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ON RANDOM PACKINGS BY NON-SPHERICAL PARTICLES

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ABSTRACT

Random sequential packings of identical rectangles and identical ellipses are respectively considered. By performing computer simulations, the values of the packing density of rectangle in the complete packing are $0.501 \sim 0.508$ for a range of aspect ratio $1.0 \leq k \leq 2.0$, while the values for ellipses in the near complete packing are $0.533 \sim 0.540$ for the same range of aspect ratio.

Key words: aspect ratio, ellipses, packing density, rectangles

INTRODUCTION

Random packing of objects into a finite region has been an important subject having many applications together with its mathematical interest. The terminology of 'packing of objects' will be used in this paper as to represent the spatial pattern of non-overlapping objects in a certain finite region B. On this subject, much work has been done with the packing of spherically symmetric objects, such as dics in the plane, spheres in 3-D space. However, the most objects we observe in the natural world are non-spherical. For example, cars in the street can be represented by rectangles better than by dics, complex metallic molecules are represented by ellipses better than by dics and so on. Then it is obviously also important to investigate packing problems of non-spherical objects.

In this paper, we consider two cases of non-spherical (non-circular) convex particles, namely, rectangles and ellipses, in the plane. We represent each particle by S. We perform computer simulation for the systems of these particles, separately. In order to represent the shape of these particles, we denote by a and b both the half of side lengths of a rectangle, and the major and minor axes of an ellipse. Thus the area of rectangle and ellipse are respectively given by $(2a) \times (2b) = 4ab$ and πab. It will be then convenient to introduce a parameter $k = a/b$ to characterize their shape, and we call it 'aspect ratio'. Let us note that another characteristic of non-sphericity is the orientation θ of particles.

In the following, our main concern is the packing density ρ which is defined by the value of

$$\rho_B = \frac{\text{Expected number of packed particles} \times |S|}{|B|}$$

in the limit of $|B| \to \infty$, where $|S|$ and $|B|$ represent the area of S and of B, respectively. It can be said that the packing density ρ_B is equal to the area fraction of the region B occupied by rectangles or ellipses. In a mathematically legitimate sense, ρ_B should depend on the size, shape and orientational distribution of the particle S. In the following, however, we only consider the shape dependence of ρ_B under the assumptions that the dependence on the size of S would be weak for a relatively large B, as given below, and that the orientational distribution of S is fixed to be the uniform distribution.

RANDOM SEQUENTIAL PACKING OF RECTANGLES

Firstly, we consider the random packing by identical rectangles. Packing procedure we concern here is based on the process of random *sequential* adsorption (e.g., Evans, 1993). However, for the packing of each rectangle, we first determine its orientation and then its location uniformly at random inside a finite region. Then the procedure of random sequential packing of rectangles (**RSPR**) can be given as follows:

Procedure RSPR

1. The direction θ of the first rectangle S_1 is sampled uniformly at random within $(0, \pi)$ and the center of S_1 is sampled uniformly at random inside the region B_θ where the center of a moving rectangle with direction θ can enter inside of B, and S_1 is settled there.

2. The second rectangle S_2 is similarly settled as S_1, but the overlap of S_2 with S_1 is not allowed. In other words, by letting the sampled direction be θ, the center of S_2 is sampled uniformly at random inside the region $R_2^\theta = B_\theta \backslash \tilde{S}_1^\theta$. Here, $\tilde{S}_1^\theta$ represents an octagon (see Fig.1) where the center of a moving rectangle with direction θ cannot enter into S_1.

3. Let θ be the uniformly sampled direction. Then, the n-th rectangle S_n is settled inside the region $R_n^\theta = B_\theta \setminus \bigcup_{j=1}^{n-1} \tilde{S}_j^\theta$ uniformly at random. Set $n \leftarrow n+1$.

4. The above procedure is continued until $R_n^\theta = \emptyset$ is attained for all $\theta \in (0, \pi)$.

We call the final state obtained by the procedure **RSPR** a 'complete packing'.

