Original Paper *Forma*, **16**, 327–338, 2001

Random Sequential Packing of Cuboids with Infinite Height

Yukinao ISOKAWA

Faculty of Education, Kagoshima University, Kagoshima 890-0065, Japan

(Received September 10, 2001; Accepted January 28, 2002)

Keywords: Random Packing, Rod Packing, Cuboid, Markov Chain

Abstract. This article investigates a problem of random sequential packing of cuboids each axis of which is parallel to one of the three axes of the Cartesian coordinate system. In the random packing process we find a six-dimensional Markov chain. The Markov chain gives us not only an insight into the random packing process but also an efficient algorithm. By the simulation using the algorithm we find several properties of the completely packed rods. Main findings are that the number of cuboids of each direction axe nearly equal and the packing density tends to 3/4 when the system size becomes large.

1. Introduction

Problems of packing geometrical objects have been investigated under a variety of formulations. Among them the most classical one is that of packing spheres in Euclidean spaces of various dimensions. In this problem main stream of research has focused on the densest packing, i.e. packing with the largest packing density, and on the regular packing, i.e. packing with symmetrical configuration of spheres (TÓTH, 1972; CONWAY and SLOAN, 1988). However, another stream of research has been maid for a long time. It deals with the problem of random packing of spheres which has a fundamental importance in various fields of science such as spatial patterns in ecological systems, adsorption of proteins on solid surfaces, and so on. RÉYNI (1958) first started the investigation of this problem and many researchers such as TANEMURA (1979, 1992) followed him.

Turning our attention to geometrical objects other than spheres, we find a pioneering work by O'KEEFFE (1977). They studied packing of cylindrical rods whose axes have directions among given three or four directions. Generalizing their findings, Ogawa and his collaborators (OGAWA *et al.*, 1996) have studied periodic 6-axes configuration of rods. Their main concern are not only with the packing density but also with the symmetry.

Inspired by these investigations, the author began to study a problem of random sequential packing of cylindrical rods with arbitrary directions. However it is not so easy as expected. Thus, in this paper, in order to gain an insight into the problem, the author studies a simpler problem of random packing of cuboids (rectangular parallelopipeds) each axis of which is parallel to one of the three axes of the Cartesian coordinate system.

In Sec. 2 we state the problem clearly and present a computer algorithm to obtain a complete packing of cuboids. Furthermore, introducing six state variables, we give a characterization of the complete packing. However the algorithm is not useful for understanding the nature of random packing and moreover, computation using the algorithm takes much time. By these reasons, in Sec. 3, we introduce a Markov chain that lies under the random packing process. In Sec. 4, using the Markov chain, we perform a large simulation. By such simulation we obtain several results concerning the state variables, the number of cuboids of each direction, and the packing density.

2. Random Sequential Packing of Cuboids

2.1. Formulation

Let us consider a cube of side length a $\{(x, y, z): 0 \le x, y, z \le a)$. Penetrating the cube, we pack rods at random and sequentially until no more rod can be packed. Here, by the word "rod", we mean a cuboid, i.e. rectanglar parallelopiped, whose section is a square of unit area and which has an infinite height.

In the course of packing rods we suppose two assumptions. First we assume that

(A1) axes of rods are parallel to the x-axis or y-axis or z-axis.

We call these three types of rods by x-rods or y-rods or z-rods respectively. Now let us consider an x-rod and make its intersection with a face of A which is contained in the yz-plane. Then the intersection is the square $[y, y+1] \times [z, z+1]$. In this case we say that the x-rod has coordinates (y, z). Thus any x-rod can be uniquely specified by coordinates (y, z). Similarly any y-rod and z-rod can be uniquely specified by coordinates (z, x) and (x, y) respectively. Then our second assumption is as follows:

(A2) all coordinates of rods are integers.

