Abstract

Title of Thesis: **An Analysis of the Dense Packing of Hard Disks**

—A Computer Simulated Approach.

Jir-Yih Tsaur, Master of Science in Mechanical Engineering, 1988.

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This thesis is concerned with the analysis of dense packing of hard disks. The Voronoi diagram and the geometric neighbours were first computed. The average number of geometric neighbours of a disk is six. It is thus more efficient to choose structural neighbours from among the geometric neighbours than from among all other disks.

Through the Monte Carlo simulation by Rosato et. al., disk configurations after pouring and subsequent shaking were provided for analysis. The mean number of geometric neighbours and the average coordination number were computed. The angular distribution of the structural neighbours was discussed. The packing fraction increases with number of shakes in a linear relationship. It seems to be packing into an ordered close packing after continued shaking.

A configuration constrained by two rigid vertical walls was analyzed. It was found the packing fraction is smallest in the vicinity of the wall and increased asymptotically to the mean packing fraction when moving away from the wall.

An Analysis of the Dense Packing of Disks —A Computer Simulated Approach

by
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To dear dad and mom.

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1 Introduction

1.1 Motivation and Literary Survey

The study of packing of spheres and disks have been of interest for modelling the structure of granular materials, liquids and glasses. A survey on related research which gives rise to the work in this thesis is presented in this Chapter.

1.1.1 The Packing of Spheres

Dated as early as 1929, the three-dimensional packing of homogeneous spheres was studied by W. O. Smith et. al. [50]. And, as late in 1983, J. G. Berryman [13] presented his definition on random close packing and found the critical packing fraction for random close packing of both spheres and disks.

J. D. Bernal [9] studied the structure of liquids by viewing it as a "heap" of particles of the same size. A liquid in Bernal's original postulate [10] was homogeneous, coherent and essentially irregular, as contrasted with a crystal, which may be called a "pile" of molecules, regularly arranged. In respect to order, a liquid is different from a crystal and resembles a gas. On the other hand, with respect to density, a liquid would resemble a crystal and differ from a gas.

Through an experiment, Bernal simulated a liquid by a heap of spheres, a close arrangement of particles, where each is in contact with a large number of others but not in any regular way. He calculated the packing density and the average number of geometric neighbour for the model he created. The packing densities were calculated to be 0.637 for random close packing and 0.60 for random loose packing, as compared to 0.74 for ordered close packing. And, the average number of geometric neighbours was calculated to be 13.6 as compared to 12 for ordered close packing.

Bernal defined the structural neighbours as those having their centroids within 1.05 diameter away from each other. The tolerance 0.05 was experimentally determined in the following procedure by Bernal. A number of steel ball bearings having a light coating of grease were packed in a balloon. Paint was then poured through the bearings. The paint was left, held by surface tension where the balls touched or nearly touched. When the paint was dry and the balloon removed, the spheres within 5% of a diameter away from each other had a dot or a ring formed at the place where they were in *contact*. By counting number of dots or rings on the surface of a sphere, the number of structural neighbours for the sphere, or the *coordination number*, was found.

Further, W. B. Haines and G. Mason [26,32] modeled the pore space in soils and rocks. J. L. Finney [19] modeled the structure of amorphous metals and alloys. C. A. Angel et. al. [4] studied the formation of glasses and gave a survey of computer experiments. D. P. Haughey [27] studied the voidage variation in equal-sized spheres and provided a review of earlier experiments on the packing of spheres. And, J. G. Berryman [11] studied the flow through aggregates of spheres.

More literature can be found in [3], [37], and [1]. For example, S. Nemat-Nasser et. al. [38] used a sample model in an experiment and found that particle rolling instead of particle sliding is the major microscopic deformation mechanism. S. B. Savage et. al. [18] derived the general conservation equations for the rapid flow of a binary mixture of smooth, inelastic, spherical granular particles following the approach of the kinetic theory for mixtures of dense gases.

Other studies of sphere packing exist in the literature, including computer- simulations and theoretical model. They are listed in the Reference and will not be discussed respectively here.

1.1.2 The Packing of Disks

While much work exists on the packing of spheres, the literature is not as extensive with regard to the nature of the structure of the packing of disks. The exact nature of disk packings is not as well understood as its three-dimensional counterpart. There seems to be no analogue to the concept of "loose" and "close" packings with regard to disks as there is for spheres. Disk packings are generally used as a model for monolayer structures.

G. T. Barnes et. al. [6] used packing of disks as a model to study the covering of a liquid surface by surfactant molecules, enabling the rate of evaporation through the "holes" in the surface layer to be deduced. The model of Barnes pictured the monolayer on the surface of water as an array of randomly placed hard disks on a plane surface, and the evaporating water molecules as hard spheres. The model assumed that water molecules could penetrate a monolayer only when void larger than a water molecule appeared in the monolayer, and that water evaporates through these voids at the usual rate for a free surface. Thus, the reduction of evaporation rate caused by a monolayer is simply a consequence of the reduction of voids in the monolayer. After obtaining the void area, Barnes calculated the evaporation/condensation rate.

Krishna K. Pillai [39] used packed disks as a model to find the cross sectional voidage variation in the vicinity of a wall for a packed bed of particles. Hard disks were used in an experiment to simulate the particles, which would appears as a monolayer of spheres and have the same front view as that of a disk model. When considering heat conduction between particles along the bed, it is necessary to know the cross-sectional area of solids perpendicular to the direction of heat flow. Though the average void fraction within the bed can be calculated, the existence of a constraining wall will alter the particle packing on the cross-sectional area of the solid in the vicinity of the wall. Through Pillai's model, the packing fraction of a cross-section at some distance x away from the wall can be calculated. A packing fraction versus x relationship was derived, which could be described by a curve oscillating in the vicinity of the wall, damped and converging to a mean value at approximately three diameters away from the wall.

Using the fact that the packing density variation near the wall is almost the same as that about a central sphere in the interior, Tory et. al. [23] introduced the molecular pair-correlation function to explain the variation in the local packing density. The results obtained agree with that of Pillai's discussed in the previous paragraph fairly well.

Quickenden and Tan [41] simulated monolayer structures using a method proposed by Stillinger et. al. [51]. This was done by randomly placing homogeneous disks on an isotropically stretched and subsequently contracted rubber film. The process modeled the compression of a monolayer on a liquid surface. The packing fraction of the disks increased with the contraction of the rubber film rapidly until a value of 0.83 was reached, after which it increased slowly and asymptotically to the value of 0.906 for a ordered close packing. It is interesting that the packing fraction of 0.83 is close to that at the phase transition, which occurs when monolayers of long chain acids or alcohols on a water surface are compressed from the liquid-condensed to the solid phase. Quickenden and Tan thus declared that it is possible to explain and calculate the position of the change from the solid to the liquid-condensed phase, purely on the basis of an array of non-interacting disks.

Following the same idea from Stillinger, Mason [33] modeled a two-dimensional packing of disks through computer simulation. Instead of contracting the coordinate system or moving the disks toward a point inside the packing, Mason kept the disks at the same coordinates and increased their size to densify the packing. Consequently, this technique produced several disks overlapping each other which is mechanically impossible for inelastic hard disks. Two disks in a overlapping pair were then moved equally apart along the line of their centers until they are just touching. This process, called *shuffling* by Mason, was repeated until no disk remained overlapped. Mason achieved the same result as Quickenden and Tan, i.e., an ordered close packing would finally be formed.

1.2 Objectives and Methods

The packing structures of assemblies of disks are analyzed. They are created via a Monte Carlo computer simulation developed by Rosato et. al [42]. A *locus method* which solves many proximity problems in computational geometry, the Voronoi diagram [58], is applied to find geometric neighbours for each disk. An algorithm originated from the one constructed by Kurt E. Brassel and Douglas Reif [14] is chosen to create the Voronoi diagram. The algorithm is implemented in Pascal because the language facilitates the handling of dynamic data structures and recursive subroutine calls. The distribution of the number of geometric neighbours possessed by a disk is computed. The average number is found to be exactly six.

Following the convention of J. D. Bernal, we define disks having their centroids within 1.05 diameter apart from each other as structural neighbours. Structural neighbours are chosen for each disk from among its geometric neighbours, which is more efficient than from among all other disks in the configuration. The distribution of the number of structural neighbours possessed by a disk, the coordination number is calculated.

Included among the geometric neighbours also is a nearest neighbour (Theorem 2, Appendix A), which is nearest to the center disk among all geometric neighbours. In case of a dense packing, which is the topic of this thesis, it is also true that the nearest neighbour is in touch with the center disk. Therefore, the nearest neighbour of a disk can be found within a even smaller subset composed of the structural neighbours. The cumulative probability of nearest neighbour radii is obtained and gives the median nearest neighbour radius.

A vector is extended from the center disk to each of its structural neighbours. An angle, which is called *structural neighbour angle* is associated with each of the vectors. For a group of disks having M structural neighbours, where M is less than or equal to six, the frequency distribution for each of the M angles is found, from which, the mean and deviation are calculated. Finally, Packing fractions are computed for all assemblies and the variation of the packing fraction in the vicinity of a wall is determined.

1.3 Outline of Chapters

Chapter Two introduces the Voronoi diagram. A variety of proximity related problems which can be solved by Voronoi diagram are discussed. The B-R method is described, which is applied to construct the Voronoi diagram.

Random close packing of hard disks is then discussed in Chapter Three. Definitions and relations are presented. The radial distribution function is introduced, which gives a better understanding of the concept of randomness. The Monte Carlo simulation is described and its output is analyzed.

The Summary and Conclusion are given in Chapter Four. The Appendix contains definitions and properties regarding Voronoi diagram, simplified flow charts for the algorithm finding next geometric neighbour and completing the Voronoi diagram, and the program *disk.pas*.

2 Voronoi Diagram

The Voronoi diagram is applied to find geometric neighbours for each disk. From the geometric neighbours, structural neighbours and the nearest neighbour can be selected efficiently. Various algorithms exist for the creation of the Voronoi diagram [15,30,48]. The algorithm by Kurt E. Brassel and Douglas Reif [14] is chosen and will be discussed in section 2.2.

2.1 Proximity Problems

Geometric objects, such as points, circles, and spheres, are sometimes used to model physical entities in the real world. In some cases we would like to have access to a suitable neighbourhood of the objects. For instance, in air traffic control it is important to keep track of the closest two aircrafts. In studying the configuration of an ensemble of granular particles, like liquid, or powdered materials, knowing the local environment of each particle as well as properties is desirable. The above are examples of proximity related problems. Some typical problems in this discipline [29] are listed below:

- (*Closest pair*): Given n points in the plane, find two points that are closest.
- (*All nearest neighbours*): Given n points in the plane, find for each point a nearest neighbour (other than itself).
- (*Euclidean minimum spanning tree, EMST*): Given n points in the plane, find a tree that interconnects all the points with minimum total edge length.

- (*Triangulation*): Given n points in the plane, construct a planar graph on the set of points such that each bounded polygon within the convex hull of the n points is a triangle.

- (*Nearest neighbour search*): Given n points in the plane (with preprocessing allowed), find the nearest neighbour of a query point. This problem is also known as the "post office problem".

- (*k Nearest neighbours search*): The same as the nearest neighbour search problem, except that the k nearest neighbours are sought.

All the above listed kinds of problems can be solved by resorting to the *locus method*—the Voronoi diagram.

2.2 The B-R Method

The algorithm constructed by Kurt E. Brassel and Douglas Reif, hence termed the B-R Method, is chosen for the creation of the Voronoi diagram. In viewing the Voronoi diagram, a *Box* was first fixed. The computation of Voronoi diagrams uses an iterative walking process, whereby the processing starts at the lower left corner of the diagram. The use of a sorted array of linked list of points provides for a dynamic data structure and efficient processing.

2.2.1 Sorting

Given an set S of n points $\{p_1, p_2, \cdots, p_n\}$, we first sort it in lexicographical order. A point $p_1(x_1, y_1)$ is lexicographically less than a point point $p_2(x_2, y_2)$ if and only if either one of the following condition is satisfied:

1. $x_1 < x_2$.

2. $x_1 = x_2$ and $y_1 \leq y_2$.

To access a point/points within a range, only this particular range will be searched. All data out of this is neglected.

A *merge sort* algorithm by Sedgewick [46] was applied in the sorting process. The running time of the merge sort is of order $n \log n$ as opposed to the n^2-order of the *insertion sort*, *selection sort*, or *bubble sort*.

2.2.2 Fixing the Viewing Box

In viewing the Voronoi diagram, we fix a *Box* containing all the centroids of the given set of disks.

Definition 1 *The viewing box for the Voronoi diagram of a disk set S is the region:*

$$\begin{aligned} Box \equiv \{(x,y) \mid \;\; & x_{min} - BoxC \cdot D_{max} \leq x \leq x_{max} + BoxC \cdot D_{max}; \\ & y_{min} - BoxC \cdot D_{max} \leq y \leq y_{max} + BoxC \cdot D_{max}\} \end{aligned}$$

in which x_{min}, x_{max}, y_{min} and y_{max} are minimum and maximum coordinates of the centroids of the disks in S, D_{max} is the maximum diameter of the disks, and $BoxC$

is a selected constant.

The choice of the constant $BoxC$ introduces slight differences in the number of "unbounded" Voronoi polygons on the boundary of the Voronoi diagram. The larger the constant $BoxC$, the smaller will be the number of unbounded Voronoi polygons on the boundary of the Voronoi diagram. A minimum number of unbounded Voronoi polygons on the boundary of the Voronoi diagram, which is exactly the number of disks with centroids located on the convex hull of the disk set, will result when the constant $BoxC$ reaches $BoxC_{l.b.}$, its lower bound.

As an example, let a set of 14 disks be given with $D_{max} = 1$ unit and $xmin = 1.5$, $xmax = 9$, $ymin = 1$, and $ymax = 9.2$. If the value of 1 is selected for the constant $BoxC$, according to Definition 1, the viewing box will be defined by the lines: $x = 0.5$, $x = 10$, $y = 0$, and $y = 10.2$ as shown in Figure 1. If the value of 10 is selected for the constant $BoxC$, the viewing box will then be defined by: $x = -8.5$, $x = 19$, $y = -9$, and $y = 19.2$ as shown in Figure 2. Refer to Figures 1 and 2 the unbounded Voronoi polygons are identified as those having an edge lying on the edges of the viewing box. The diagram in Figure 2 has 9 unbounded Voronoi polygons, while the diagram in Figure 1 has 10 unbounded Voronoi polygons.

