharply defined or inherently vague. Dilatancy has recently been associated with a phase transition measured by the response of the material to shear [SN], which answers the question for this phenomenon. The case of random close packing is controversial and awaits further experiment; see [TT,R]. Our main goal here is to analyze this question with respect to random loose packing, to determine whether or not traditional theoretical approaches to granular matter predict a sharply defined random loose packing density. It is clear that any experimental determination of a random loose packing density will vary with physical conditions such as coefficient of friction. It is possible, however, that there is a precise geometrical quantity which underlies the phenomenon, and it is our goal to investigate this question.

We will eventually specialize to a certain two dimensional model, but we begin our discussion more ambitiously. Consider a model using a large collection of impenetrable, unit mass, unit diameter spheres in a large container, acted on by gravity and with infinite coefficient of friction between themselves and with the container. We will not try to understand a random loose packing density as an absolute minimum at which the spheres can form a bulk material. Rather, we will use a probabilistic framework in the spirit of Edwards’ theory of granular matter [EO]. More specifically, we expect, but cannot show, that the following is true, and use it as our motivation. Consider a probability density on the set of all mechanically stable packings of the spheres in their container, with the probability density of a packing $c$ proportional to $\exp[-E(c)]$, where $E(c)$ is the sum of the heights, from the floor of the container, of the centers of the spheres in the packing $c$. We expect that such an ensemble will exhibit a gradient in the volume fraction, with volume fraction decreasing with height, and that there is a well-defined random loose packing density as one approaches the top of the packing, where the (ana-
logue of hydrostatic pressure goes to zero. More specifically, we expect that as one takes an infinite volume limit, the probability distribution for the volume fraction of the top layer of the packing becomes concentrated at a single nonzero value. We emphasize that we are focusing on a bulk property near the top of the configuration, not a surface phenomenon.

To analyze random loose packing in such a probabilistic framework we make several simplifications of the above model, first to an ensemble of those packings which are limits, as the gravitational constant goes to zero, of mechanically stable packings; we effect this by setting \( E(c) = 0 \) in the relative density \( \exp[-E(c)] \). With this simplification configurations are now, in their entirety, representative of the top layer in the original model. Next we consider the two dimensional version of the above: congruent frictional unit disks in mechanically stable configurations under vanishingly small gravity. Note that each such disk must be in contact with either a pair of supporting disks below it or part of the container. (Here and elsewhere in this paper we neglect events of probability zero, such as one sphere perfectly balanced on another.) We simplify the model one last time by replacing the disks by congruent squares, with edges aligned with the sides of the (rectangular) container, each square in contact with either a pair of supporting squares below it or the floor of the container. This is now a granular version of the old model of “(equilibrium) hard squares” [H], which is a simplification of “hard disks” and “hard spheres” (see [AH] for a review), in which gravity is neglected but kinetic energy plays a significant role. We emphasize that in our granular model there is no longer any need to concentrate on the “top layer”; in fact we will eventually be concerned with an infinite volume limit which, as usual, focuses on the middle of the collection of squares and lets the boundaries grow to infinity.

It is this granular model which is the focus of this paper. We have run Markov chain Monte Carlo simulations on the model, with the following results. We initialize the squares in an allowed configuration of some well-defined volume fraction anywhere between 0.5 and 1. If the initial volume fraction \( \phi \) is not approximately 0.76, the packing expands or contracts, relatively quickly, into the range 0.76 ± 0.01; see Figs. 1 and 2.

The process is insensitive to the tightness of fit of the initial configuration in the containing box except for absolute extremes. If the side walls of the containing box abut a closely-packed initial configuration, the simulation cannot significantly change the volume fraction; alternatively if the width of the box is much larger than that of the initial configuration the simulation will drive the configuration to a monolayer on the floor; but both extremes are negligible and the equilibrium volume fraction is otherwise insensitive to the fit of the initial configuration in the box. More precisely, we found that the equilibrium volume fraction should be accurate if the floor length is between \( 2\sqrt{N} \) and \( 8\sqrt{N} \), where \( N \geq 100 \) is the number of squares. Since we will be conjecturing the behavior of the model in the infinite volume limit, the equilibrium configuration should be a single bulk pile, so the floor length should be on the order of \( \sqrt{N} \). To understand the lower bound, note that, at any volume fraction, a configuration occupies the least amount of floor space when the squares
are arranged in a single full triangle. The bottom level of such a triangle has just under $\sqrt{2N}$ squares. Assume the containing box fits tightly around the triangle. If the triangle has volume fraction greater than 0.754 then the configuration will not be able to decrease to this equilibrium volume fraction; we avoid this by ensuring that the floor length is at least $(0.754)^{-1}\sqrt{2N}$. To arrive at the upper bound we performed simulations on fixed particle number and let the floor length vary. We saw that the equilibrium volume fraction was reliable so long as the floor length was less than about $8\sqrt{N}$, at least for $N \geq 100$.

We conclude that, for floor lengths in the aforementioned acceptable range, the equilibrium volume fraction is found to depend only on the number of squares in the system. The main goal of our work is an analysis of the distribution of volume fraction – both the mean and standard deviation – as the number of particles increases. We conclude that the limiting standard deviation as particle number goes to infinity is zero, so the model exhibits a sharp value for the random loose packing density, which we estimate to be approximately 0.754.