2.2. An algorithm of packing

Suppose that, in an intermediate stage of random packing process, we have the number N_x of x-rods, the number N_y of y-rods, and the number N_z of z-rods whose coordinates form sets

$$R_x = \{(y_i, z_i): i = 1, 2, ..., N_x\},$$

$$R_y = \{(z_i, x_i): i = 1, 2, ..., N_y\},$$

$$R_z = \{(x_i, y_i): i = 1, 2, ..., N_z\},$$

respectively. We make projections of these coordinate sets

$$R_{x,y} = \{y_i: (y_i, z_i) \in R_x\},\ \ R_{x,z} = \{z_i: (y_i, z_i) \in R_x\},$$

$$R_{y,z} = \{z_i: (z_i, x_i) \in R_y\},\ \ R_{y,x} = \{x_i: (z_i, x_i) \in R_y\},$$

$$R_{z,x} = \{x_i: (x_i, y_i) \in R_z\}, \ R_{z,y} = \{y_i: (x_i, y_i) \in R_z\}.$$

Obviously we have

$$R_x \subset R_{x,y} \times R_{x,z}, \ R_y \subset R_{y,z} \times R_{y,x}, \ R_z \subset R_{z,x} \times R_{z,y},$$

where the notation “×” denotes the operation to form the direct product of two sets.

Furthermore, setting $A = \{0, 1, 2, ..., a - 1\}$, we make sets

$$S_x = A \times A - A \times R_{y,z} - R_{z,y} \times A - R_x,$$

$$S_y = A \times A - A \times R_{z,x} - R_{x,z} \times A - R_y,$$

$$S_z = A \times A - A \times R_{x,y} - R_{y,z} \times A - R_z.$$

These sets are candidates of coordinates that are allowed for newly packed rods. Let us denote the number of elements of sets S_x, S_y, S_z by M_x, M_y, M_z respectively.

Now we state an algorithm of random sequential packing.

Step 1 Compute the numbers M_x, M_y, M_z and $M = M_x + M_y + M_z$. At the next time, we will pack an x-rod or y-rod or z-rod with probability M_x/M, M_y/M, M_z/M respectively.

Step 2 When we pack a x-rod at the next time, choose an element at random from the set S_x and pack an x-rod which has this element as its coordinates. When we pack a y-rod or z-rod at the next time, we do in a similar way.

Step 3 When we arrive at the state that no more rod can packed, our packing process stops. Otherwise we return to Step 1 and repeat both Step 1 and 2.

2.3. Complete packing

After iterating Step 1 and 2 finite times, we finally arrive at the stage that no more rod can packed. At this time we say that our packing is complete. When rods axe completely packed, a configuration of rods has a simple structure. In order to describe the configuration, we introduce six state variables

$$Y_1 = {}^{\#}R_{x,y}, \ Z_2 = {}^{\#}R_{x,z}, \ Z_1 = {}^{\#}R_{y,z}, \ X_2 = {}^{\#}R_{y,x}, \ X_1 = {}^{\#}R_{z,x}, \ Y_2 = {}^{\#}R_{z,y},$$

where the notation “#” denotes the number of elements of a set.

Then we can see easily that when rods are completely packed, all the coordinates sets R_x, R_y, R_z, are of forms of direct products,

$$R_x = R_{x,y} \times R_{x,z}, \ R_y = R_{y,z} \times R_{y,x}, \ R_z = R_{z,x} \times R_{z,y} \tag{1}$$

and moreover

$$X_1 + X_2 = Y_1 + Y_2 = Z_1 + Z_2 = a. \tag{2}$$

An example of configuration of completely packed rods are displayed in Fig. 1.