It is desirable to generate a Voronoi diagram which contains only Voronoi points at the neighbourhood of the configuration. This is achieved by assigning a small value, a value of 1 for example, for the constant $BoxC$ in Definition 1, and by adding some dummy points to the query point in each processing loop discussed in the following

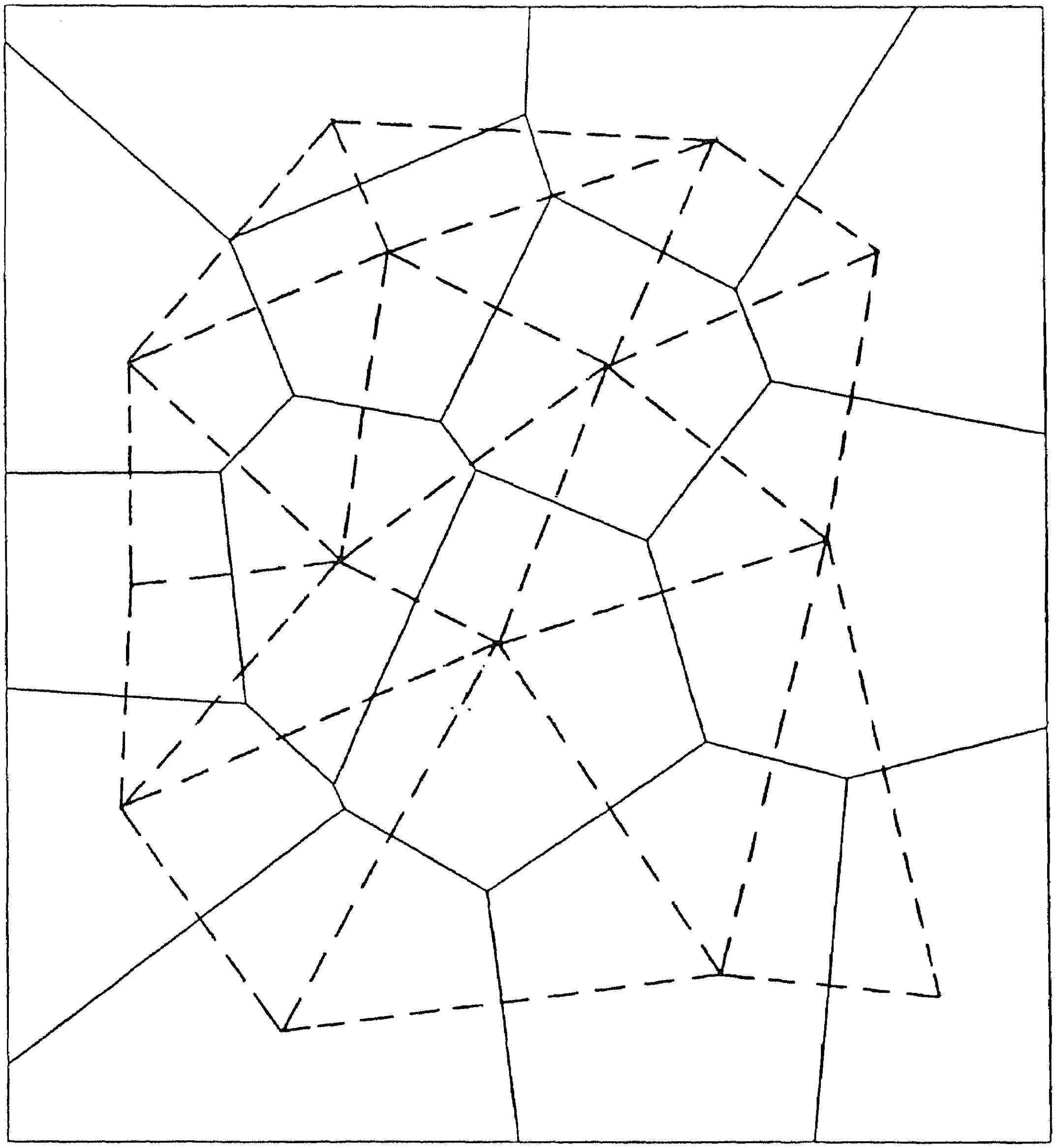


Figure 1: The Voronoi diagram and Delaunay triangulation of 14 disks with a selected value of 1 for the constant $BoxC$.

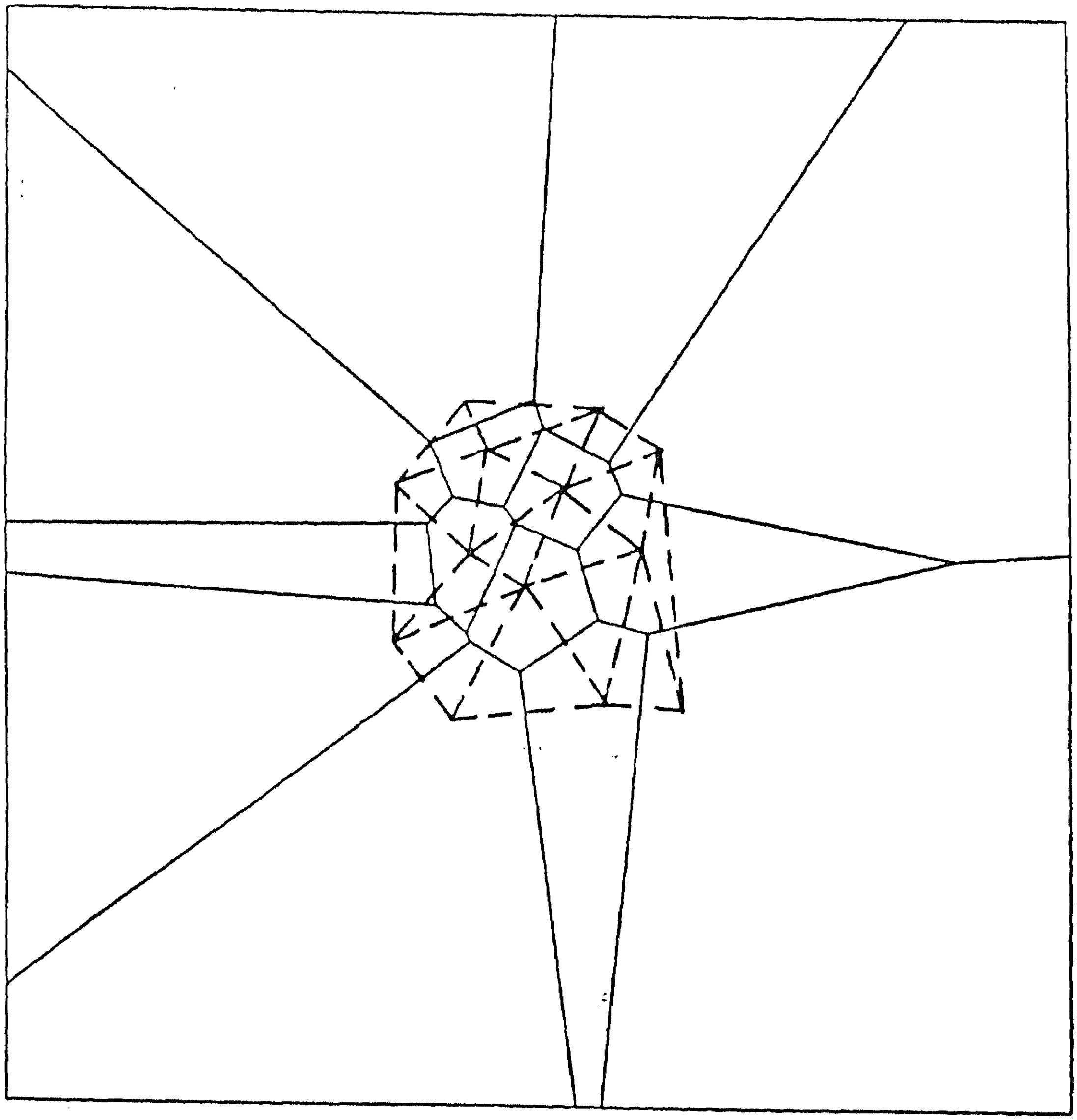


Figure 2: The Voronoi diagram and Delaunay triangulation of 14 disks with a selected value of 10 for the constant *BoxC*.

section.

2.2.3 Processing Loop

Beginning with the set of disk center coordinates, a set of points, the box is fixed as previously described and the processing loop begins. The point nearest to the lower left corner of the box, point A in Figure 3, is selected as the query point in the first loop. Some assignment are executed before the first loop commences.

Four dummy points dummy1, dummy2, dummy3, and dummy4 are introduced so that the perpendicular bisectors between point A and the four dummy points coincide with the four edges of the viewing box. In Figure 3 it can be seen that dummy4 and dummy1 are neighbours of point A, and V_0 is a vertex of Voronoi polygon about point A. Further searching for the next clockwise neighbour, i.e., the next neighbour clockwise to dummy1 will be performed in the loop as described in the following.

The procedure to search for the next clockwise neighbour is based on the following properties given in Appendix A.

- Corollary 1 — Voronoi polygon are always star-shaped.

- Corollary 2 — For a point having a bounded Voronoi polygon, the next clockwise neighbour is always located in the right half plane of the vector from the query point to the present neighbour. (By the introduction of the four dummy points, Voronoi polygons associated with the given set of points are all bounded.)

- Lemma 3 — A point p equidistant to three points p_i, p_j, and p_k is a true Voronoi

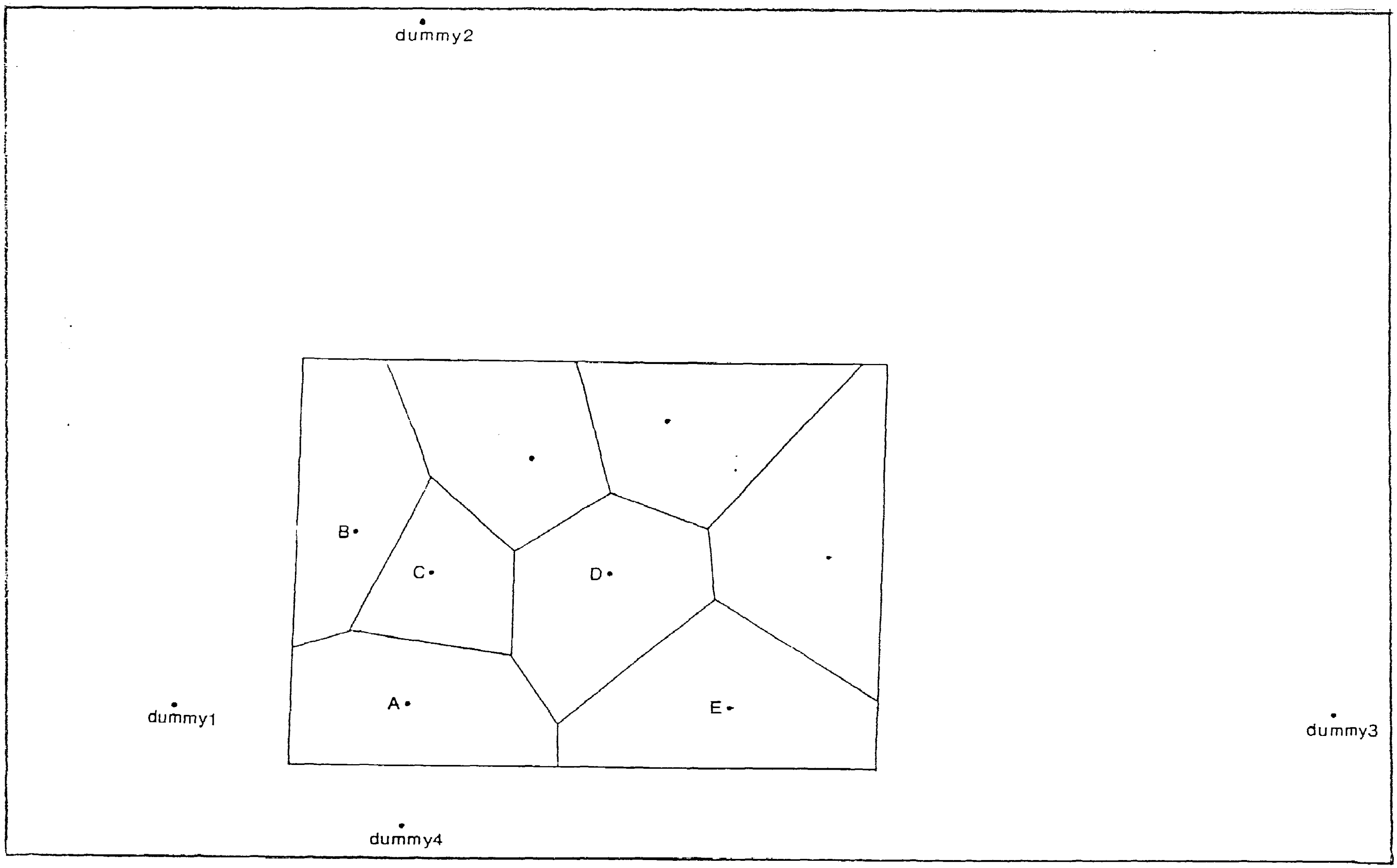


Figure 3: Geometric neighbours and dummy points associated with point A, the first point processed.

point if no other point is located within a circle centered at point p with radius the distance from point p to either one of the three points p_i, p_j, and p_k.

Based on the three properties, we use the following strategy in the processing loop finding the remaining geometric neighbours of a disk. Take disk A for example, in which dummy4 and dummyl were two geometric neighbours and V_0 was one Voronoi point already known; dummy4 is predefined as $NbrFirst[1]$[1], dummyl is predefined as $NewNbr$[2]:

1. Define the two half planes $E_r(A, NewNbr)$ and $E_l(A, NewNbr)$, such that $E_r(A, NewNbr)$ is the right half plane of vector $\overrightarrow{A\,NewNbr}$. $E_l(A, NewNbr)$ is the left half plane of vector $\overrightarrow{A\,NewNbr}$.

2. Assign the first clockwise dummy point in the right half plane $E_r(A, NewNbr)$ as the potential new neighbour, denoted $PNewNbr$, of A. Find the point V equidistant to A, $NewNbr$, and $PNewNbr$ by intersecting perpendicular bisectors $B(A, NewNbr)$ and $B(NewNbr, PNewNbr)$. V is termed the potential new vertex. A, $NewNbr$, and $PNewNbr$ form a circle (V, R) with center V and radius R.

3. Search for point P' among the given point set, which is both in the right half plane $E_r(A, NewNbr)$ and inside the circle (V, R). If such a point P' exists,

[1] The symbol $NbrFirst[k]$ will be used for the first geometric neighbour found for the kth query disk undergoing processing.