The heart of our argument is the degree to which we can demonstrate that in this model there is a sharp value, approximately 0.754, for the equilibrium volume fraction of large systems, and we postpone analysis of error bars to later sections. But to understand the value 0.754, consider the following crude estimate of the volume in phase space of all allowable packings at fixed volume fraction $\phi$. First notice that the conditions of the model prevent the possibility of any “holes” in a configuration. Furthermore, if we consider any rectangle in the interior of a configuration, each horizontal row in the rectangle contains the same number of squares. (One consequence is that in the infinite volume limit each individual configuration must have a sharply defined volume fraction; of course this is quite distinct from the degree of spread of the volume fraction among all configurations.) Now consider a very symmetrical configuration of squares at any desired volume fraction $\phi$, with the squares in each horizontal row equally spaced, and gaps between squares each of size $(1-\phi)/\phi$ centered over squares in the next lower horizontal row; see Fig. 3. Consider these squares to represent average positions, fix all but one square in such a position, and consider the (horizontal) degree of motion allowed to the remaining square. There are two constraints on its movement: the gap size separating it from its two neighbors in its horizontal row, and the length to which its top edge and bottom edge intersects the squares in the horizontal rows above and below it. These two constraints are to opposite effect: increasing the gap size decreases the necessary support in the rows above and below. A simple calculation shows that the square has optimum allowed motion when the gap size is $1/3$, corresponding to a volume fraction of 0.75, roughly as found in the simulations. In other words, this crude estimate suggests that the volume in phase space (which we effectively estimate, for $N$ squares, to be $L^N$ where $L$ is the allowed degree of motion of one square considered above) is maximized among allowed packings of fixed volume fraction by the packings of volume fraction about 0.75.

To obtain accurate physical measurements a method of sedimentation has been developed to prepare samples of millions of grains in a controlled manner; see [JS]
and references therein for the current state of the experimental data. In these experiments monodisperse grains sediment in a fluid. The sediment is of uniform volume fraction, at or above 0.55 depending on various experimental parameters. To achieve the low value (0.55 ± 0.001 [JS]), the grains need to have a high friction coefficient and the fluid needs to have mass density only slightly lower than the grains, to minimize the destabilizing effect of gravity. (In the absence of gravity one could still produce a granular bed by pressure; we do not know of experiments reporting a random loose packing value for such an environment.)

Our results suggest that whatever the initial local volume fraction of the bed, on sedimentation (in low effective gravity) most samples would have a well-defined volume fraction, the random loose packing density of about 0.55, with no intrinsic lower bound on the sharpness of the value. This should be verifiable by a sequence of experiments of increasing dimensions.

There have been previous probabilistic interpretations of the random loose packing density, for instance [MP,PC]. A distinguishing feature of our results is our analysis of the degree of sharpness of the basic notion, which, as we shall see below, requires unusual care in the treatment of error analysis.

2. Results

We performed Markov chain Monte Carlo simulations on our granular model, which we now describe more precisely. We begin with a fixed number of unit edge squares contained in a large rectangular box $B$. A collection of squares is “allowed” if they do not overlap with positive area, their edges are parallel to those of the box $B$, and the lower edge of each square intersects either the floor of the box $B$ or the upper edge of each of two other squares; see Fig. 3. Note that although the squares have continuous translational degrees of freedom in the horizontal direction, this is not in evidence in the vertical direction because of the stability condition: the squares inevitably appear at discrete horizontal “levels”.

Markov chain simulations were performed as follows. In the rectangular container $B$ a fixed number of squares are introduced in a simple “crystalline” configuration: squares are arranged equally spaced in horizontal rows, the spacing determined by a preassigned volume fraction $\phi$, and with squares centered above the centers of the gaps in the row below it; see Fig. 4. The basic step in the simulation is the following. A square is chosen at random from the current configuration and all possible positions are determined to which it may be relocated and produce an allowed configuration. Note that if the chosen square supports a square above it then it can only be allowed a relatively small horizontal motion; otherwise it may be placed atop some pair of squares, or the floor. So the boundary of the configuration plays a crucial role in the ability of the chain to change the volume fraction. In any case the positions to which the chosen square may be moved constitute a union of intervals. A random point is selected from this union of intervals and the square is moved. The random movement of a random square is the basic element of the Markov chain. It is easy to see that this protocol is transitive and satisfies
detailed balance, so the chain has the desired uniform probability distribution as its asymptotic state [NB]. See Fig. 5 for a configuration of 399 squares after $10^6$ moves. Our interest is in random loose packing, which occurs in the top (bulk) layer of a granular pile, and we assume that the entirety of each of our configurations represents this top layer. We emphasize that our protocol is not particularly appropriate for studying other questions such as the statistical shape of the boundary of a granular pile, or properties associated with high volume fraction, such as random close packing.

After a prescribed number of moves, a volume fraction is computed for the collection of squares as follows. Within horizontal level $L_j$, where $j = 0$ corresponds to the squares resting on the floor, the distances between the centers of neighboring squares is computed. (Such a distance is $1 + g$ where $g$ is the gap between the squares.) Suppose that $n_j$ of these neighboring distances are each less than 2, and that the sum of these distances in the level is $s_j$. At this point our procedure will be complicated by the desire to obtain information during the simulation about inhomogeneities in the collection, for later use in analyzing the approach to equilibrium. For this purpose we introduce a new parameter, $p$. For fixed $0 < p < 1$ we consider those levels, beginning from $j = 0$, for which $n_j$ is at least $0.75p$ times the length of the box’s floor. Suppose $L_{J(p)}$ is the highest level such that it, and all levels below it, satisfy the condition. We then assign the volume fraction

$$
\phi(p) = \frac{\sum_{j=0}^{J(p)} n_j}{\sum_{j=0}^{J(p)} s_j}
$$

(1)

to the assembly of squares. (The factor 0.75 represents the volume fraction we expect the box’s floor to reach in equilibrium. Note that any two such calculations of volume fraction of the same configuration may only differ by a term proportional to the length of the boundary of the configuration, so any inhomogeneity is limited to this size.) Such a calculation of volume fraction was performed regularly, after approximately $10^6$ moves, producing a time series of volume fractions $\phi_t$ for the given number of squares. (We suppress reference to the variable $p$ for ease of reading. As will be seen later all our results correspond to the choice $p = 0.4$, so one can, without much loss, ignore other possible values.) Variables $\phi_t$ and $\phi_{t+1}$ are highly dependent, but we can be guaranteed that if the series is long enough then the sample mean:

$$
\frac{1}{N} \sum_{t=1}^{N} \phi_t
$$

(2)

will be a good approximation to the true mean of the target (uniform) probability distribution for the given number of squares [KV].