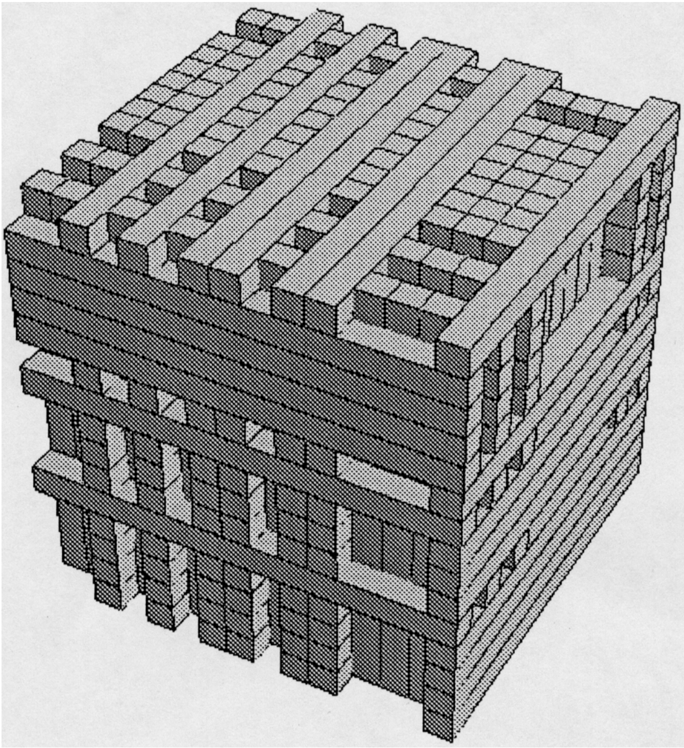

Fig. 1. An example of the configuration of completely packed rod (a = 15).

3. A Markov Chain that Underlies the Random Packing Process

3.1. Why we consider a Markov chain?

Although the assumptions (A1) and (A2) considerably simplify our random sequential packing problem, it seems difficult to understand the nature of the packing problem and to treat it rigorously by mathematical analysis. Furthermore its simulation needs a long time for large a. By these reasons we will focus our attention on a Markov chain that underlines the random packing process.

Before introducing a Markov chain, we reconsider the random packing process in some detail. First, concerning Step 1 of the algorithm, we see that

$$M_x = (a - Y_2)(a - Z_1) - N_x,$$

$$M_y = (a - Z_2)(a - X_1) - N_y,$$

$$M_z = (a - X_2)(a - Y_1) - N_z$$

and

$$0 < N_x \le Y_1Z_2,\ \ 0 < N_y \le Z_1X_2,\ \ 0 < N_z \le X_1Y_2.$$

Next we turn our attention to Step 2 of the algorithm. Let us suppose that we pack a x-rod with coordinates (y, z) at the next time. Then the following four cases will occur:

1. If $(y, z) \in (A - R_{z,y} - R_{x,y}) \times (A - R_{y,z} - R_{x,z})$, then both Y_1 and Z_2 increase by 1 at the next time.
2. If $(y, z) \in (A - R_{z,y} - R_{x,y}) \times R_{x,z}$, then only Y_1 increases by 1 and Z_2 remains unchanged at the next time.
3. If $(y, z) \in R_{x,y} \times (A - R_{y,z} - R_{x,z})$, then only Z_2 increases by 1 and Y_1 remains unchanged at the next time.
4. If $(y, z) \in R_{x,y} \times R_{x,z} - R_x$, then neither Y_1 nor Z_2 increase at the next time.

Now it can be easily seen that

$$^{\#}(A - R_{z,y} - R_{x,y}) \times (A - R_{y,z} - R_{x,z}) = (a - Y_1 - Y_2)(a - Z_1 - Z_2)$$

$$^{\#}(A - R_{z,y} - R_{x,y}) \times R_{x,z} = (a - Y_1 - Y_2)Z_2$$

$$^{\#}R_{x,y} \times (A - R_{y,z} - R_{x,z}) = Y_1(a - Z_1 - Z_2)$$

$$^{\#}(R_{x,y} \times R_{x,z} - R_x) = Y_1Z_2 - N_x$$

and

$$(a - Y_1 - Y_2)(a - Z_1 - Z_2) + (a - Y_1 - Y_2)Z_2 + Y_1(a - Z_1 - Z_2) + (Y_1Z_2 - N_x) = M_x.$$

Thus, at the next time,

1. both Y_1 and Z_2 increase by 1 with probability $(a - Y_1 - Y_2)\,(a - Z_1 - Z_2)/M_x$.
2. only Y_1 increases by 1 with probability $(a - Y_1 - Y_2)Z_2/M_x$.
3. only Z_2 increases by 1 with probability $Y_1(a - Z_1 - Z_2)/M_x$.
4. neither Y_1 nor Z_2 increase with probability $(Y_1Z_2 - N_x)/M_x$.