[2] The symbol $NewNbr$ will be used for the new geometric neighbour found for the disk undergoing processing.

assign P' as the $PNewNbr$, calculate potential new vertex V' and new radius R', where $R' < R$.

4. Repeat Step 3 until there is no point in the given point set which is both in the right half plane $E_r(A, NewNbr)$ and in the circle (V, R), or (V', R') if exists. Then, declare $PNewNbr$ as $NewNbr$ and V' as the new vertex.

5. Redefine half planes $E_r(A, NewNbr)$ and $E_l(A, NewNbr)$. Repeat Steps 2, 3, and 4 until a complete walk around A is completed; i.e., until a $NewNbr$ is identical with $NbrFirst[1]$, the first neighbour of the query point A. At this point, all geometric neighbours of point A have been computed.

Following the above strategy and referring to Figure 3, the geometric neighbours of point A are calculated in the following sequence:

1. Dummy4 is known as the first neighbour and dummy1 is known as $NewNbr$. Define half planes $E_r(A, dummy1)$ and $E_l(A, dummy1)$.

2. Select dummy2 as the $PNewNbr$. Compute V_6 and R by intersecting bisectors of $\overline{A\, dummy1}$ and $\overline{A\, dummy2}$. Search for a point among given point set which both lies in $E_r(A, dummy1)$ and in the circle (V_6, R). The search is in the lexicographical order indicated by the dashed line in Figure 3. Since B is both in $E_r(A, dummy1)$ and (V_6, R), it is assigned the $PNewNbr$. Compute V_1 and R'. As no other point is within (V_1, R'), B is declared as the $NewNbr$, and V_1 the new vertex.

3. Redefine half planes $E_r(A,B)$ and $E_l(A,B)$. Again, the $PNewNbr$ starts from dummy2. Compute (V,R). Find C within $E_r(A,B)$ and (V,R). Assign C to be the $PNewNbr$, compute (V_2,R'). Since there is no point within (V_2,R'), declare C as the $NewNbr$, V_2 the new vertex.

4. Redefine half planes $E_r(A,C)$ and $E_l(A,C)$. This time the $PNewNbr$ starts from dummy3. Compute (V,R). Find F as the second $PNewNbr$, compute (V',R'). Find D within $E_r(A,C)$ and (V',R'), assign D the $PNewNbr$, compute (V_3,R'). No point exists in (V_3,R'). Declare D as the $NewNbr$, V_3 the new vertex.

5. Redefine half planes $E_r(A,D)$ and $E_l(A,D)$. Select dummy3 as the first $PNewNbr$, compute (V,R). Find E both lies in $E_r(A,D)$ and (V,R), assign E the $PNewNbr$, compute (V_4,R'). No other point lies in (V_4,R'), E is declared the $NewNbr$, and V_4 the new vertex.

6. Redefine half planes $E_r(A,E)$ and $E_l(A,E)$. Dummy4 is assigned the first $PNewNbr$, (V_5,R) are computed. No point in the given point set lies in (V_5,R), dummy4 is declared the $NewNbr$.

7. Now that the $NewNbr$ is identical with $NbrFirst$, a completed walk around point A has been completed; i.e., the Voronoi polygon about point A has been constructed.

Because each vertex V_i pertains to three Voronoi polygons, all neighbourhood relationships are mutual. Once a vertex is found, it is stored and the mutual relationships among the centroids involved are recorded in a bookkeeping process. Referring to Figure 3 again, when point B was found as a geometric neighbour of point A, with a common Voronoi point V_1 among points A, dummy1, and B, point A was also recorded as a geometric neighbour of point B. And, when point C was found as the next geometric neighbour of point A, with a common Voronoi point V_2 among points A, B, and C, point C is also recorded as a geometric neighbour of point B. When the first loop ceases, five records exist in the bookkeeping and record geometric neighbours for points A, B, C, D, and E.

Once the first loop which processes point A has been completed, point B, the first *non-dummy* geometric neighbour of point A is processed next. The processes continue until all points have been processed and the Voronoi diagram completed. Consider the eight points in Figure 4, the complete process is tabulated in the following. Whenever a new vertex V_i is found, the bookkeeping for the three related centroids will be modified and appear in bold face in the table. Though dummy points are also shown for better understanding of the complete mutual relationship, they will not be recorded in the bookkeeping. Also, a centroid or vertex which has previously been recorded will not be recorded in duplicate and will be put in a pair of parentheses.

V_0: **A — dummy4, dummy1**

dummy4 — dummy1, A

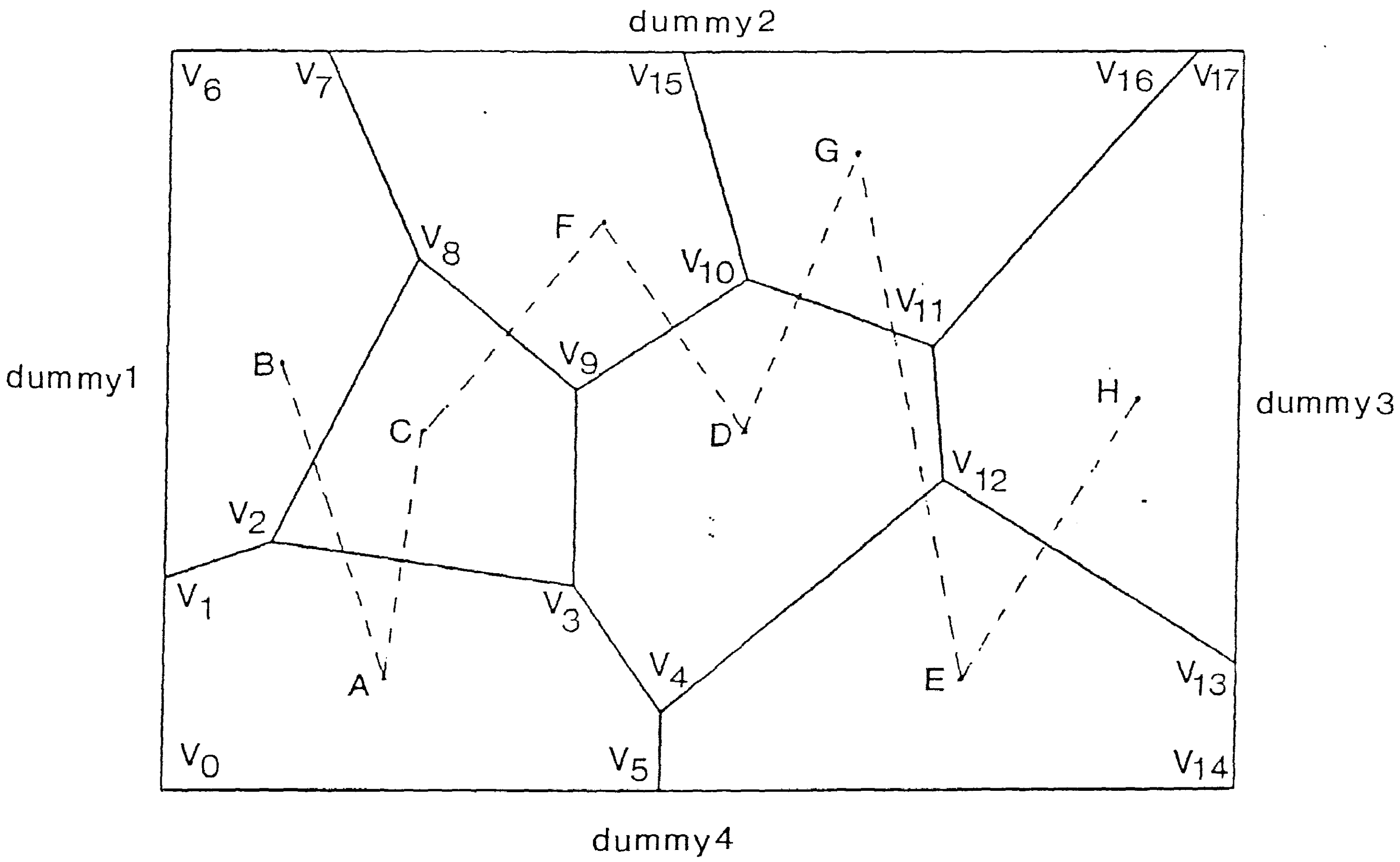


Figure 4: An ensemble of 8 disks.

dummy1 — A, dummy4

V_1: **A** — dummy4, **dummy1, B**

dummy4 — dummy1, A

dummy1 — B, A, dummy4

B — A, dummy1

V_2: **A** — dummy4, dummy1, **B, C**

dummy4 — dummy1, A

dummy1 — B, A, dummy4

B — C, A, dummy1

C — A, B

V_3: **A** — dummy4, dummy1, B, **C, D**

dummy4 — dummy1, A

dummy1 — B, A, dummy4

B — C, A, dummy1

C — D, A, B

D — A, C

V_4: **A** — dummy4, dummy1, B, C, **D, E** dummy4 — dummy1, A

dummy1 — B, A, dummy4

B — C, A, dummy1

C — D, A, B

D — **E, A,** C

E — **A, D**

V_5: **A** — dummy4, dummy1, B, C, D, **E, (dummy4)**

dummy4 — dummy1, **A, E**

dummy1 — B, A, dummy4

B — C, A, dummy1

C — D, A, B

D — E, A, C

E — **dummy4, A,** D

(**dummy4** — **A, E**)

Now that the $NewNbr$ dummy4 was the first neighbour, the geometric neighbours of A have all been found and the Voronoi polygon about A has been completed. The first geometric neighbour of point A is now to be processed. By skipping the dummy points dummy4 and dummy1, we choose point B with known neighbours C and A, where C is the first neighbour and A is the $NewNbr$. Shift the dummy point to new positions such that the bisectors of the dummy points and B generate the four edges of the viewing box. To continue:

(V_1): **B** — C, **A, dummy1**

C — D, A, B

D — E, A, C

E — A, D

(**A — dummy1, B**)

dummy1 — B, A

V_6: **B** — C, A, **dummy1, dummy2**

C — D, A, B

D — E, A, C

E — A, D

dummy1 — dummy2, B, A

dummy2 — B, dummy1

V_7: **B** — C, A, dummy1, **dummy2, F**

C — D, A, B

D — E, A, C

E — A, D

dummy1 — dummy2, B, A

dummy2 — F, B, dummy1

F — **B, dummy2**

V_8: **B** — C, A, dummy1, dummy2, **F, (C)**

C — D, A, **B, F**

D — E, A, C

E — A, D

dummy1 — dummy2, B, A

dummy2 — F, B, dummy1

F — **C, B,** dummy2

(**C** — **B, F**)

The Voronoi polygon about B is now completed. Now, start processing C with known neighbours D, A, B, and F.

V_9: **C** — D, A, B, **F, (D)**

D — E, A, **C, F**

E — A, D

F — **D, C,** B

(**D** — **C, F**)

The Voronoi polygon about C is now completed. The next point to be processed will be D, with known neighbours E, A, C, and F.

V_{10}: **D** — E, A, C, **F, G**

E — A, D

F — **G, D,** C, B

G — **D, F**

V_{11}: **D** — E, A, C, F **G, H**

E — A, D

F — G, D, C, B

G — **H, D,** F

H — **D, G**

V_{12}: **D** — E, A, C, F, G, **H, (E)**

E — A, **D, H**

F — G, D, C, B

G — H, D, F

H — **E, D,** G

(**E** — **D, H**)

Continuing on:

V_{13}: **E** — A, D, **H, dummy3**

F — G, D, C, B

G — H, D, F

H — **dummy3, E,** D, G

dummy3 — E, H

V_{14}: **E** — A, D, H, **dummy3, dummy4**

F — G, D, C, B

G — H, D, F

H — dummy3, E, D, G

dummy3 — dummy4, E, H

dummy4 — E, dummy3

(V_5): **E** — A, D, H, dummy3, **dummy4, (A)**

F — G, D, C, B

G — H, D, F

H — dummy3, E, D, G

dummy3 — dummy4, E, H

dummy4 — A, E, dummy3

(A — E, dummy4)

To keep on:

(V_7): **F** — G, D, C, **B, dummy2**

G — H, D, F

H — E, D, G

(B — dummy2, F)

dummy2 — F, B

V_{15}: **F** — G, D, C, B **dummy2, (G)**

G — H, D, **F, dummy2**

H — E, D, G

dummy2 — G, F, B

(**G — F, dummy2**)

For point G:

(V_{15}): **G** — H, D, **F, dummy2**

H — E, D, G

(**F — dummy2, G**)

dummy2 — G, F,

V_{16}: **G** — H, D, F, **dummy2, (H)**

H — E, D, **G, dummy2**

dummy2 — H, G, F

(**H — G, dummy2**)

Finally, for the last centroid H:

(V_{16}): **H** — E, D, **G, dummy2**

(**G — dummy2, H**)

dummy2 — H, G

V_{17}: **H** — E, D, G, **dummy2, dummy3**

dummy2 — dummy3, H, G

dummy3 — H, dummy2

(V_{13}): **H** — E, D, G, dummy2, **dummy3, (E)**

dummy2 — dummy3, H, G

dummy3 — E, H, dummy2

(E — H, dummy3)

After a *NewNbr E* is found which is the same as *NbrFirst* of the query point *H*, the last Voronoi polygon is completed. The Voronoi diagram is also finished because all points have been processed. The complete frameworks finding the next geometric neighbour and completing the Voronoi diagram are shown in Appendices B and C.

Once the entire diagram is completed, an array of linked list of geometric neighbours and another array of linked list of vertices are created and stored in two different files. Each element of these arrays is associated with a point of the set. Using the array in the two files the Voronoi diagram and the Delaunay triangulation [16] can be drawn. The Voronoi diagrams associated with the set are shown in solid lines in Figures 1 and 2, and the Delaunay taiangulations are shown in dashed lines.

3 Random Close Packing

3.1 Definition

Given an ensemble of disks, first, is it an ordered packing or a random packing? Second, is it a close packing or not?

A random packing differs from a ordered packing in that the latter has a regular periodic structure with a fixed lattice spacing. Berryman [13] had given the following geometric interpretation of random packing:

1. A *random* packing is a packing containing no statistically significant short- or long- range order.

2. A *random close* packing is a random packing so dense such that the density of it will not be increased without signigicant increase in short-range order.

3. From (1) and (2) above, it is derived that a disk in a random close packing must be in contact with several others.

4. Any decrease in density makes a random close packing not *close*, though still random, anymore. It is because a given disk will not necessarily be in contact with another disk when the density is decreased.