Figure 1 shows a sample pattern of the intermediate stage of random sequential packing of rectangles. In Fig. 1, each rectangle written in thick lines represents a particle settled in the region. Letting θ_0 be the angle which is sampled for the settlement of a new rectangular particle in this figure, polygons written in dotted lines associated with respective rectangles represent the 'excluded' regions $\tilde{S}^{\theta_0}$. It will be easy to understand that the shape of the latter comes to be an octagon in general as can be seen in Fig. 1. It is because this is the locus of the center of the new rectangle obtained by contacting with a settled rectangle at a fixed angle θ_0. Then, it is also easy to see that the area which is not covered by these octagons in this figure comes to be the region R^{θ_0} which is accessible for the center of the new particle. Let us note that if the value of sampled angle is different from the case in Fig. 1, then the shapes of the associated octagons change accordingly.

Figure 1: A sample of intermediate stage of random sequential packing of rectangles.

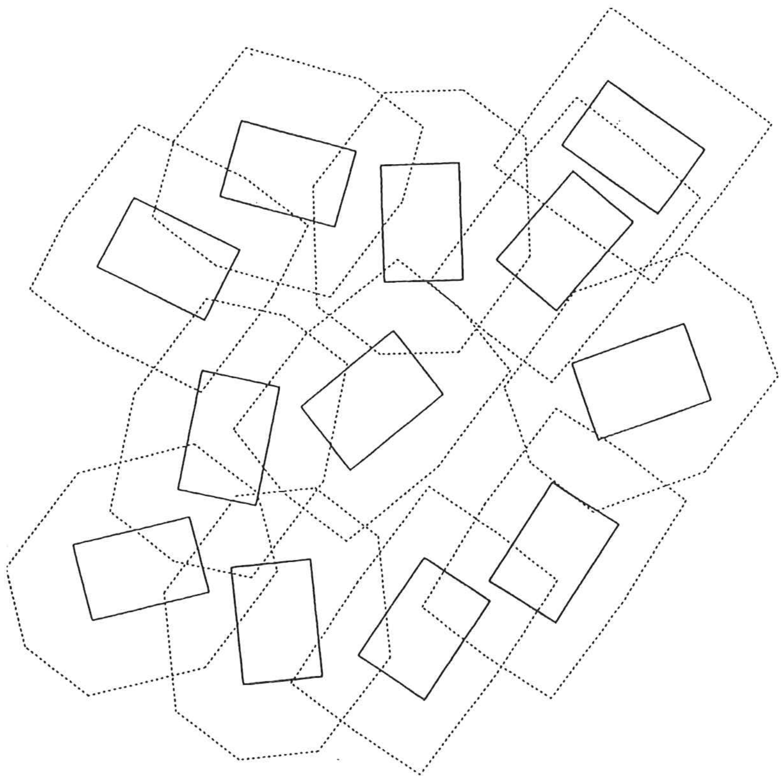

Table 1: Result of computer simulation of random sequential complete packing of rectangles.

k	B	Sample size	$\overline{\rho}_B$	$\hat{\sigma}_\rho$
1.0	10.0×10.0	100	0.5014	0.0180
1.2	10.0×10.0	100	0.5062	0.0170
1.4	10.0×10.0	100	0.5051	0.0166
1.6	10.0×10.0	100	0.5075	0.0164
1.8	10.0×10.0	100	0.5080	0.0161
2.0	10.0×10.0	100	0.5037	0.0161
1.0 ($\theta = 0$)	10.0×10.0	100	0.5636	0.0256

By implementing an efficient algorithm for **RSPR**, we performed computer simulation for several values of aspect ratio k in the range $1.0 \leq k \leq 2.0$. In the simulation, the periodic boundary condition is used throughout. The unit of length is selected as $2a = 1$.