Now we decide to neglect the case that neither Y_1 nor Z_2 increase. Then, noting that

$$(a - Y_1 - Y_2)(a - Z_1 - Z_2) + (a - Y_1 - Y_2)Z_2 + Y_1(a - Z_1 - Z_2) = (a - Y_2)(a - Z_1) - Y_1Z_2$$

which we denote by $\tilde{M}_x$, we have

1. both Y_1 and Z_2 increase by 1 with probability $(a - Y_1 - Y_2)\,(a - Z_1 - Z_2)/\tilde{M}_x$.
2. only Y_1 increases by 1 with probability $(a - Y_1 - Y_2)Z_2/\tilde{M}_x$.
3. only Z_2 increases by 1 with probability $Y_1\,(a - Z_1 - Z_2)/\tilde{M}_x$.

When we pack y-rod or z-rod at the next time, we proceed in a similar way.

3.3. *Definition of a Markov chain*

Taking into account of the discussion stated above, we consider a sixdimensional

Markov chain

$$(X_1(t), Y_1(t), Z_1(t), X_2(t), Y_2(t), Z_2(t)); t = 0, 1, 2 \ldots$$

whose transition probabilities are defined as follows:

1. $Y_1(t+1) = Y_1(t) + 1$ and $Z_2(t+1) = Z_2(t) + 1$ and all other variables remain unchanged with probability

$$\frac{(a - Y_1(t) - Y_2(t))(a - Z_1(t) - Z_2(t))}{M(t)},$$

2. $Y_1(t + 1) = Y_1(t) + 1$ and all other variables remain unchanged with probability

$$\frac{(a - Y_1(t) - Y_2(t))Z_2(t)}{M(t)},$$

3. $Z_2(t + 1) = Z_2(t) + 1$ and all other variables remain unchanged with probability

$$\frac{Y_1(t)(a - Z_1(t) - Z_2(t))}{M(t)},$$

4. $Z_1(t+1) = Z_1(t) + 1$ and $X_2(t+1) = X_2(t) + 1$ and all other variables remain unchanged with probability

$$\frac{(a - Z_1(t) - Z_2(t))(a - X_1(t) - X_2(t))}{M(t)},$$

5. $Z_1(t + 1) = Z_1(t) + 1$ and all other variables remain unchanged with probability

$$\frac{(a - Z_1(t) - Z_2(t))X_2(t)}{M(t)},$$

6. $X_2(t + 1) = X_2(t) + 1$ and all other variables remain unchanged with probability

$$\frac{Z_1(t)(a - X_1(t) - X_2(t))}{M(t)},$$

7. $X_1(t+1) = X_1(t) + 1$ and $Y_2(t+1) = Y_2(t) + 1$ and all other variables remain unchanged with probability

$$\frac{(a - X_1(t) - X_2(t))(a - Y_1(t) - Y_2(t))}{M(t)},$$

8. $X_1(t + 1) = X_1(t) + 1$ and all other variables remain unchanged with probability

$$\frac{(a - X_1(t) - X_2(t))Y_2(t)}{M(t)},$$

9. $Y_2(t + 1) = Y_2(t) + 1$ and all other variables remain unchanged with probability

$$\frac{X_1(t)(a - Y_1(t) - Y_2(t))}{M(t)}.$$

In the above we put

$$\begin{aligned} M(t) = {} & (a - Y_2(t))(a - Z_1(t)) + (a - Z_2(t))(a - X_1(t)) \\ & + (a - X_2(t))(a - Y_1(t)) - Y_1(t)Z_2(t) - Z_1(t)X_2(t) - X_1(t)Y_2(t). \end{aligned}$$

Recalling the characterization (1) and (2) of the complete packing, we are concerned with the final state $(X_1(t), Y_1(t), Z_1(t), X_2(t), Y_2(t), Z_2(t))$ when $X_1(t) + X_2(t) = Y_1(t) + Y_2(t) = Z_1(t) + Z_2(t) = a$.

4. Results of Simulation

4.1. Method of simulation

When the author began to study the present problem, he first performed a simulation using the naive algorithm presented in Subsec. 2.2. However, even when a is as small as 100, it takes rather long time (it takes about as much as 18 hours using a PC with Athlon 1.2 GHz CPU). Thus I have abandoned the naive simulation and we decide to simulate the Markov chain introduced in the previous section, because the computation of the Markov chain is much faster than that of the naive simulation. In the following we present results of simulation of 10^6 times, and the variables $X_1(t), Y_1(t), Z_1(t)$ at the final state will be simply denoted by X_1, Y_1, Z_1.