Obviously, Berryman's description was based on geometry only and was independent of thermodynamic interpretation.

Based on the previous concepts, Berryman had made the following definitions:

Definition 2 *Let D be the diameter of the disks in the random packing, $P(r \leq R)$ be the cumulative probability that the nearest neighbour of a disk at the origin is at some radius r in the range $D < r < R$. Then, for a fixed packing fraction η, the median nearest neighbour radius $R_{MNN}(\eta)$ is defined implicitly by*

$$P(r \leq R_{MNN}) = \frac{1}{2}. \tag{1}$$

For a dilute packing of disks, the median nearest neighbour radius will be large, tending to infinity as the packing density η approaches 0. As the density increases toward random close packing, the median nearest neighbour radius will approach D. Furthermore, it follows from our previous discussion that

$$R_{MNN} = D \tag{2}$$

is characteristic of random close packing since each disk must be touching its nearest neighbour in such a packing. Thus, the problem of determining whether a disk configuration forms a close packing can be answered by checking if Eq. (2) is satisfied. However, it has been found that R_{MNN} never reaches D if a digital computer with some fixed precision is used. The median nearest neighbour radius calculated for a 1,000 disk configuration after different number of shakes are listed in Table 1. To conquer this problem, a tolerance is introduced and Eq. (2) is modified as follows while using a computer:

$$R_{MNN} = (1 + tolerance) \cdot D \tag{3}$$

The choice of the tolerance will be discussed in Section 3.4.3.

cycle no.	R_{MNN}/D	cycle no.	R_{MNN}/D
0	1.00181	8	1.00201
1	1.00195	9	1.00194
2	1.00182	10	1.00179
3	1.00217	11	1.00182
4	1.00192	12	1.00201
5	1.00202	13	1.00203
6	1.00202	14	1.00221
7	1.00204	15	1.00175

Table 1: Normalized median nearest neighbour radii versus cycle number for a 1,000 disk configuration.

Eqs. (2) and 3 are also characteristic of all configurations with a packing fraction greater than the packing fraction of a random close packing. Thus, a definition is given below which defines the packing fraction of a random close packing, denoted η_{RCP}:

Definition 3 *The packing fraction of a random close packing is the minimum packing fraction, such that $R_{MNN}(\eta) = D$. Explicitly,*

$$\eta_{RCP} \equiv min\{\eta | R_{MNN}(\eta) = D\} \tag{4}$$

The problem of determining η_{RCP} can now be reduced to one of estimating $R_{MNN}(\eta)$ for dilute packings of disks and then extrapolating to higher densities to find the point at which Eq. (4) is satisfied. This is where the Voronoi diagram comes into play. However, this will require more configurations with much more distributed packing fractions. And, it is not the topic of this thesis. So, no more discussion will be focussed on it.

3.2 Radial Distribution Function Characteristics of A Random Close Packing

The concept of randomness can be understood by introducing RDF, the radial distribution function [36]. This function, denoted by g, gives the number of disk centers, N_c, within an annulus (or shell in three dimensions) located at a radial distance r from a central disk of diameter D, in which N_c is normalized by $2\pi\frac{r}{D}$. Hence, in two dimensions,

$$g(r/D) = \frac{N_c}{2\pi(r/D)} \tag{5}$$

Clearly, $g(r/D) = 0$ if $r/D < 1$. At $r/D = 1$, an estimate of the average coordination number cab be calculated from Eq. (5). Also,

$$\frac{g(r/D)}{\Delta(r/D)} = \frac{N_c}{2\pi(r/D)\Delta(r/D)}$$

tends to the number density ρ, the number of disks per unit area, as r/D becomes large. If

$$\rho = \lim_{r/D\to\infty} \frac{g(r/D)}{\Delta(r/D)}$$

then the packing fraction, PF, defined as the fraction of a unit area which is occupied by disks, can be expressed as:

$$PF = \frac{\pi}{4}\rho D^2 \tag{6}$$

In the case of an two-dimensional ordered close packing, also termed HCP (hexagonal close packing), or crystallographic packing, the RDF has peaks at some discrete values of r/D and zeroes in between. These locations can be easily determined and are listed in Table 2.

Peak	1	2	3	4	5	6	7
r/D	1	$\sqrt{3}$	2	$\sqrt{7}$	3	$2\sqrt{3}$	$\sqrt{13}$

Table 2: Radial distribution peaks in a two-dimensional ordered close packing.

This feature possessed by the ordered close packing does not occur for a random close packing. Therefore a comparison of the RDF of a random packing with that of an HCP will give a measure of the "randomness" of the configuration.

In this work, attention is not focused on the RDF and plots of this function are given only to demonstrate that the generated packings are indeed random. Rather, the main thrust here is on the analysis of the packing through the use of Voronoi diagram.

3.3 Monte Carlo Simulation

The work by Rosato et. al. [42,43] has been discussed in Chapter One. The "pouring" and "shaking" of hard disks were simulated based on a Monte Carlo method. It was able to model the dynamical many-particle process, which occurs during the shaking of disks. Horizontal boundary conditions could be either non-periodic or periodic, i.e., with or without hard vertical walls. The one with periodic condition simulates closely the behaviour of an infinite system, while the non-periodic one gives a model which shows the effects of walls.

The initial coordinates of the disk centers, which form a configuration, are created by a random number generator. For any possible variation, a trial configuration is created by moving one disk at a time within a small predefined neighbourhood, usually some fraction of the disk diameter and denoted δ. A trial configuration is accepted as the new configuration based on the change in the system—inter-particle and gravitational potential energy variation δE, using the Boltzmann distribution. The details of the algorithm will not be repeated here, and may be found in [42]. An attempt to move all of the disks once is defined as a pass. In general, many passes are necessary to attain the equilibrium configuration. The simulation is run so as to allow no upward movements of disks, so that the gravitational potential is permitted only to decrease. This simulates a process whereby the initially randomly placed disks slowly settle to the bottom of the container.

To simulate a shaking, the disks are first lifted uniformly by a specific amount, called amplitude. Then, using the Monte Carlo method again, they are allowed to settle to an equilibrium state. This process is called a cycle. A cycle ceases when the change of the average system energy is less then a preselected tolerance. The disks are now packed at the bottom and a new cycle may begin. Figure 34 shows an assembly of 1,000 disks after a pouring of 60,000 passes and Figure 35 shows the same assembly after 20 cycles of shaking.

3.4 Analysis of the Monte Carlo Simulation Output

Some analysis of the output given by the code briefly described in the previous section will be discussed in this section. This includes (1) the radial distribution function, (2) the average count of geometric neighbours, (3) the average count of structural neighbours, (4) the angular distribution of structural neighbours, (5) the packing

case study		1	2
disk number		1,000	1,250
cell width		8 in. with periodic b.c.	9 in. with non-periodic b.c.
disk dia. (D)		0.3 in.	0.25 in.
pouring	passes	60,000	60,000
	δ in each pass	1 / 3 D	1 / 3 D
shaking	amplitude	1 / 3 D	1 / 3 D
	passes per shake	20,000	20,000
	δ in each pass	1 / 6 D	1 / 6 D
no. of shakes		20	19

Table 3: Cases Studied.

fraction, and (6) the rigid wall effect. The case studies include: (1) 1,000 disks in a cell with horizontal periodic boundary conditions and (2) 1,250 disks in a cell with impenetrable vertical walls. The maximum allowed movement, δ, for each disk during a pass was equal to one sixth of the disk diameter, while the shaking amplitude for both cases was one third of the disk diameter. The details are shown in Table 3.

3.4.1 Radial Distribution Function

The radial distribution functions, denoted by g, for the case study (1), 1,000 disks with periodic boundary condition are shown in Figure 5 and 6 for the poured configuration and the one after 20 cycles of shake respectively. After shaking, the peaks become more pronounced since the packing has become more dense and less random, as depicted in Figures 34 and 35.

The value of the first peak at $r/D = 1$ has also increased after shaking. It is calculated as 0.654809 for the poured case and 0.761822 for the shaken one. It yields an estimate of the average coordination number as mentioned in Section 3.2. Using

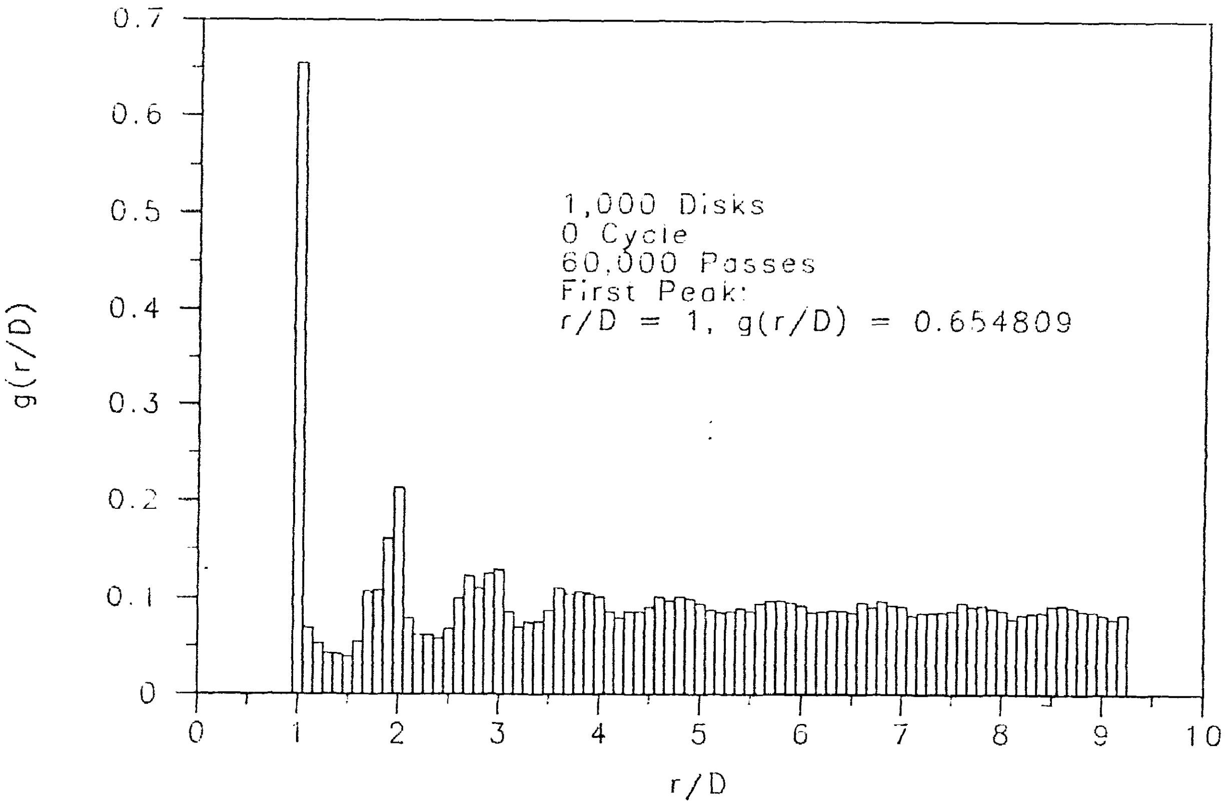


Figure 5: Radial distribution function for a 1,000 disk configuration after pouring.

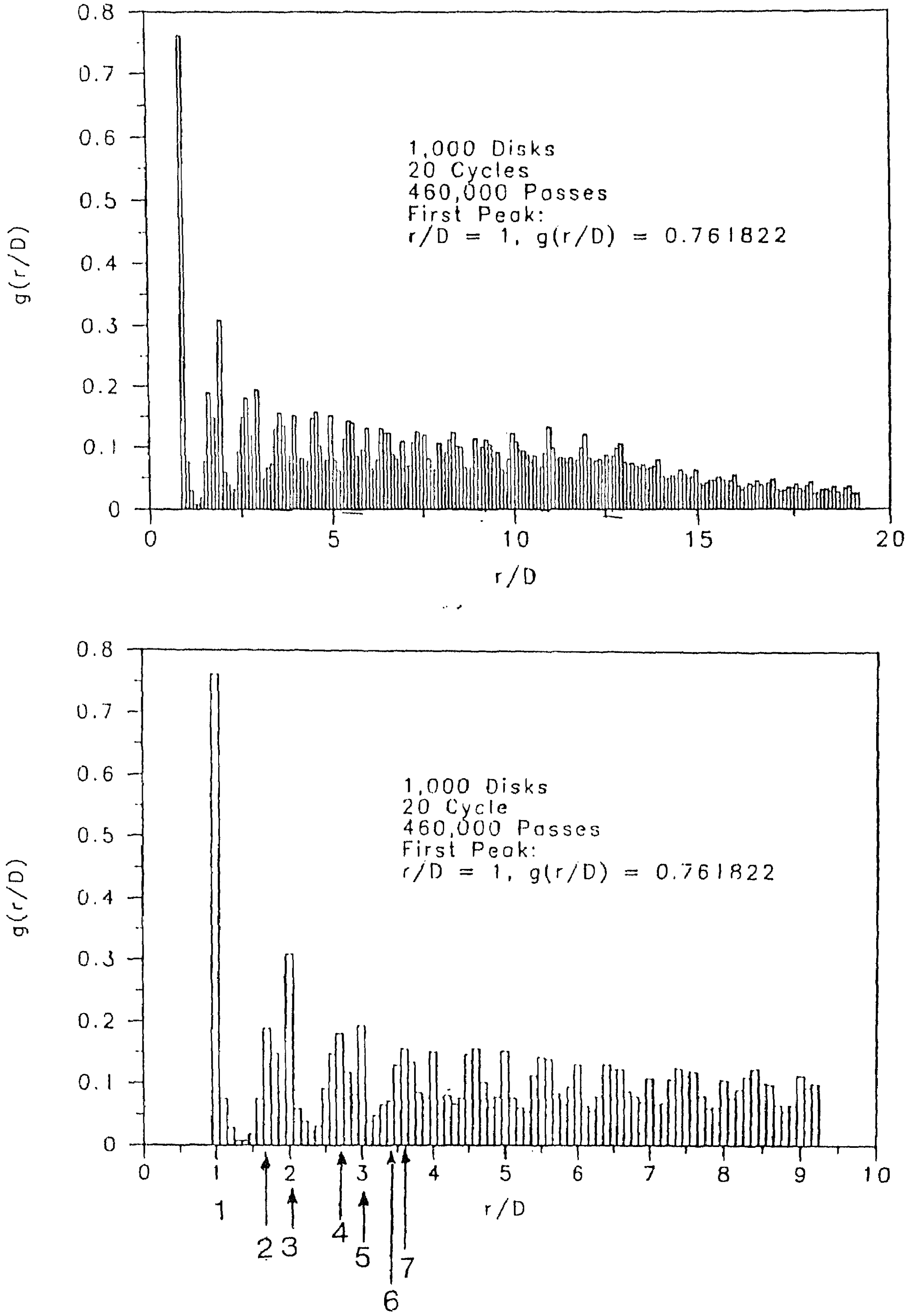


Figure 6: Radial distribution function of a 1,000 disk configuration after 20 cycles of shakings.