We created such time series $\phi_t$, each of about $10^4$ terms (roughly $10^{10}$ elementary moves), using values $p = 0.2, 0.4, 0.6, 0.8$, on systems for the following numbers of squares: $100m$, and $1000m$, for $m = 1, 2, \ldots, 9$, with varying initial volume fractions. For each system we needed to determine the initialization period – the
number of moves necessary to reach equilibrium – and then the total number of moves to be performed. Both of these determinations were made based on variants of the (sample) autocorrelation function \( f(k) \) of the time series \( \{\phi_t \mid 1 \leq t \leq T\} \) of volume fractions, defined for \( 1 \leq k \leq T \) by:

\[
f(k) = \frac{1}{T-k+1} \sum_{t=1}^{T-k+1} (\phi_t - \bar{\phi})(\phi_{t+k} - \bar{\phi}),
\]

where \( \bar{\phi} \) is the mean of the series. This function is easily seen to give less reliable results as \( k \) increases, because of limited data, so it is usual to work with functions made from it as follows. One way to avoid difficulties is to restrict the domain of \( f \); we define the “unbiased” autocorrelation \( f_1(k) \) by \( f_1(k) = f(k) \) for \( k \leq T/10 \).

Another variant we consider is the “biased” autocorrelation \( f_2 \), defined for all \( 1 \leq k \leq T \) by:

\[
f_2(k) = \frac{1}{T} \sum_{t=1}^{T-k+1} (\phi_t - \bar{\phi})(\phi_{t+k} - \bar{\phi}),
\]

which reduces the value of \( f(k) \) for large \( k \). (See pages 321-324 of Priestley [P] for a discussion of this biased variant.) We consider both variants of autocorrelation; to refer to either we use the term \( f_j \).

With these autocorrelations we determined the smallest \( k = k_z \) such that \( f_j(k) = 0 \). We then computed the sample standard deviation \( \sigma_{f_j} \) away from zero of \( f_j \) restricted to \( k \geq k_z \), and defined \( k_I \) to be the smallest \( k \) such that \( |f_j(k)| \leq \sigma_{f_j} \); see Fig. 6. (For ease of reading we sometimes do not add reference to \( j \) to quantities derived using \( f_j \).) This defined the initialization period. Then starting from \( \phi_{k_I} \) we recomputed the autocorrelation \( \tilde{f}_j \) and \( \sigma_{\tilde{f}_j} \) and determined the mixing time, the smallest \( k = k_M \) such that \( |\tilde{f}_j(k)| \leq \sigma_{\tilde{f}_j} \). \( k_M \) was interpreted as the separation \( k \) needed such that the random variables \( \tilde{\phi}_t \) and \( \tilde{\phi}_{t+k} \) are roughly independent for all \( t \geq k \). (We performed the above using the different definitions of volume fraction corresponding to different values of \( p \), allowing us to analyze different geometrical regions of the samples. For each system of squares we selected, for initialization and mixing times, the largest obtained as above corresponding to the various values of \( p \), which was always that for \( p = 0.2 \), corresponding to the lowest layers of the configuration.)

Once we determined \( k_I \) and \( k_M \) we ran the series to \( \phi_F \), where \( F = k_I + T k_M \) for some \( T \geq 20 \). The values of \( k_I \) and \( k_M \) are given in Tables 1 and 2; the empirical means and standard deviations of volume fraction are given in Tables 3 and 4.

In all our results we use \( p = 0.4 \) to minimize the boundary effects presumably associated with small or large \( p \). (With large \( p \) the lowest level may have undue influence on the volume fraction; with small \( p \), the surface levels could have undue influence. Note that the arrangements of squares on the lowest level and the surface levels are not restricted by the arrangements of squares below and above them, respectively, and so the corresponding volume fractions are not bound to the logic,
discussed above, which suggested that each level should equilibrate at a volume fraction of about .75. In spite of this, we found that using any series corresponding to \( p \) in the range \( 0.2 \leq p \leq 0.8 \) generated a similar result.) For all systems the volume fraction quickly settles to the range \( 0.76 \pm 0.01 \) and we can easily see from Table 4 that the empirical standard deviations decrease with increase of particle number. In Fig. 7 we plot the empirical standard deviations against particle number, and in Fig. 8 the data is replotted using logarithmic scales. In Fig. 8 we include the best least-squares fit to a straight line \( y = ax + b \), obtaining \( a = -0.5004 \) and \( b = -0.8052 \). The corresponding curve is included in Fig. 7. Also included in both graphs are 90\% confidence intervals for the true standard deviations, obtained as described in the next section, using \( f_2 \). (There was not enough data to obtain a confidence interval by this method for the system with 8995 squares.) The same data is reanalyzed in Figs. 9 and 10 with confidence intervals derived using \( f_1 \).

We use the close fit to the line in Figs. 8 or 10, corresponding to 33 data points in a range of particle number varying from 100 to 9000, to extend the agreement to arbitrarily large particle number, and therefore to claim that the standard deviation is zero in the infinite volume limit, or that there is a sharp value for the random loose packing density. The argument is supported from the theoretical side by noting the closeness of the slopes in Figs. 8 and 10 to \(-1/2\). A slope of \(-1/2\) would be expected if it were true that an equilibrium configuration of \( N \) squares could be partitioned into similar subblocks which are roughly independent – a proposition which would not be surprising given a phase interpretation of granular media [R]. Verifying such independence might be of some independent interest but would require much more data and much longer running times.