4.2. The number of x-rod, y-rods, and z-rods

Recalling the characterization (1) and (2) of the complete packing, we can see that

$$N_x = Y_1(a - Z_1), \quad N_y = Z_1(a - X_1), \quad N_z = X_1(a - Y_1).$$

About the state variables X_1, Y_1, Z_1 our simulation gives the following results:

1. Figure 2 displays a graph with a as abscissa and the mean of X_1 as ordinate. The straight line denotes the graph of a linear function $a/2$. Similar results hold for the means

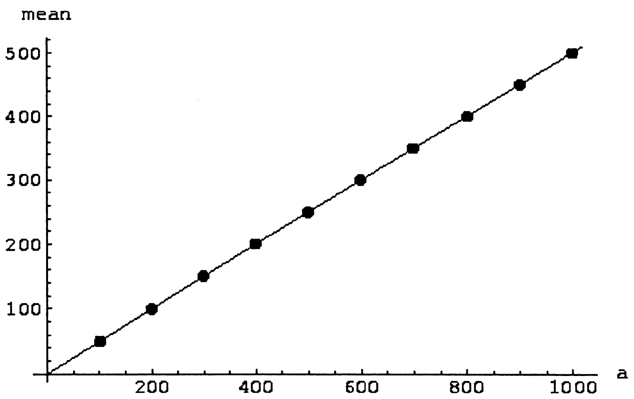

Fig. 2. The mean of X_1. The straight line denotes the graph of a linear function $a/2$.

of Y_1 and Z_1.

2. Figure 3 displays a graph with a as abscissa and the variance of X_1 as ordinate. The straight line denotes the graph of a linear function of a. Similar results hold for the variances of Y_1 and Z_1.

3. The correlation between X_1 and Y_1, that between Y_1 and Z_1 and that between Z_1 and X_1 are all nearly equal to a constant which do not depend on a.

These experimental results strongly suggest that

$$\begin{cases} E(X_1) = E(Y_1) = E(Z_1) = \dfrac{a}{2}, \\ Var(X_1) = Var(Y_1) = Var(Z_1) = k_1 a, \\ Corr(X_1, Y_1) = Corr(Y_1, Z_1) = Corr(Z_1, X_1) = -k_2, \end{cases} \tag{3}$$

where the symbol E denotes expectation, Var denotes variance, $Corr$ denotes correlation, and k_1, k_2 are positive constants (k_1 is about 0.28 and k_2 is about 0.39). Hence, noting that

$$\begin{aligned} E(N_x) &= E(Y_1(a - Z_1)) \\ &= a \cdot E(Y_1) - Corr(Y_1, Z_1)\sqrt{Var(Y_1)}\sqrt{Var(Z_1)} - E(Y_1)E(Z_1), \end{aligned}$$

we have

$$E(N_x) = \frac{a^2}{4}\left(1 + \frac{4k_1k_2}{a}\right). \tag{4}$$

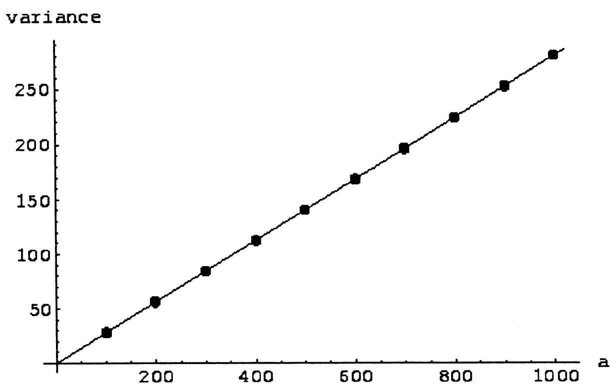

Fig. 3. The variance of X_1. The straight line denotes the graph of a linear function k_1a where k_1 is about 0.28.