Eq. (5), the average coordination number estimated are:

- $2\pi g(r/D) \mid_{r/D=1}= 4.11429$, for the poured case.

- $2\pi g(r/D) \mid_{r/D=1}= 4.78667$, for the shaken case.

3.4.2 Average Number of Geometric Neighbours

It is well known that the average number of edges per Voronoi polygon is six [49]. That is, the average count of geometric neighbours of a disk is six, independent of the randomness and the density of the packing.

To obtain an acceptable statistical result, the number of disk in the configuration to be analyzed is supposed to be great enough so that the finite size effect, sometimes called edge effect, would be eliminated. However, to utilize the minimum space and time on computer for each study, the size of the system to be processed is restricted.

To minimize the edge effects rooted from a small configuration, an inner box adjusted within the viewing box introduced in Definition 1, was fixed. The method of fixing the inner box is described below with reference to Figure 7.

1. Define disks having an unbounded Voronoi polygon as the boundary disks. All boundary disks form the boundary of a disk configuration.

2. Find *Corner1*, *Corner2*, *Corner3*, and *Corner4*, the disks closest to the lower left, upper left, upper right, and lower right corners of the viewing box respectively. The four corners divide the boundary of the disk configuration into four divisions, namely *left*, *top*, *right*, and *bottom boundaries*

3. Find the most inner disk on each of the four boundaries; i.e., (x_l, y_l)–the right most disk on the left boundary, (x_t, y_t)–the bottom most disk on the top boundary, (x_r, y_r)–the left most disk on the right boundary, and (x_b, y_b)–the top most disk on the bottom boundary.

4. Walk twice the maximum disk diameter further toward the center to get the constraint on the four edges of the inner box:

$$x \geq x_l + 2D_{max}; \qquad y \leq y_t - 2D_{max};$$

$$x \leq x_r - 2D_{max}; \qquad y \geq y_b + 2D_{max}$$

Each and every disk in the ensemble is then checked and discarded from the analysis if it lies completely outside of the inner box. The analysis is then be performed on disks possessing no *edge disk characteristics*.

What is the edge disk characteristics? For instance, a disk on the edge of an ensemble would possess significantly fewer geometric neighbours on the average than the inner disks. Through the introduction of the inner box, the edge disks are taken out and the result will be closer to that of an infinite ensemble.

A geometric neighbour number distribution for the inner disks of a finite disk configuration composed of 1,000 disks, after 15 cycles of shaking, is presented in figure 8. The average count of it is calculated to be 5.99875. The small deviation from six is due to the remaining finite size effect and the machine error.

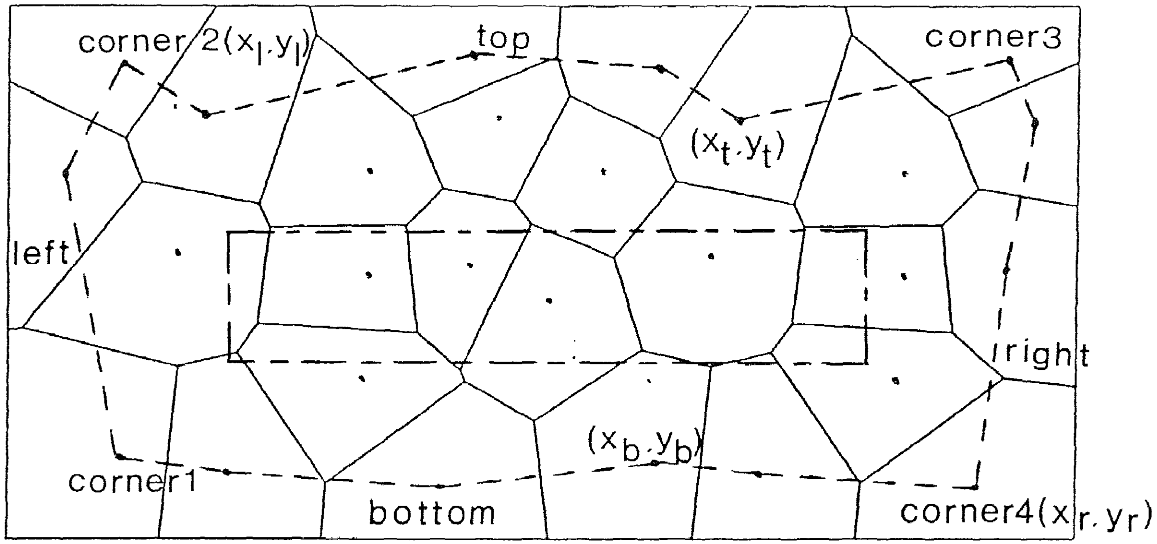


Figure 7: The fixing of a inner box within the viewing box.

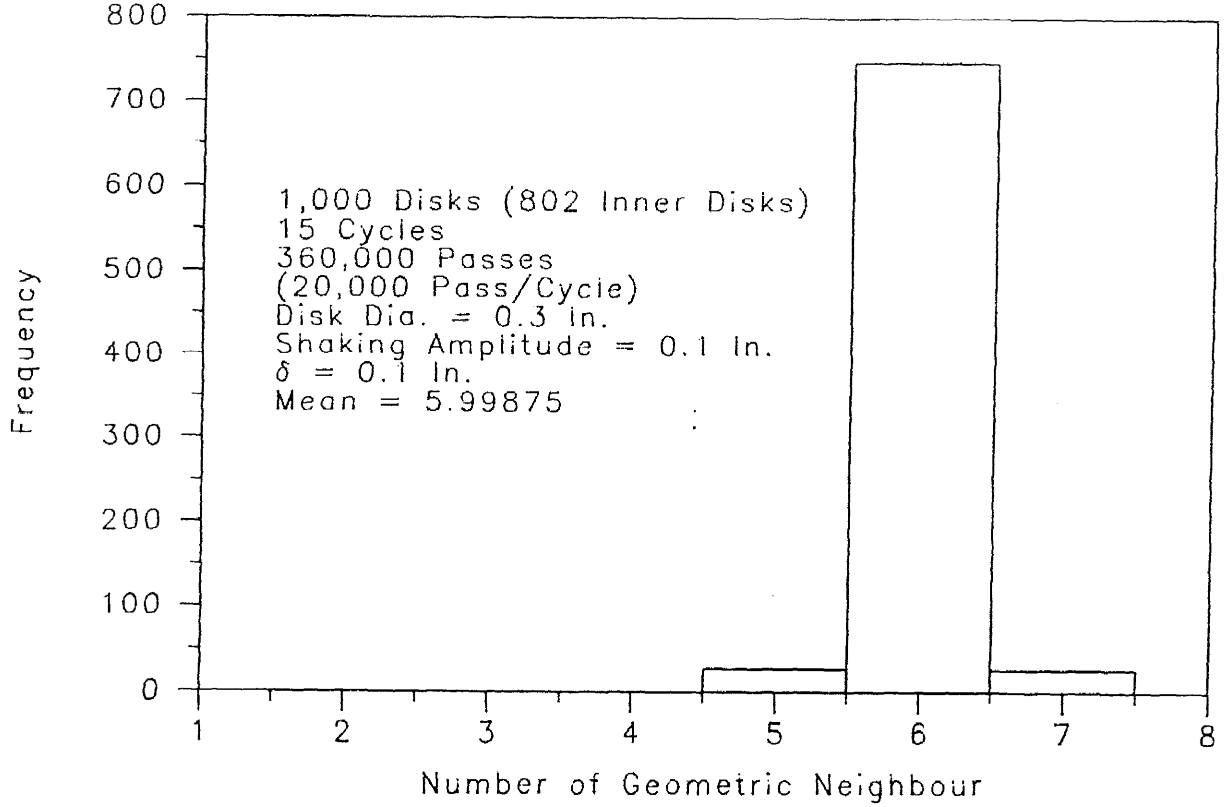


Figure 8: Distribution of geometric neighbour number.

3.4.3 Average Number of Structural Neighbours — Mean Coordination Number

The structural neighbours of a disk are contained in its geometric neighbours and are those disks in *contact* with it. The number of structural neighbours is called coordination number. It is well known that all disks in a ordered close packing have six geometric neighbours and the geometric neighbour set for each disk in such a packing is also the structural neighbour set. Therefore, the average coordination number of a ordered close packing is six, the same as the average number of geometric neighbour. A Voronoi diagram and its Delaunay triangulation for an ordered close packing are shown in Figure 9 and 10. It can be seen that each inner Voronoi polygon has exactly six edges and each vertex in the Delaunay triangulation has six lines incident upon it.

Unlike the ordered packing the coordination number may vary from disk to disk. Thus, we can only speak of coordination numbers in a statistical mean sense for a random close packing.

For this work, the accuracy of the digital computer must be considered. Let the distance between one geometric neighbour and its center disk be r, and let their radii be r_1 and r_2 respectively. For the case in which the geometric neighbour is in contact with the center disk, the following is true:

$$r = r_1 + r_2$$

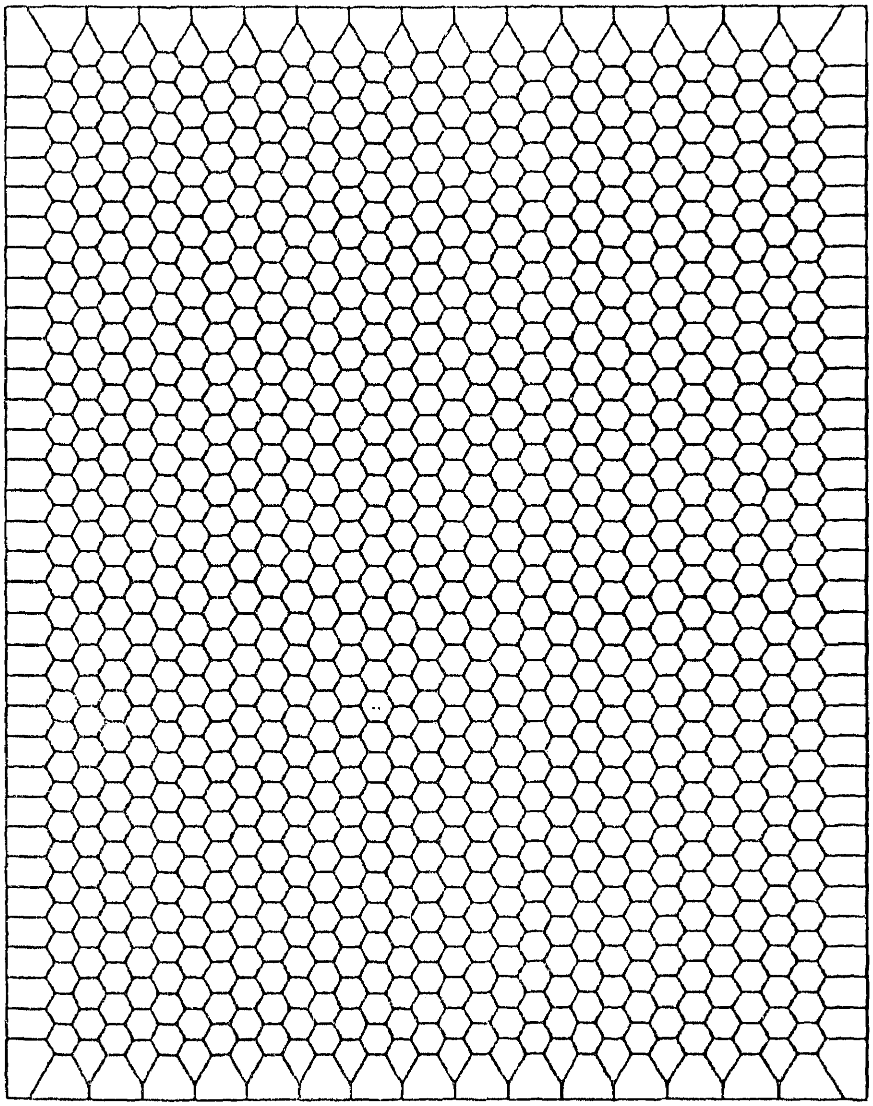


Figure 9: Voronoi diagram for an ordered close packing.

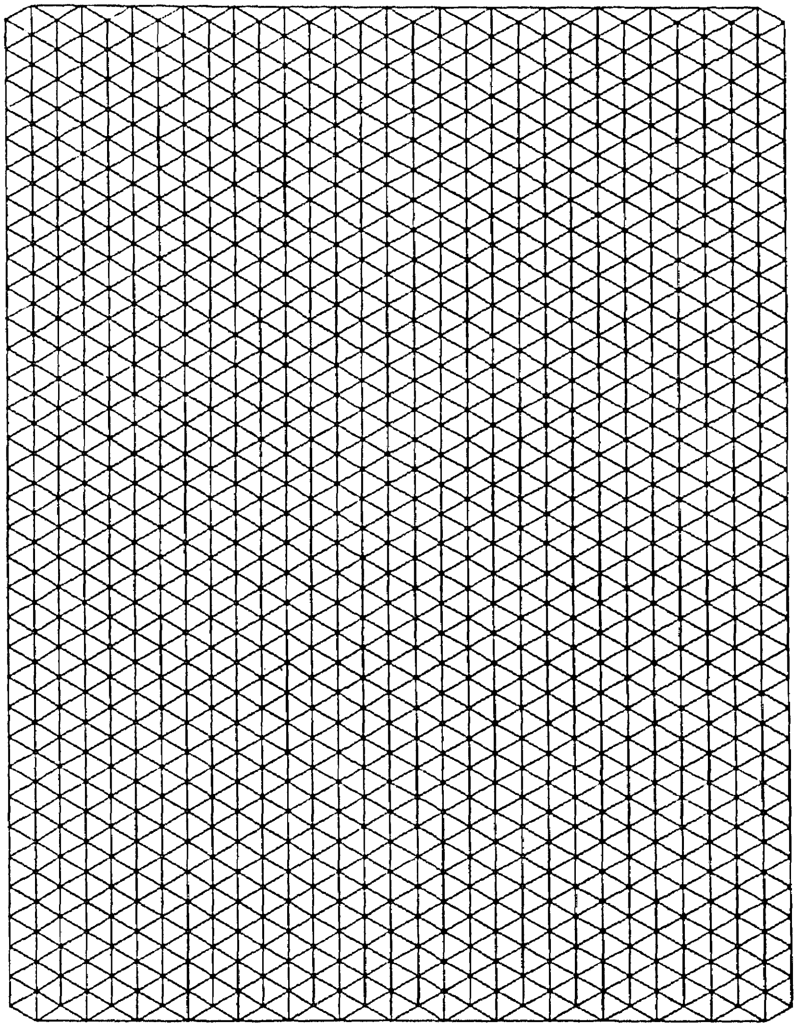


Figure 10: Delaunay triangulation for an ordered close packing.