Table 1 shows the result of our simulation for rectangles. In this table, $\overline{\rho}_B$ is meant by the sample mean of ρ_B and $\hat{\sigma}_\rho$ the sample standard deviation of $\overline{\rho}_B$. The value in the last line of the table indicates the result of simulation for the homothetic (the angle θ is fixed to 0) random sequential packing of squares ($k = 1$). Regarding to this, the value of homothetic packing of square is known to be $\rho \sim 0.5644$ in the limit $|B| \to \infty$ (Solomon et al., 1986).

The mean value $\overline{\rho}_B = 0.5636$ for $B = 10.0 \times 10.0$ in our table indicates a good coincidence with this limiting value. We believe this is due to the periodic boundary condition used in our simulation. Thus, the packing density values in our table for a rahter 'small' region B would be considered to well approximate the corrsponding limiting values.

The plot of packing density against aspect ratio in this case is shown in Figure 2. The mean value is represented by a cross and its one sigma range is indicated by dotted lines. Although a certain trend is found from this plot, it might be said that the value of density is in a rather narrow range $0.501 \sim 0.508$ and hence the density of random sequential complete packing is fairly invariant for the value of aspect ratio in the range $1.0 \leq k \leq 2.0$.

RANDOM SEQUENTIAL PACKING OF ELLIPSES

The situation of random sequential packing of ellispes is similar to that of rectangles, but the procedure **RSPR** should be changed in the following point: The meaning of $\tilde{S}^\theta$ in the steps 2 and 3 of **RSPR** changes as to represent the region where the center of moving ellipse with direction θ cannot enter into S. The shape of $\tilde{S}^\theta$ is too much complicated to represent in a simple analytic form.

It is because that the 'exclude' region $\tilde{S}^\theta$ is determined, similarly to the case of the packing of rectangles, by the locus of the center of one moving ellipse which is in contact with the other fixed ellipse at a definite given angle. Since the equation of each ellipse is represented by a quadratic form, the form of the equation for the locus of two contacting ellipses comes to be too much complicated in general. Then, in this case it is difficult to implement an efficient algorithm similar to **RSPR**.

However, by using a large number of random numbers, we can obtain a nearly complete packing of ellipses by implementing a simplified version of algorithm. This implementation is done by simply iterating the following process: sample the angle θ and the center x of a trial ellipse in the range $0 \leq \theta < \pi$ and in the whole region $x \in B$ irrespective of the number of settled ellipses; check if the trial ellipse overlaps with the settled ellipses, and accept it if it does not, or reject it if it does. It is obvious, by the use of this algorithm, the settlement of a new ellipse tends to be more difficult as the settled ellipses become more dense. Although it is inefficient, we can obtain a nearly complete packing of ellipses if we generate a sufficiently large number of trial ellipses.

Table 2 is the result of the computer simulation for random sequential packing of ellipses by the use of this simplified version of algorithm. In this simulation, we generated 10^6 trial ellipses throughout. Notations in this table is the same to those of Table 1. Let us investigate the value of the mean of packing density for the aspect ratio $k = 1.0$, that is, for the discs. In Table 2, this value is 0.5332. As for the random sequential packing of discs, we have already estimated, by systematic simulations, the value 0.5473 as the limiting packing density ρ (Tanemura, 1979; Tanemura, 1988). By comparing these two values, we note a good coincidence between them.