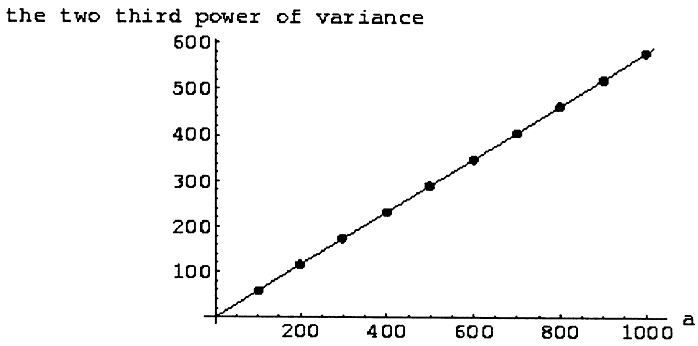

Fig. 4. The 2/3-th power of the variance of N_x. The straight line denotes the graph of a linear function of k_3a where k_3 is about 0.58.

Thus we see that when a grows, the ratio of the mean N_x to a^2 gradually tends to 1/4. Furthermore our simulation also shows the following:

Figure 4 displays a graph with a as abscissa and the 2/3-th power of the variance of N_x as ordinate. The straight line denotes the graph of a linear function of a. Similar results hold for N_y and N_z.

This suggests the fact

$$Var(N_x) = Var(N_y) = Var(N_z) = k_3a^{3/2} + o(a^{3/2}) \tag{5}$$

where k_3 is a positive constant and $o(a^{3/2})$ denotes a term whose order is lower than $a^{3/2}$. From Eqs. (4) and (5) we obtain

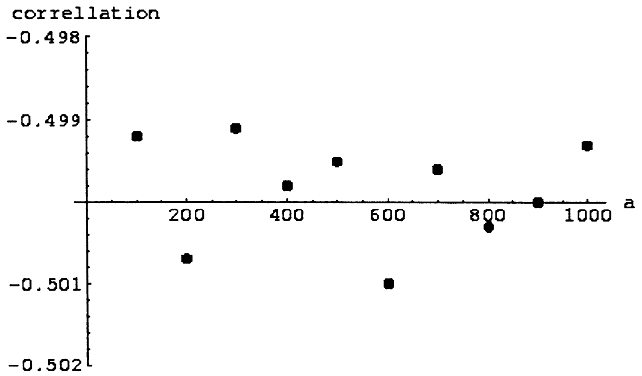

Fig. 5. The correlation between N_x and N_y. The horizontal line denotes the graph of a constant function (–1/2).

$$\lim_{a\to\infty}\frac{N_x}{a^2}=\lim_{a\to\infty}\frac{N_y}{a^2}=\lim_{a\to\infty}\frac{N_z}{a^2}=\frac{1}{4}. \tag{6}$$

About the correlation between N_x and N_y, our simulation shows the following result: Figure 5 displays a graph with a as abscissa and the correlation between N_x and N_y as ordinate. The horizontal line denotes the graph of a constant function (–1/2). Similar results hold for the correlation between N_y and N_z, and that between N_z and N_x.

Thus we can see that

$$Corr\left(N_x, N_y\right)=Corr\left(N_y, N_z\right)=Corr\left(N_z, N_x\right)=-\frac{1}{2}. \tag{7}$$

4.3. Packing density

Let us denote the packing density of rods by p. Obviously

$$p=\frac{N_x+N_y+N_z}{a^2}.$$

From Eq. (4) it immediately follows that

$$E(p)=\frac{3}{4}+\frac{3k_1k_2}{a}. \tag{8}$$

Moreover, by Eq. (6), we obtain

$$\lim_{a\to\infty} p=\frac{3}{4}. \tag{9}$$

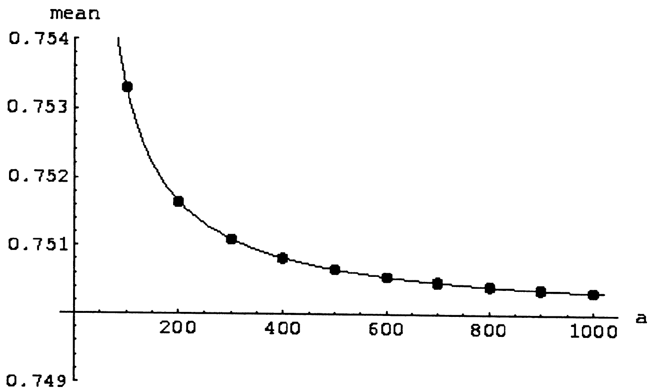

Fig. 6. The mean of p. The solid line denotes the graph of a function $3/4 + k_4/a$ where k_4 is about 0.33.