However, since the equality can never be exactly obtained, a tolerance is introduced:

$$r \leq (1 + tolerance) \cdot (r_1 + r_2) \tag{7}$$

A disk is classified as a structural neighbour if Eq. 7 is satisfied.

Figure 11 and 12 give the cumulative probability of the normalized nearest neighbour radius, r/D, that is, $P(r/D \leq R)$, for the poured and shaken (with 15 cycles) configurations. In Figure 12,

$$\lim_{x \to 1.03} P(r/D \leq R) = 1$$

It seems to indicate that a tolerance of 0.03 would be appropriate. This value is regarded as a lower bound on the tolerance. The upper bound is chosen to be 0.05 following Bernal's [9] convention. In all of the analysis, the upper bound value was used. Figure 13 indicates that the average coordination number increases with tolerance.

Also, the structural neighbour number distributions for the 1,000 disk configuration after pouring and after 15 cycles of shaking respectively respectively are shown in Figures 14 and 15. It is observed that that shaking increases the average coordination number. Figures 16 and 17 clearly exhibit this trend for case studies 1 and 2. This is physically reasonable since it is expected more disks would be in contact with each other after shaking.

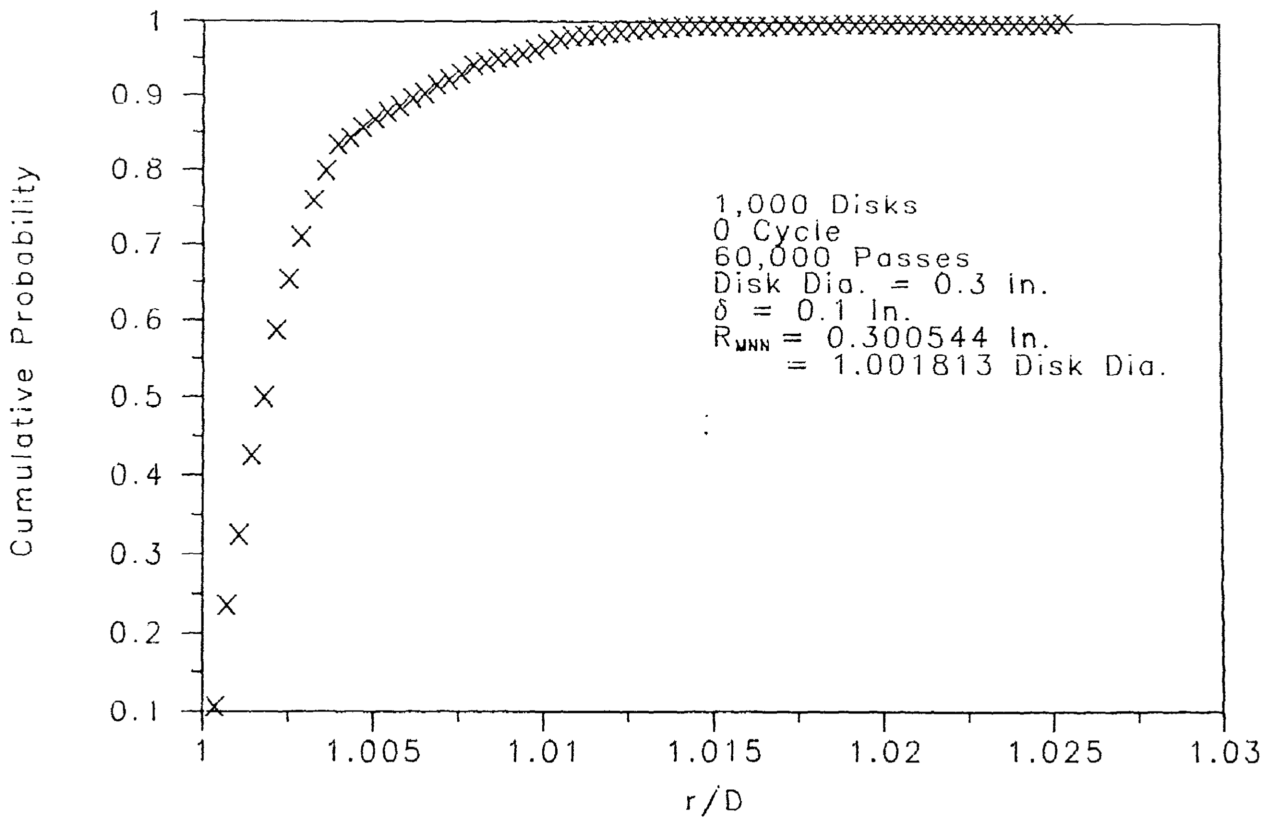


Figure 11: Cumulative probability of the normalized nearest neighbour radius r/D for 1,000 disks after pouring.

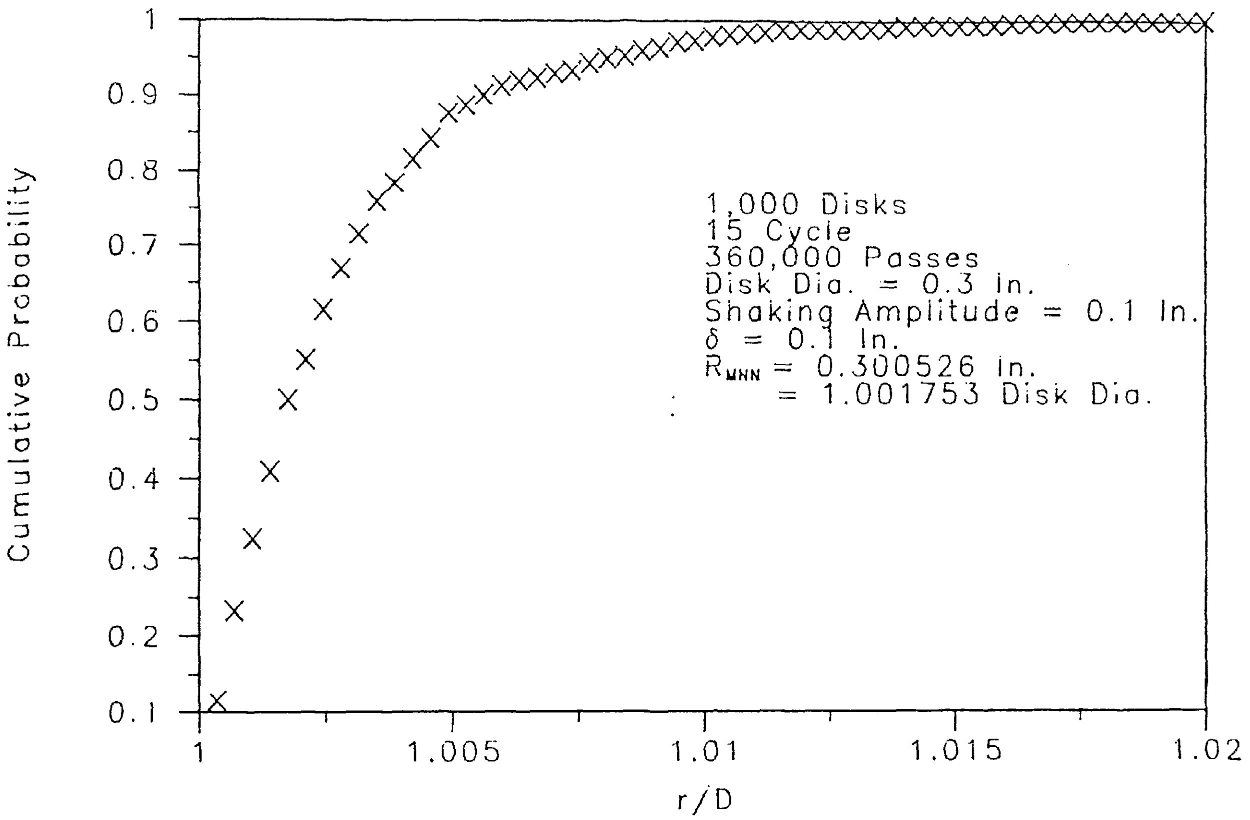


Figure 12: Cumulative probability of the normalized nearest neighbour radius r/D for 1,000 disks after shaking.

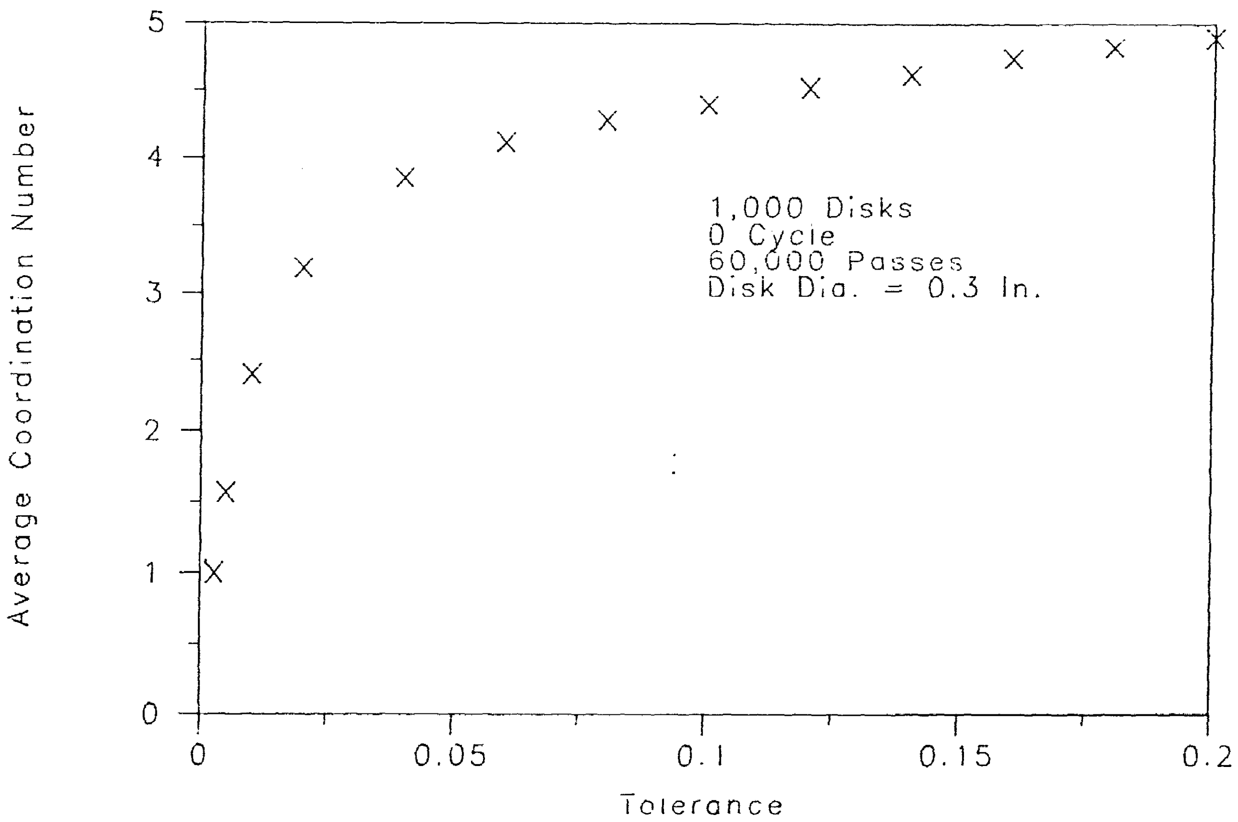


Figure 13: Relationship between coordination number and tolerance.

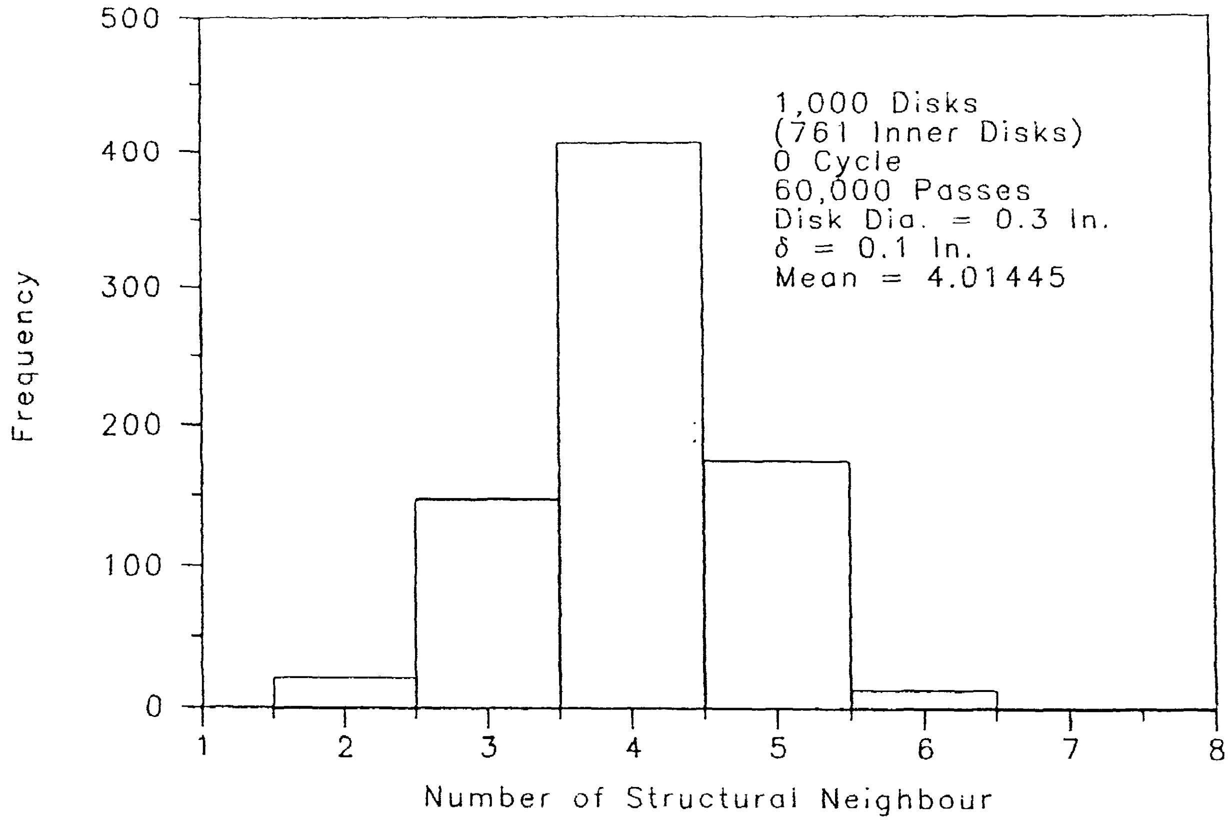


Figure 14: Distribution of structural neighbour number after pouring.