This is our main result, since it shows how to make sense of a perfectly well-defined random loose packing density within a granular model of the standard Edwards’ form.

As to the actual asymptotic value of the volume fraction in the limit of large systems, we assume that our simulations suffer from a surface error proportional to \( \sqrt{N} \) for a system of \( N \) squares. The least-squares fit of a function of form \( A + B/\sqrt{N} \) to the data (see Figs. 11 and 12) yields \( A = 0.7541 \), and the good fit suggests an (asymptotic) random loose packing density in our granular model of about 0.754.

Our argument concerning asymptotically large systems depends on the fit of our standard deviation data to a curve, and the degree to which this fit is convincing depends on the confidence intervals associated with our simulations. In the next section we explain how we arrived at our confidence intervals.

3. Simulation data analysis

A good source for common ways to analyze the data in Markov chain Monte Carlo simulation is chapter 3 in Newman and Barkema [NB]. We will give a more detailed analysis, following the paper by Geyer [Gey] in the series put together for this purpose by the statistics community [Gel]. As will be seen, our argument is based on the precision of estimates of various statistical quantities, and necessitates
a delicate treatment.

Our simulations produce a time series $c_j$ of (dependent) random configurations of squares. From this we produce other series $g(c_j)$ using functions $g$ on the space of possible configurations $c$, in particular the volume fraction $g_1(c) = \phi$ and $g_2(c) = (\phi - K)^2$ for constant $K$.

We use the common method of batch means. As described in the previous section, we first determine an initialization time $k_I$ and a mixing time $k_M$ for our series $c_j$ from autocorrelations. After removing the initialization portion of the series, we break up the remaining $W$ terms of the series into $w \geq 2$ equal size consecutive batches (subintervals), each of the same length $W/w$, discarding the last few terms from the series if $w$ does not divide $W$ evenly.

It should be emphasized that rarely, if ever, are conclusions drawn from a finite number of Monte Carlo simulations a literal proof of anything interesting. We are going to obtain confidence intervals (using the Student’s t-test) for the mean and standard deviation of the volume fraction of our systems of fixed particle number. The t-test’s results would be mathematically rigorous if in our simulations we had performed infinitely many moves; of course this is impossible, so we will try to make a convincing case that we have enough data to give reliable results. Ultimately, this is the most sensitive point in our argument.

Assume fixed some function $g$, and denote the true mean of $g(c)$ by $\mu_g$. Assume, temporarily, that enough moves have been taken for the t-test to be reliable. (We will come back to this assumption below.) With the notation $\overline{g(c)}$ for the empirical average $(1/w) \sum_k (g(c))_k$ of $g(c)$, the variable:

$$\frac{\overline{g(c)} - \mu_g}{\sqrt{\frac{1}{w(w-1)} \sum_k ((g(c))_k - \overline{g(c)})^2}}$$

has a t-distribution, allowing one to compute confidence intervals for $\mu_g$.

The above outline explains how (given the validity of the t-test) we could compute confidence intervals for the mean value of the volume fraction for the time series associated with our simulations for fixed numbers of squares. A small variation allows us to give confidence intervals for the standard deviations of these variables, as follows.

Denote the true standard deviation of $g(c)$ by $\sigma_g$. Using conditioning,

$$\text{Prob}(\mu_g \in I \text{ and } \sigma_g \in J) = \text{Prob}(\mu_g \in I) \text{Prob}(\sigma_g \in J \mid \mu_g \in I)$$

$$= \text{Prob}(\mu_g \in I) \sum_i \text{Prob}(\sigma_g \in J \mid \mu_g \in I_i) \text{Prob}(\mu_g \in I_i \mid \mu_g \in I),$$

where $\{I_i\}$ is a partition of $I$. We have discussed how to obtain $I$ so that the factor $\text{Prob}(\mu_g \in I)$ is at least 0.95. We now want to obtain $J$ so that the factor $\text{Prob}(\sigma_g \in J \mid \mu_g \in I)$ is also at least 0.95, and therefore $\text{Prob}(\mu_g \in I \text{ and } \sigma_g \in J)$ is at least $(0.95)(0.95) > 0.90.$
Consider, for each constant $K$, the random variable

$$\Sigma_K = \sqrt{\frac{1}{w} \sum_j [\langle g(c) \rangle_j - K]^2}. \tag{7}$$

Using (5) with $(g(c) - K)^2$ playing the role of $g(c)$, we can obtain a 95% confidence interval for the mean of $\Sigma_K^2$, which we translate into a 95% confidence interval $J_K$ for the mean of $\Sigma_K$. Assume the partition so fine that within the desired precision $J_K = J_i$ only depends on $i$, where $K \in I_i$. Note that if $K = \mu_g$, then the random variable $\Sigma_K$ has as its mean the standard deviation $\sigma_g$. So if we let $J = \cup_i J_i$, then $\text{Prob}(\sigma_g \in J \mid \mu_g \in I_i) > 0.95$ for all $i$, and therefore $\text{Prob}(\sigma_g \in J \mid \mu_g \in I) > 0.95$.

In practice the union $J = \cup_i J_i$ is easy to compute.

In the above arguments we have assumed that enough moves have been taken to justify the t-test, which has independence and normality assumptions which are not strictly satisfied in our situation. We now consider how to deal with this situation. Some guidance concerning independence can be obtained from the following toy model.

Assume that for the time series of the simulation one can determine some number $k_M$, perhaps but not necessarily derived as above from the autocorrelation $f(k)$, such that variables $\phi_i$ and $\phi_{i+k}$ in the time series are roughly independent if $k \geq k_M$. We model this transition between independent random variables as follows.