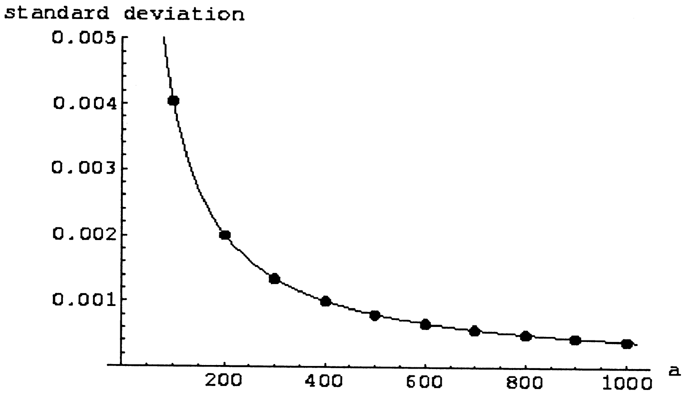

Fig. 7. The standard deviation of p. The solid line denotes the graph of a function k_5/a where k_5 is about 0.40.

The conclusion (9) can be also verified directly by simulation:

1. Figure 6 displays a graph with a as abscissa and the mean of p as ordinate. The solid line denotes the graph of a function $3/4 + k_4/a$ where k_4 is about 0.33.

2. Figure 7 displays a graph with a as abscissa and the standard deviation (the square root of the variance) of p as ordinate. The solid line denotes the graph of a function k_5/a where k_5 is about 0.40.

It is interesting to see that the packing density 3/4 is identical to that of the densest regular packing with 3-axes which has been studied in Ogawa and his collaborates (OGAWA *et al.*, 1996).

5. Conclusion

By this research we make two findings. One is that, under the packing process of cuboids, there lies a Markov chain. Using the Markov chain we can obtain some insight into the original packing process on one hand, and on the other hand, we can carry out more efficient simulation than simulation by a naive packing algorithm.

Second finding is about configuration of completely packed rods and as follows:

1. Coordinates sets of x-rods, y-rods, and z-rods have forms of a rectangle of sides Y_1, $a - Z_1$, that of sides Z_1, $a - X_1$, and that of sides X_1, $a - Y_1$ respectively. All the means of X_1, Y_1, Z_1 are equal to $a/2$.
2. When a is large, all the mean numbers of x-rods, y-rods, and z-rods are nearly equal each other and equal to $a^2/4$. Their deviations from $a^2/4$ are of order a $a^{3/2}$.
3. When a is large, the packing density is nearly equal to 3/4. Its deviation from 3/4 is of order a^{-1}.

REFERENCES

CONWAY, J. H. and SLOANE, N. J. A. (1988) *Sphere Packings*, Lattices and Groups, Springer-Verlag, New York.

OGAWA, T., TESHIMA, Y. and WATANABE, Y. (1996) Geometry and crystallography of self-supporting rod structures, in *KATACHI U SYMMETRY*, pp. 239–246, Springer-Verlag, Heidelberg.

O'KEEFFE, M. (1977) Rod packings and crystal chemistry, *Acta Cryst*., **A33**, 914–923.

RÉNYI (1958) On a one-dimensional problem concerning random space filling, *Publ. Math. Inst. Hung. Acad. Sci*., **3**, 109–127.

TANEMURA, M. (1979) On random complete packing by discs, *Ann. Inst. Stat. Math*., **31B**, 351–365.

TANEMURA, M. (1992) Models and simulations of random structures of particles, *Acta Stereol*., **II**/Suppl., 41–52.

TÓTH, L. F. (1972) *Lagerungen in der Ebene, auf der Kugel und im Raum*, Springer-Verlag, Heidelberg.