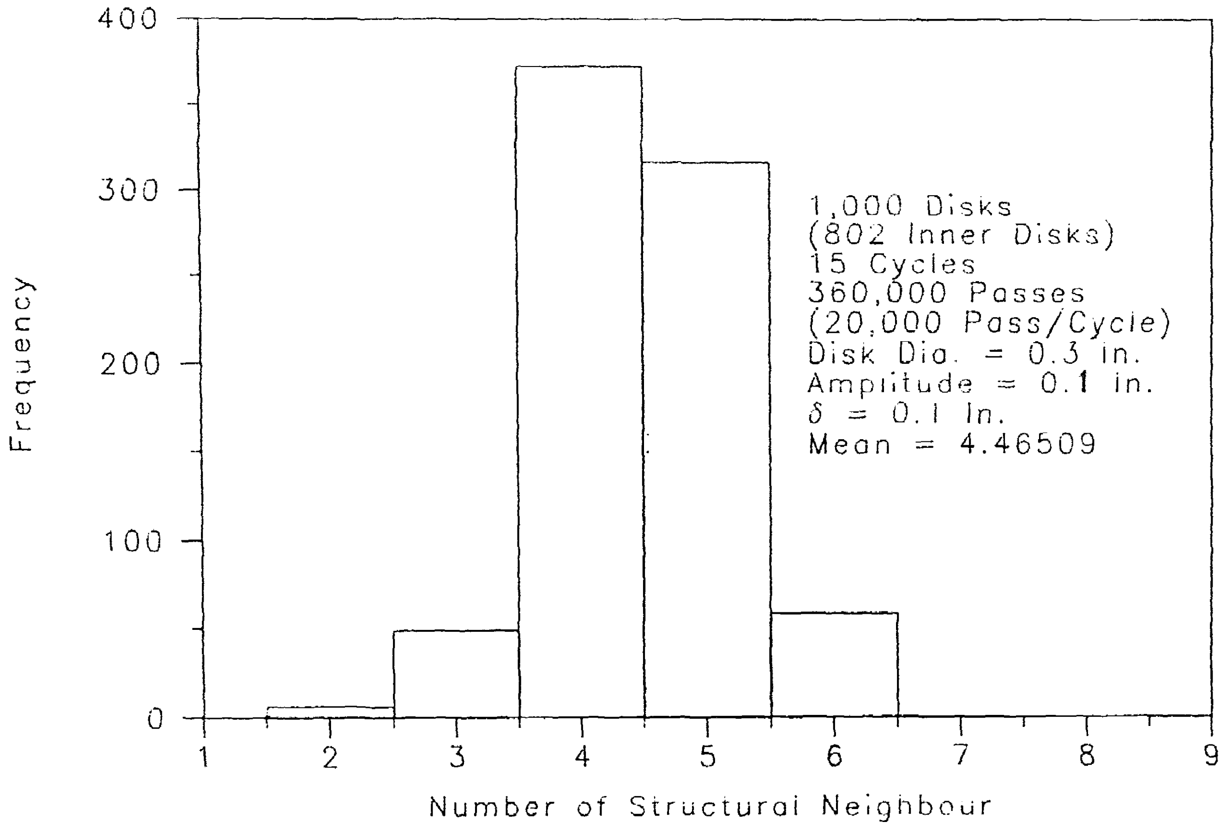


Figure 15: Distribution of structural neighbour number after shaking.

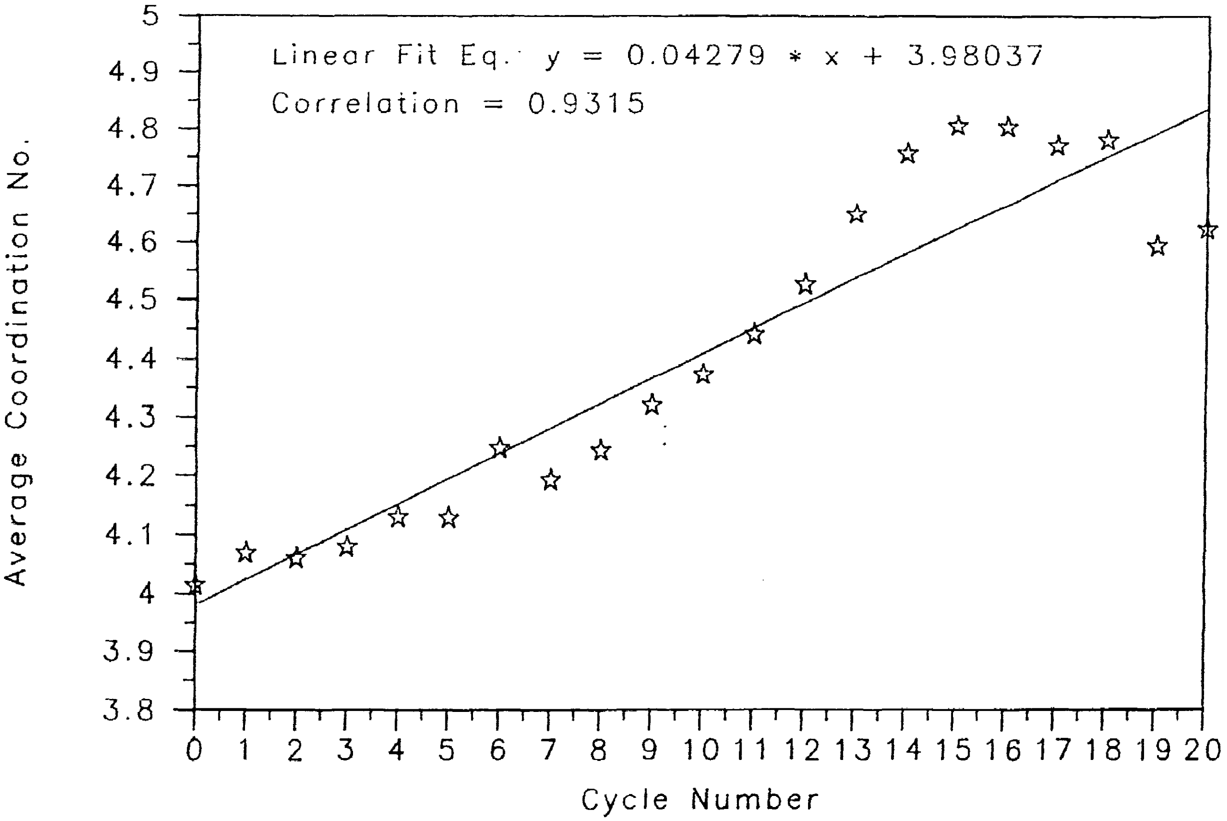


Figure 16: Average coordination number versus shaking: 1,000 disks with periodic boundary conditions.

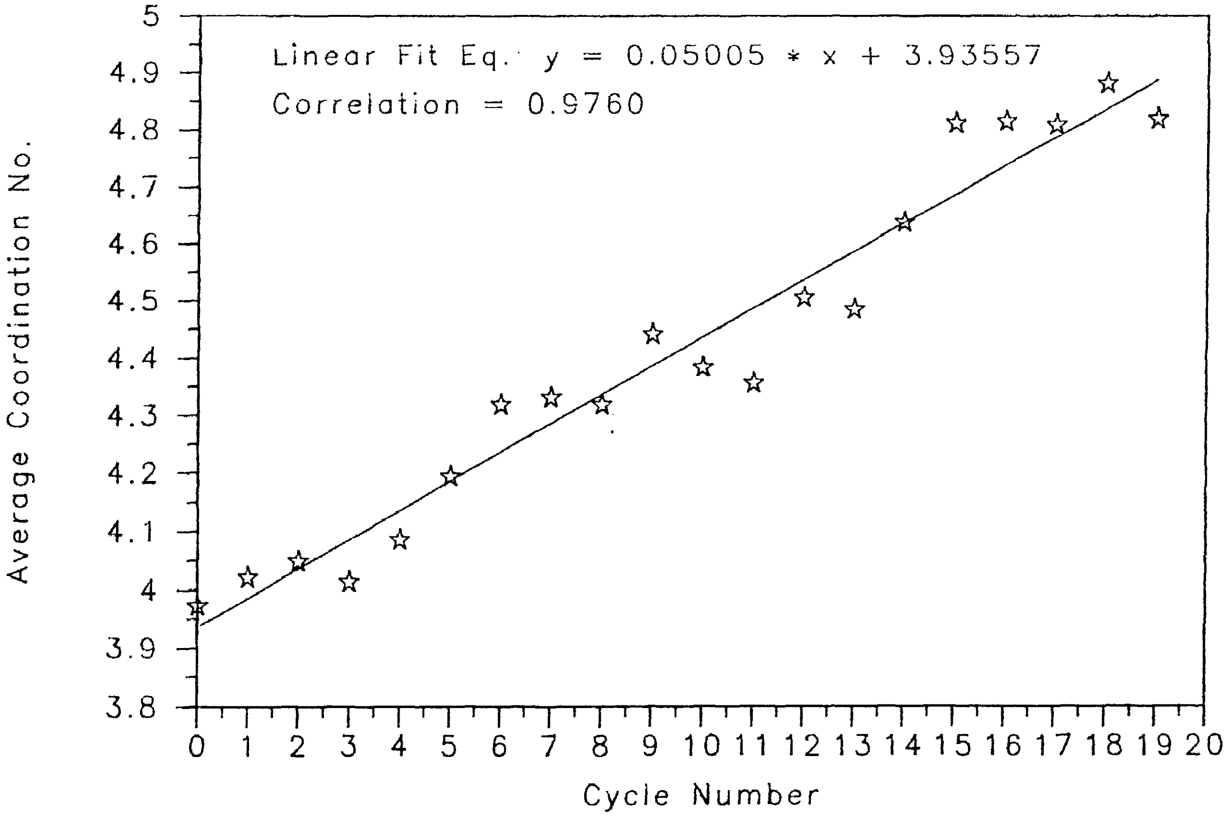


Figure 17: Average coordination number versus shaking: 1,250 disks with non-periodic boundary conditions.

3.4.4 Angular Distribution of Structural Neighbours

As discussed in the previous section, structural neighbours are those geometric neighbours which satisfy Eq. (7). Under a selected tolerance, a disk will have a number of structural neighbours, less than or equal to six. The structural neighbours "park" on the circumference of the center disk and each one has an associated structural neighbour angle. The structural neighbour angle is defined as follows:

Definition 4 *Let p and q be the centroids of a disk and one of its structural neighbour respectively. The structural neighbour angle associated with this structural neighbour is the angle measured from the positive x-direction to vector $\overrightarrow{pq}$ in counterclockwise direction.*

A disk in a random close packing, possessing M structural neighbours, will have M structural neighbour angles. It is interesting to determine the distribution of structural neighbour angles for those disks having M = 1, 2, 3, 4, 5, or 6 structural neighbours.

To accomplish this task, the disks were first categorized into groups with the same number, M, of structural neighbours. The M structural neighbour angles for each disk possessing M structural neighbour were then sorted in descending order such that the first structural neighbour had the largest structural neighbour angle and the Mth one had the smallest structural neighbour angle.

The distributions of the first through the Mth angles were computed, resulting in M distributions. These distributions are presented in Figures 18 to 22 for the 1,000

number of structural neighbour	mean value for structural neighbour in sequence					
	1	2	3	4	5	6
2	292.3	136.9				
3	293.0	188.5	73.08			
4	312.3	233.0	132.0	54.07		
5	326.4	260.5	191.4	115.9	48.54	
6	349.6	289.5	229.0	169.6	109.8	49.28

Table 4: Mean values for each structural neighbour angle.

number of structural neighbour	standard deviation for structural neighbour in sequence					
	1	2	3	4	5	6
2	40.53	94.68				
3	45.69	54.35	53.17			
4	24.36	26.06	28.39	24.97		
5	28.18	31.95	35.64	26.40	23.55	
6	20.28	21.30	20.92	20.85	20.97	20.47

Table 5: Standard deviation for each structural neighbour angle.

disk configuration after 15 cycles of shakings. The mean value and standard deviation were derived from the distribution and were presented in Tables 4 and 5.

3.4.5 Packing Fraction

Knowledge of the packing fraction gives an estimate of the density of the granular mass. In addition, the use of Voronoi diagram permits the determination of the distribution of void fraction for each Voronoi polygon. Such information is of use in modelling the behavior of powdered materials. However, calculations of the void fraction distributions has not been done in this study. Rather, the packing fraction for the whole configuration has been determined for pouring and subsequent shaking of disk assemblies. The purpose of the shaking is to densify the assembly.