Let $T$ and $M$ be nonnegative (integer) constants. For $0 \leq t \leq T$ and $1 \leq m \leq M - 1$ we first define independent, identically distributed random variables $X_{tM}$ and from these define:

$$X_{tM+m} = \left(1 - \frac{m}{M}\right)X_{tM} + \frac{m}{M}X_{(t+1)M}, \tag{8}$$

together defining $X_t$ for $0 \leq t \leq TM - 1$. Note that variables $X_t$ and $X_{t+m}$ are independent for $m \geq 2M - 1$.

A simple calculation shows that:

$$\sum_{m=0}^{M-1} X_{tM+m} = \left(\frac{M+1}{2}\right)X_{tM} + \left(\frac{M-1}{2}\right)X_{(t+1)M}. \tag{9}$$

Then another simple calculation shows that:

$$S_T \equiv \frac{1}{TM} \sum_{m=0}^{TM-1} X_m = \frac{1}{T} \left[\sum_{t=1}^{T-1} X_{tM} + \frac{1}{2}(X_0 + X_{TM}) + \frac{1}{2M}(X_0 - X_{TM})\right]. \tag{10}$$

In other words $S_T$ is the mean of roughly $K$ independent variables.

Returning to the question of the assumptions in the t-test, the toy model suggests that the independence assumption is easily satisfied. The normality assumption is usually taken as the more serious [Gey]. But we note from [DL] that
the t-test is quite robust with respect to the normality assumption. Although the robustness of the t-test is well known and is generally relied on, in practice one still has to pick specific batch partitions in a reliable way. This is not covered in [Gey]. We arrived at a standard for batches of length 10 times mixing time for our series as follows. In outline, we use mixing times as computed above to standardize comparison between our systems with different particle number. Those for which our runs constituted at least 800 mixing times are assumed to give accurate values for the mean volume fraction. Various initial segments of these runs are then used, with various choices of batch partitions, to see which choices (if any) give reliable results for confidence intervals. Batches of size 10 mixing times proved reliable even for initial segments in the range of 20-100 mixing times, so this choice was then used for all systems. We emphasize that we are using this method to determine a minimum reliable batch size on the sequence of configurations, and then we apply this to the time series $\phi_t$ as well the time series $[\phi_t - K]^2$. We now give more details.

For most of the systems of particle numbers 100-900 we have over 500 mixing times worth of data, yet for some of the systems of particle numbers 1000-9000 we have, for practical reasons, less than one tenth that depth of data. We want to choose a fixed multiple of mixing time as batch length for all of our batches. To decide what range of mixing times will be reliable we used various portions of the data from those of our longest runs, and then applied the conclusions we drew to the other 3/4 of the runs.

More specifically, we treat as “reliable” the empirical volume fraction of the longest runs, those of length at least 800 times mixing time. We then consider a range of batch partitions of these systems to see which ones give accurate t-test results. We are looking for 95% confidence intervals, so we expect such intervals to contain the true volume fraction 95% of the time; since the true volume fraction is unknown we instead check how frequently the intervals contain the empirical volume fraction, which for the longer runs we have assumed is reliable. We do this for each of the runs of length 800 or more times mixing time. The results on these systems are the following.

For each of our longer runs (of at least 800 mixing times), we considered various initial portions of the run in each of six ranges of mixing times: 20-100, 100-200, 300-400, 400-500, and 500-600. For each of these truncated runs we considered batch partitions of the data into equal size batches of a variety of multiples of mixing time: 1-5, 6-10, 11-15, 16-20, 21-30, 31-40 and 41-50. For each size run and for each batch size we computed a 95% confidence interval for the true mean of the volume fraction, and determined whether or not the confidence interval covers the sample mean for the full run (which we are assuming is interchangeable with the true mean). The fraction of the more than 200 cases in each category for which the sample mean lies within the confidence interval is recorded in Table 5. From this it appears that using batches of size 1-5 mixing times would be unreliable, but that size 10 times mixing times would be reliable. (Table 5 is based on mixing times obtained using the autocorrelation $f_2$. Table 6 is similar, using the autocorrelation $f_1$, and again justifies the use of batches of size 10 times mixing time.)
We then used batches of size 10 times mixing times to obtain 95% confidence intervals for the true mean of all the systems, obtaining the results tabulated in Table 3 and included in Figs. 17 and 18.

Finally, we applied the above batch criterion to obtain 90% confidence intervals for the true standard deviation of all our systems, using the method described earlier in this section. The results are in Table 4 and in Figs. 7 to 10.

4. Conclusion

We have performed Markov chain Monte Carlo simulations on a two dimensional model of low pressure granular matter of the general Edwards probabilistic type [EO]. Our main result, superficially summarized in Fig. 8, is that in this model the standard deviation of the volume fraction decays to zero as the particle number increases, which indicates a well-defined random loose packing density for the model. This suggests that real granular matter exhibits sharply defined random loose packing; this could be verified by repeating the sedimentation experiments [JS] at a range of physical dimensions. Our argument is only convincing to the extent that the confidence intervals in Fig. 8 are small and justified, which required a statistical treatment of the data unusual in the physics literature. We hope that our detailed error analysis may be useful in other contexts.
Figure 1. Plot of volume fraction versus number of moves, from an initial volume fraction of 0.9991, for 970 squares.

Figure 2. Plot of volume fraction versus number of moves, from an initial volume fraction of 0.5192, for 994 squares.
Figure 3. An allowed configuration

Figure 4. A uniform configuration

Figure 5. 399 squares after $10^6$ moves.
Figure 6a. Plot of biased autocorrelation (for 8000 particles) versus number of moves, with horizontal lines denoting one standard deviation away from zero.