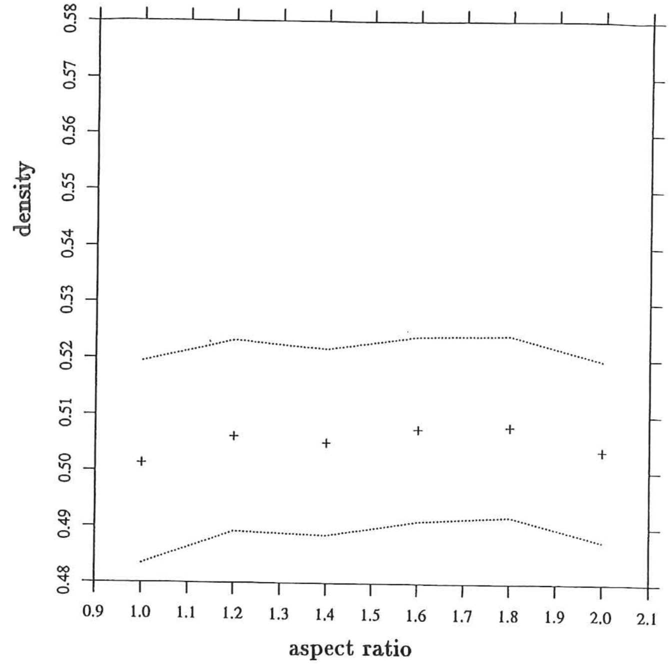

Figure 2: Plot of density vs. aspect ratio for rectangles.

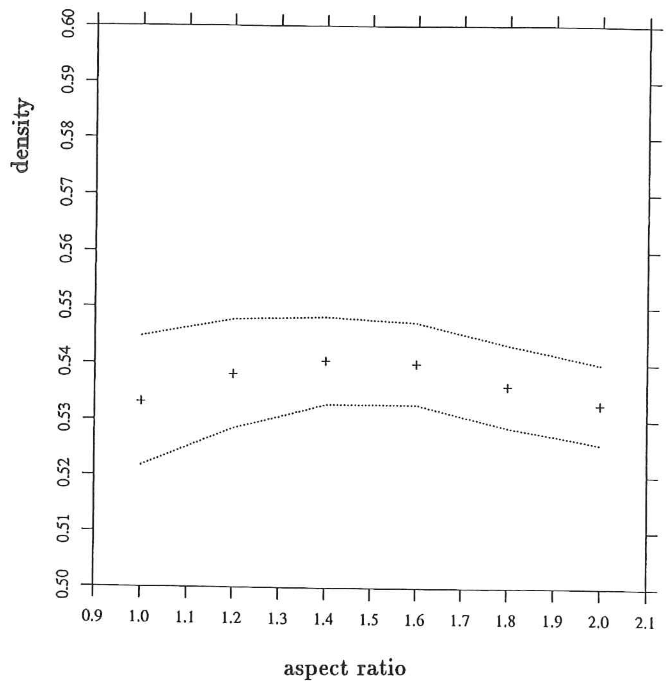

Figure 3: Plot of density vs. aspect ratio for ellipses.

Table 2: Result of computer simulation of random sequential packing of ellipses.

k	B	Sample size	$\overline{\rho}_B$	$\hat{\sigma}_\rho$
1.0	15.0×15.0	100	0.5332	0.0115
1.2	15.0×15.0	100	0.5381	0.0096
1.4	15.0×15.0	100	0.5405	0.0077
1.6	15.0×15.0	100	0.5400	0.0072
1.8	15.0×15.0	100	0.5360	0.0073
2.0	15.0×15.0	100	0.5328	0.0071

This is partly attributed to the periodic boundary condition used in this computer simulation. Although we are certain that a complete packing might not be attained in almost cases of the above simulation, we can say that a nearly complete packing of ellipses is attained in all cases. Then, the behaviour of the values of packing density against the aspect ratio k will have a meaning. Figure 3 shows the plot of packing density against the aspect ratio, corresponding to Table 2. From Fig.3, we observe a maximum of density at a certain value of k. It is interesting to point out that a similar behaviour of the packing density of ellipses is obtained by Sherwood (1990). But, rather, we would like to stress the fact that the density of random sequential packing of ellipses keeps a fairly similar value for a moderate range of aspect ratio values.

In summary, the density of random sequential packing of identical rectangles and of identical ellipses is respectively shown to be fairly invariant for a moderate range of aspect ratio.

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