Figure 6b. Close-up of the above plot, with initialization time.
Figure 7. Plot of the standard deviation of the volume fraction versus number of squares, using $f_2$ for confidence intervals.
Figure 8. Plot of the standard deviation of the volume fraction versus number of squares, using log scales and $f_2$ for confidence intervals. The line is $y = -0.5004 \, x - 0.8052$. 
Figure 9. Plot of the standard deviation of the volume fraction versus number of squares, using $f_1$ for confidence intervals.
Figure 10. Plot of the standard deviation of the volume fraction versus number of squares, using log scales and $f_1$ for confidence intervals. The line is $y = -0.5003x - 0.8055$. 
Figure 11. Plot of the mean of the volume fraction versus number of squares, using $f_2$ for confidence intervals. The curve is $y = 0.7541 + 0.0998 x^{-1/2}$. 
Figure 12. Plot of the mean of the volume fraction versus number of squares, using $f_1$ for confidence intervals. The curve is $y = 0.7541 + 0.0998 \, x^{-1/2}$. 
Table 1
Basics
(using unbiased autocorrelation $f_1$)

| number of squares in packing | number of moves in units of $10^9$ | step size in units of $10^6$ moves | $k_I$ (init. time) in units of step size using $f_1$ | $k_M$ (mixing time) in units of step size using $f_1$ | run length in units of mixing time using $f_1$ |
|-----------------------------|-----------------------------------|-----------------------------------|---------------------------------|---------------------------------|---------------------------------|
| 99                          | 0.4                               | 0.2                               | 1                              | 1                              | 1998                            |
| 100                         | 0.4                               | 0.2                               | 1                              | 1                              | 1998                            |
| 195                         | 0.4                               | 0.2                               | 1                              | 1                              | 1998                            |
| 205                         | 0.4                               | 0.2                               | 1                              | 1                              | 1998                            |
| 294                         | 0.4                               | 0.2                               | 5                              | 5                              | 398                             |
| 294                         | 0.4                               | 0.2                               | 4                              | 4                              | 498                             |
| 399                         | 2                                 | 0.2                               | 10                             | 10                             | 998                             |
| 413                         | 2                                 | 0.2                               | 9                              | 9                              | 1110                            |
| 497                         | 2                                 | 0.2                               | 17                             | 17                             | 587                             |
| 504                         | 2                                 | 0.2                               | 17                             | 17                             | 587                             |
| 600                         | 2                                 | 0.2                               | 12                             | 12                             | 832                             |
| 603                         | 2                                 | 0.2                               | 23                             | 23                             | 433                             |
| 690                         | 2                                 | 0.2                               | 14                             | 14                             | 713                             |
| 690                         | 2                                 | 0.2                               | 20                             | 20                             | 498                             |
| 790                         | 2                                 | 0.2                               | 43                             | 43                             | 231                             |
| 803                         | 2                                 | 0.2                               | 14                             | 14                             | 713                             |
| 913                         | 2                                 | 0.2                               | 34                             | 34                             | 293                             |
| 913                         | 2                                 | 0.2                               | 75                             | 75                             | 135                             |
| 996                         | 12                                | 1                                 | 13                             | 13                             | 953                             |
| 1001                        | 12                                | 1                                 | 16                             | 16                             | 755                             |
| 1955                        | 12                                | 1                                 | 38                             | 38                             | 318                             |
| 2980                        | 12                                | 1                                 | 44                             | 44                             | 277                             |
| 3003                        | 12                                | 1                                 | 51                             | 53                             | 234                             |
| 3933                        | 12                                | 1                                 | 64                             | 63                             | 193                             |
| 4008                        | 12                                | 1                                 | 99                             | 75                             | 158                             |
| 4995                        | 12                                | 1                                 | 193                            | 174                            | 68                              |
| 5908                        | 12                                | 1                                 | 163                            | 96                             | 125                             |
| 6030                        | 12                                | 1                                 | 143                            | 143                            | 84                              |
| 7037                        | 12                                | 1                                 | 223                            | 261                            | 46                              |
| 7161                        | 12                                | 1                                 | 222                            | 181                            | 48                              |
| 8015                        | 12                                | 1                                 | 132                            | 120                            | 100                             |
| 8991                        | 12                                | 1                                 | 283                            | 287                            | 41                              |
| 8995                        | 12                                | 1                                 | 632                            | 631                            | 18                              |
Table 2

Basics
(using biased autocorrelation $f_2$)

| number of squares in packing | number of moves in units of $10^9$ | step size in units of $10^6$ moves | $k_I$ (init. time) in units of step size using $f_2$ | $k_M$ (mixing time) in units of step size using $f_2$ | run length in units of mixing time using $f_1$ |
|-----------------------------|-----------------------------------|------------------------------------|---------------------------------|---------------------------------|-----------------|
| 99                          | 0.4                               | 0.2                                | 1                               | 1                               | 1998            |
| 100                         | 0.4                               | 0.2                                | 3                               | 2                               | 998             |
| 195                         | 0.4                               | 0.2                                | 1                               | 1                               | 1998            |
| 205                         | 0.4                               | 0.2                                | 1                               | 1                               | 1998            |
| 294                         | 0.4                               | 0.2                                | 5                               | 5                               | 398             |
| 294                         | 0.4                               | 0.2                                | 4                               | 4                               | 498             |
| 399                         | 2                                 | 0.2                                | 12                              | 12                              | 832             |
| 413                         | 2                                 | 0.2                                | 11                              | 11                              | 908             |
| 497                         | 2                                 | 0.2                                | 20                              | 20                              | 498             |
| 504                         | 2                                 | 0.2                                | 19                              | 19                              | 525             |
| 600                         | 2                                 | 0.2                                | 12                              | 12                              | 832             |
| 603                         | 2                                 | 0.2                                | 23                              | 23                              | 433             |
| 690                         | 2                                 | 0.2                                | 14                              | 15                              | 665             |
| 690                         | 2                                 | 0.2                                | 25                              | 20                              | 498             |
| 790                         | 2                                 | 0.2                                | 43                              | 44                              | 226             |
| 803                         | 2                                 | 0.2                                | 15                              | 14                              | 713             |
| 913                         | 2                                 | 0.2                                | 36                              | 38                              | 262             |
| 913                         | 2                                 | 0.2                                | 77                              | 75                              | 132             |
| 996                         | 12                                | 1                                 | 18                              | 18                              | 687             |
| 1001                        | 12                                | 1                                 | 16                              | 16                              | 755             |
| 1955                        | 12                                | 1                                 | 38                              | 38                              | 318             |
| 2980                        | 12                                | 1                                 | 56                              | 56                              | 218             |
| 3003                        | 12                                | 1                                 | 51                              | 54                              | 230             |
| 3933                        | 12                                | 1                                 | 76                              | 78                              | 156             |
| 4008                        | 12                                | 1                                 | 101                             | 88                              | 135             |
| 4995                        | 12                                | 1                                 | 191                             | 177                             | 67              |
| 5908                        | 12                                | 1                                 | 179                             | 100                             | 120             |
| 6030                        | 12                                | 1                                 | 139                             | 151                             | 80              |
| 7037                        | 12                                | 1                                 | 220                             | 290                             | 41              |
| 7161                        | 12                                | 1                                 | 199                             | 186                             | 47              |
| 8015                        | 12                                | 1                                 | 131                             | 126                             | 95              |
| 8991                        | 12                                | 1                                 | 282                             | 355                             | 33              |
| 8995                        | 12                                | 1                                 | 565                             | 609                             | 19              |
| number of squares in packing | sample value | end points of 95% confidence interval for true value, using $f_1$ | end points of 95% confidence interval for true value, using $f_2$ |
|-----------------------------|--------------|-------------------------------------------------|-------------------------------------------------|
| 99                          | 0.7637       | 0.7637±0.0007                                   | 0.7637±0.0007                                   |
| 100                         | 0.7631       | 0.7631±0.0007                                   | 0.7631±0.0007                                   |
| 195                         | 0.7617       | 0.7617±0.0005                                   | 0.7617±0.0005                                   |
| 294                         | 0.7608       | 0.7608±0.0005                                   | 0.7608±0.0005                                   |
| 294                         | 0.7598       | 0.7598±0.0004                                   | 0.7598±0.0004                                   |
| 399                         | 0.7596       | 0.7596±0.0002                                   | 0.7596±0.0002                                   |
| 413                         | 0.7593       | 0.7593±0.0002                                   | 0.7593±0.0002                                   |
| 497                         | 0.7590       | 0.7590±0.0002                                   | 0.7590±0.0002                                   |
| 504                         | 0.7590       | 0.7590±0.0003                                   | 0.7590±0.0002                                   |
| 600                         | 0.7583       | 0.7583±0.0002                                   | 0.7583±0.0002                                   |
| 603                         | 0.7588       | 0.7588±0.0002                                   | 0.7588±0.0002                                   |
| 690                         | 0.7581       | 0.7581±0.0002                                   | 0.7581±0.0002                                   |
| 690                         | 0.7583       | 0.7583±0.0003                                   | 0.7583±0.0003                                   |
| 790                         | 0.7578       | 0.7578±0.0003                                   | 0.7578±0.0003                                   |
| 803                         | 0.7579       | 0.7579±0.0002                                   | 0.7579±0.0002                                   |
| 913                         | 0.7575       | 0.7575±0.0002                                   | 0.7575±0.0002                                   |
| 913                         | 0.7578       | 0.7578±0.0003                                   | 0.7578±0.0003                                   |
| 996                         | 0.7575       | 0.7575±0.0001                                   | 0.7575±0.0001                                   |
| 1001                        | 0.7574       | 0.7574±0.0001                                   | 0.7574±0.0001                                   |
| 1955                        | 0.7565       | 0.7565±0.0002                                   | 0.7565±0.0002                                   |
| 2980                        | 0.7558       | 0.7558±0.0002                                   | 0.7558±0.0001                                   |
| 3003                        | 0.7559       | 0.7559±0.0002                                   | 0.7559±0.0002                                   |
| 3933                        | 0.7554       | 0.7554±0.0002                                   | 0.7554±0.0002                                   |
| 4008                        | 0.7558       | 0.7558±0.0003                                   | 0.7558±0.0003                                   |
| 4995                        | 0.7555       | 0.7555±0.0004                                   | 0.7555±0.0005                                   |
| 5908                        | 0.7549       | 0.7549±0.0003                                   | 0.7549±0.0003                                   |
| 6030                        | 0.7551       | 0.7551±0.0004                                   | 0.7551±0.0003                                   |
| 7037                        | 0.7545       | 0.7545±0.0005                                   | 0.7545±0.0004                                   |
| 7161                        | 0.7550       | 0.7550±0.0005                                   | 0.7550±0.0007                                   |
| 8015                        | 0.7551       | 0.7551±0.0004                                   | 0.7551±0.0004                                   |
| 8991                        | 0.7551       | 0.7551±0.0004                                   | 0.7551±0.0012                                   |
| 8995                        | 0.7550       | none                                            | none                                            |
| number of squares in packing | sample value | end points of 90% confidence interval for true value, using $f_1$ | end points of 90% confidence interval for true value, using $f_2$ |
|-----------------------------|--------------|---------------------------------------------------------------|---------------------------------------------------------------|
| 99                          | 0.0160       | 0.0160±0.0005                                                | 0.0160±0.0005                                                |
| 100                         | 0.0157       | 0.0157±0.0006                                                | 0.0157±0.0006                                                |
| 195                         | 0.0110       | 0.0110±0.0004                                                | 0.0110±0.0004                                                |
| 205                         | 0.0108       | 0.0108±0.0004                                                | 0.0108±0.0004                                                |
| 294                         | 0.0090       | 0.0090±0.0003                                                | 0.0090±0.0003                                                |
| 399                         | 0.0078       | 0.0078±0.0001                                                | 0.0078±0.0002                                                |
| 413                         | 0.0076       | 0.0077±0.0001                                                | 0.0077±0.0001                                                |
| 497                         | 0.0070       | 0.0070±0.0001                                                | 0.0070±0.0001                                                |
| 504                         | 0.0069       | 0.0069±0.0001                                                | 0.0069±0.0001                                                |
| 600                         | 0.0064       | 0.0064±0.0001                                                | 0.0064±0.0001                                                |
| 603                         | 0.0064       | 0.0064±0.0001                                                | 0.0064±0.0001                                                |
| 690                         | 0.0060       | 0.0061±0.0002                                                | 0.0060±0.0001                                                |
| 690                         | 0.0060       | 0.0060±0.0002                                                | 0.0060±0.0001                                                |
| 790                         | 0.0055       | 0.0055±0.0002                                                | 0.0055±0.0002                                                |
| 803                         | 0.0055       | 0.0055±0.0002                                                | 0.0055±0.0002                                                |
| 913                         | 0.0052       | 0.0052±0.0002                                                | 0.0052±0.0002                                                |
| 913                         | 0.0053       | 0.0053±0.0001                                                | 0.0053±0.0001                                                |
| 996                         | 0.0050       | 0.0050±0.0001                                                | 0.0050±0.0001                                                |
| 1001                        | 0.0049       | 0.0049±0.0001                                                | 0.0049±0.0001                                                |
| 1955                        | 0.0036       | 0.0036±0.0001                                                | 0.0036±0.0001                                                |
| 2980                        | 0.0028       | 0.0028±0.0001                                                | 0.0028±0.0001                                                |
| 3003                        | 0.0029       | 0.0029±0.0001                                                | 0.0029±0.0001                                                |
| 3933                        | 0.0024       | 0.0025±0.0001                                                | 0.0025±0.0001                                                |
| 4008                        | 0.0025       | 0.0025±0.0001                                                | 0.0025±0.0002                                                |
| 4995                        | 0.0022       | 0.0022±0.0002                                                | 0.0022±0.0002                                                |
| 5908                        | 0.0021       | 0.0021±0.0002                                                | 0.0021±0.0002                                                |
| 6030                        | 0.0020       | 0.0020±0.0002                                                | 0.0020±0.0002                                                |
| 7037                        | 0.0018       | 0.0019±0.0002                                                | 0.0019±0.0002                                                |
| 7161                        | 0.0019       | 0.0020±0.0003                                                | 0.0021±0.0004                                                |
| 8015                        | 0.0016       | 0.0017±0.0002                                                | 0.0017±0.0002                                                |
| 8991                        | 0.0017       | 0.0017±0.0003                                                | 0.0021±0.0008                                                |
| 8995                        | 0.0016       | none                                                          | none                                                          |
Table 5

Fraction of times the given batch size gives acceptable confidence interval for given segment of total data of long runs, using unbiased autocorrelation $f_1$

|                | 20-100 mixing times of total data | 100-200 mixing times of total data | 200-300 mixing times of total data | 300-400 mixing times of total data | 400-500 mixing times of total data | 500-600 mixing times of total data |
|----------------|-----------------------------------|-------------------------------------|------------------------------------|------------------------------------|------------------------------------|------------------------------------|
| number of mixing times per batch | 1-5 | 0.0849 | 0.0867 | 0.1119 | 0.1191 | 0.1938 | 0.2082 |
|                | 6-10 | 0.9410 | 0.9394 | 0.9830 | 1.0000 | 1.0000 | 1.0000 |
|                | 11-15 | 0.9648 | 0.9231 | 0.9656 | 1.0000 | 1.0000 | 1.0000 |
|                | 16-20 | 0.9524 | 0.9095 | 0.9777 | 0.9879 | 1.0000 | 1.0000 |
|                | 21-31 | 0.9650 | 0.9177 | 0.9673 | 1.0000 | 1.0000 | 1.0000 |
|                | 31-40 | 0.9712 | 0.9042 | 0.9643 | 1.0000 | 1.0000 | 0.9957 |
|                | 41-51 | 0.9375 | 0.8869 | 0.9402 | 0.9511 | 0.9783 | 0.9402 |

Table 6

Fraction of times the given batch size gives acceptable confidence interval for given segment of total data of long runs, using biased autocorrelation $f_2$

|                | 20-100 mixing times of total data | 100-200 mixing times of total data | 200-300 mixing times of total data | 300-400 mixing times of total data | 400-500 mixing times of total data | 500-600 mixing times of total data |
|----------------|-----------------------------------|-------------------------------------|------------------------------------|------------------------------------|------------------------------------|------------------------------------|
| number of mixing times per batch | 1-5 | 0.0833 | 0.0924 | 0.1182 | 0.1259 | 0.2006 | 0.2326 |
|                | 6-10 | 0.9245 | 0.9784 | 0.9805 | 0.9524 | 0.9762 | 1.0000 |
|                | 11-15 | 0.9107 | 0.9451 | 0.9607 | 0.9524 | 0.9707 | 1.0000 |
|                | 16-20 | 0.9728 | 0.9212 | 0.9745 | 0.9493 | 0.9655 | 1.0000 |
|                | 21-31 | 0.9486 | 0.9059 | 0.9592 | 0.9547 | 0.9744 | 1.0000 |
|                | 31-40 | 0.9780 | 0.9190 | 0.9592 | 0.9704 | 0.9852 | 1.0000 |
|                | 41-51 | 0.9000 | 0.8639 | 0.9441 | 0.9565 | 0.9814 | 1.0000 |
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