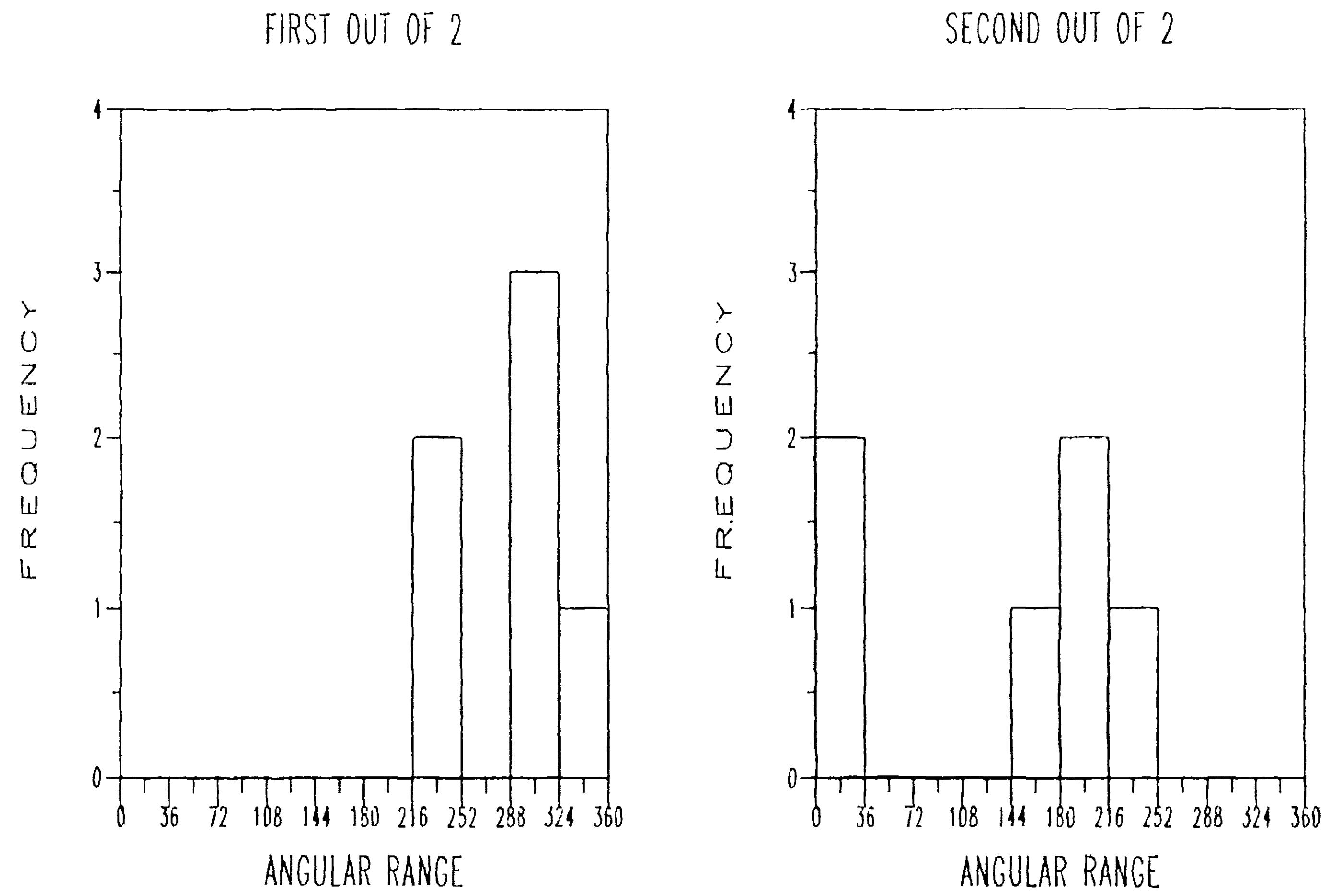


Figure 18: Angular distribution of each structural neighbour for disks possessing two structural neighbours.

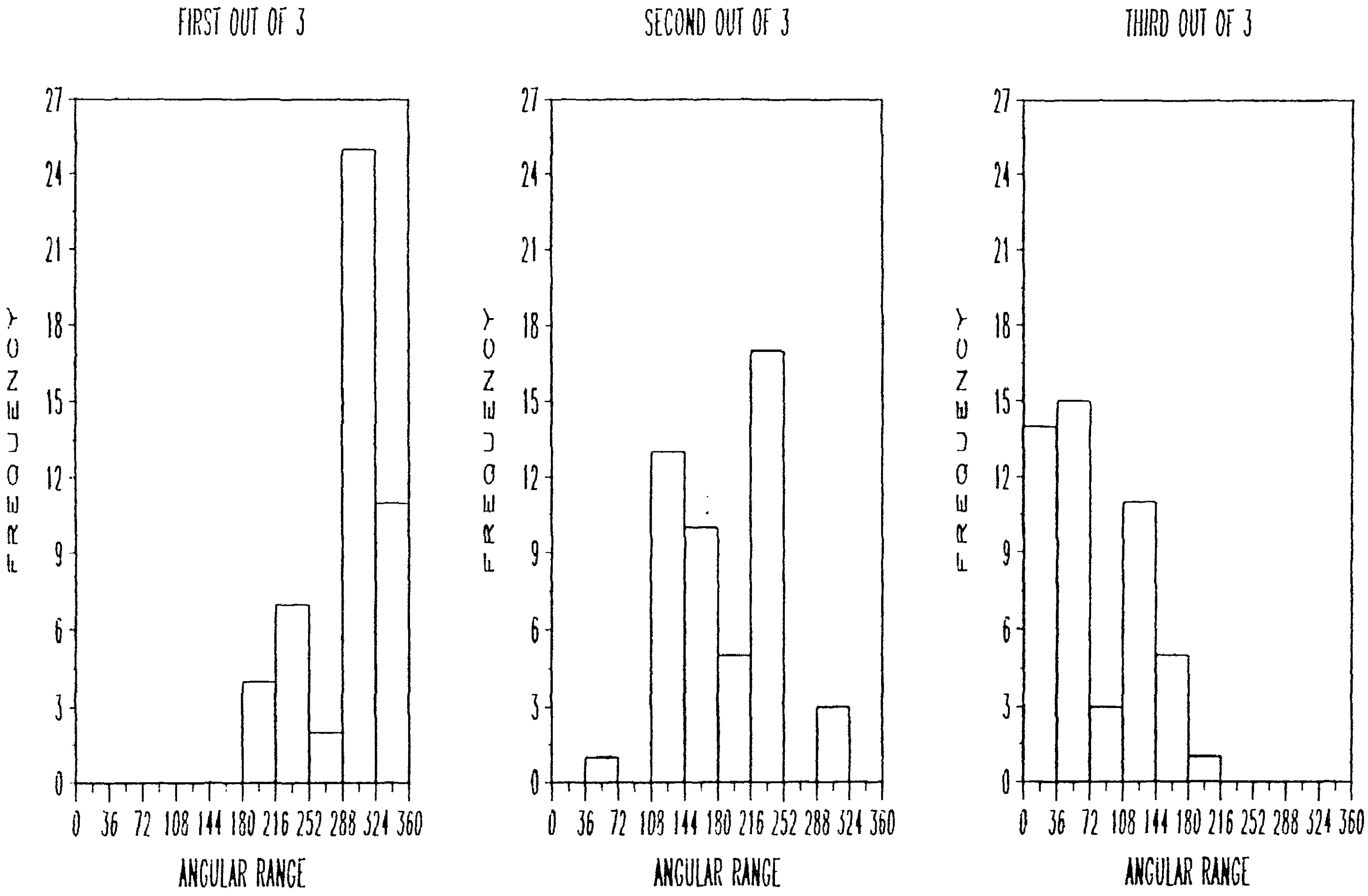


Figure 19: Angular distribution of each structural neighbour for disks possessing three structural neighbours.

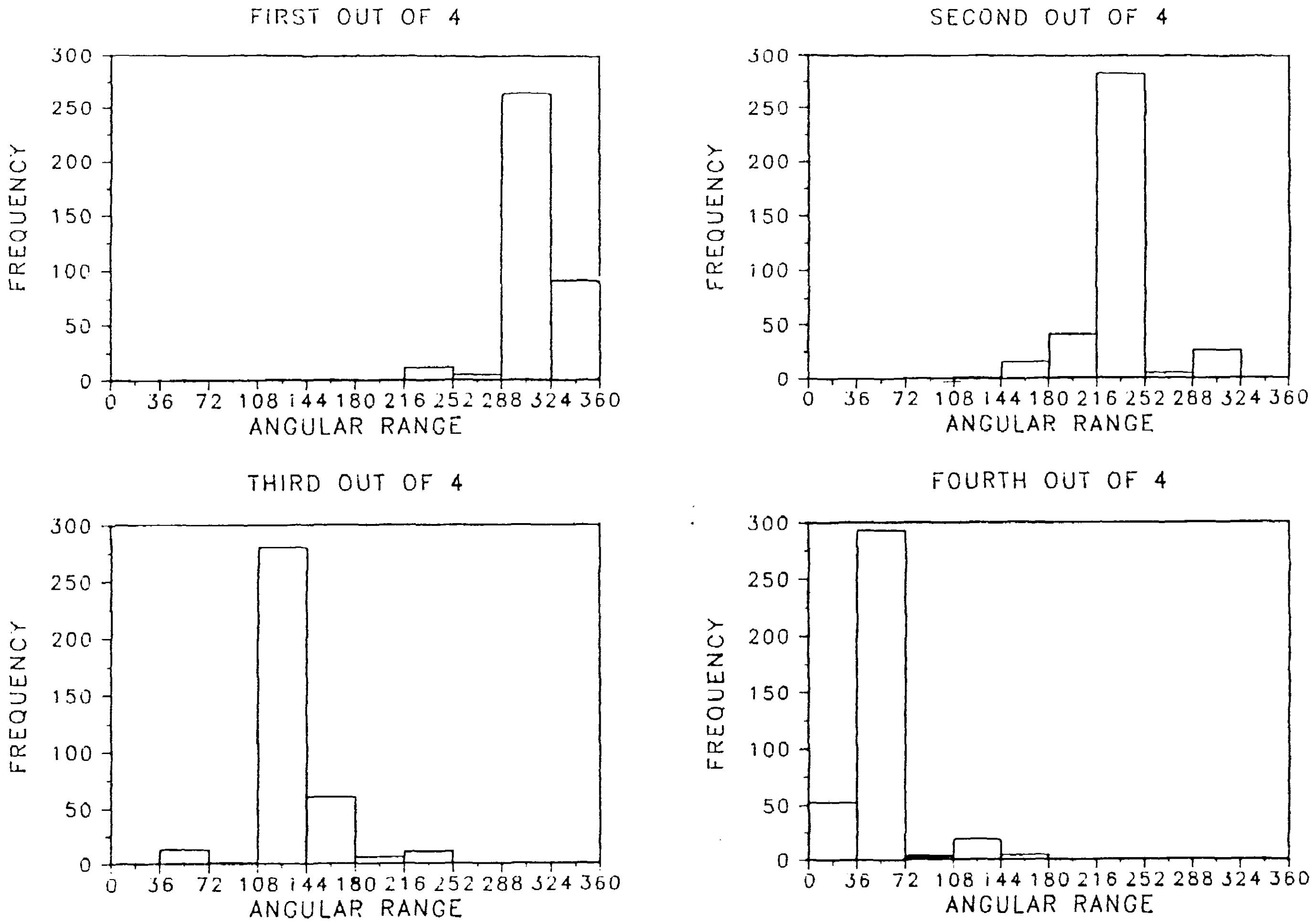


Figure 20: Angular distribution of each structural neighbour for disks possessing four structural neighbours.

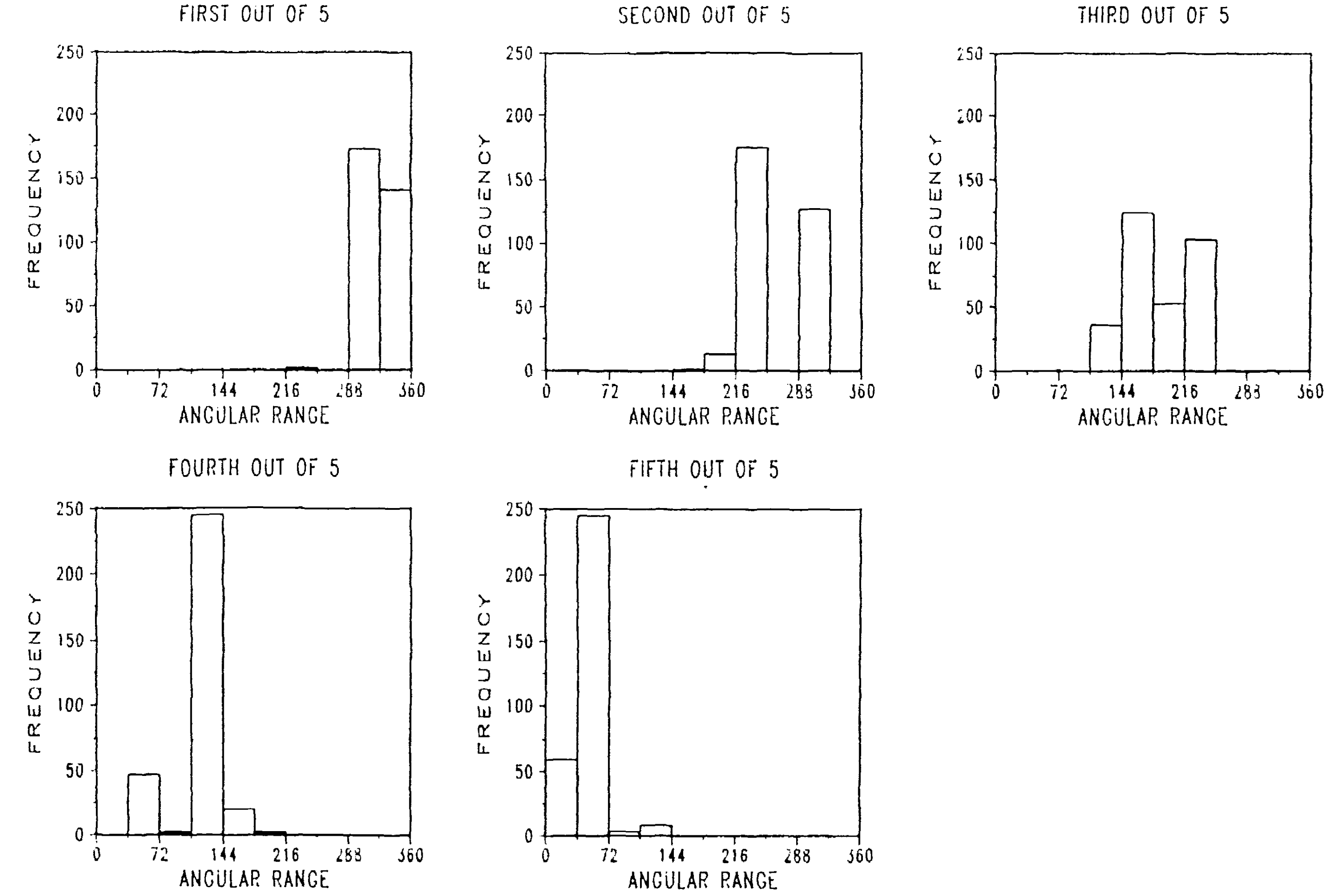


Figure 21: Angular distribution of each structural neighbour for disks possessing five structural neighbours.

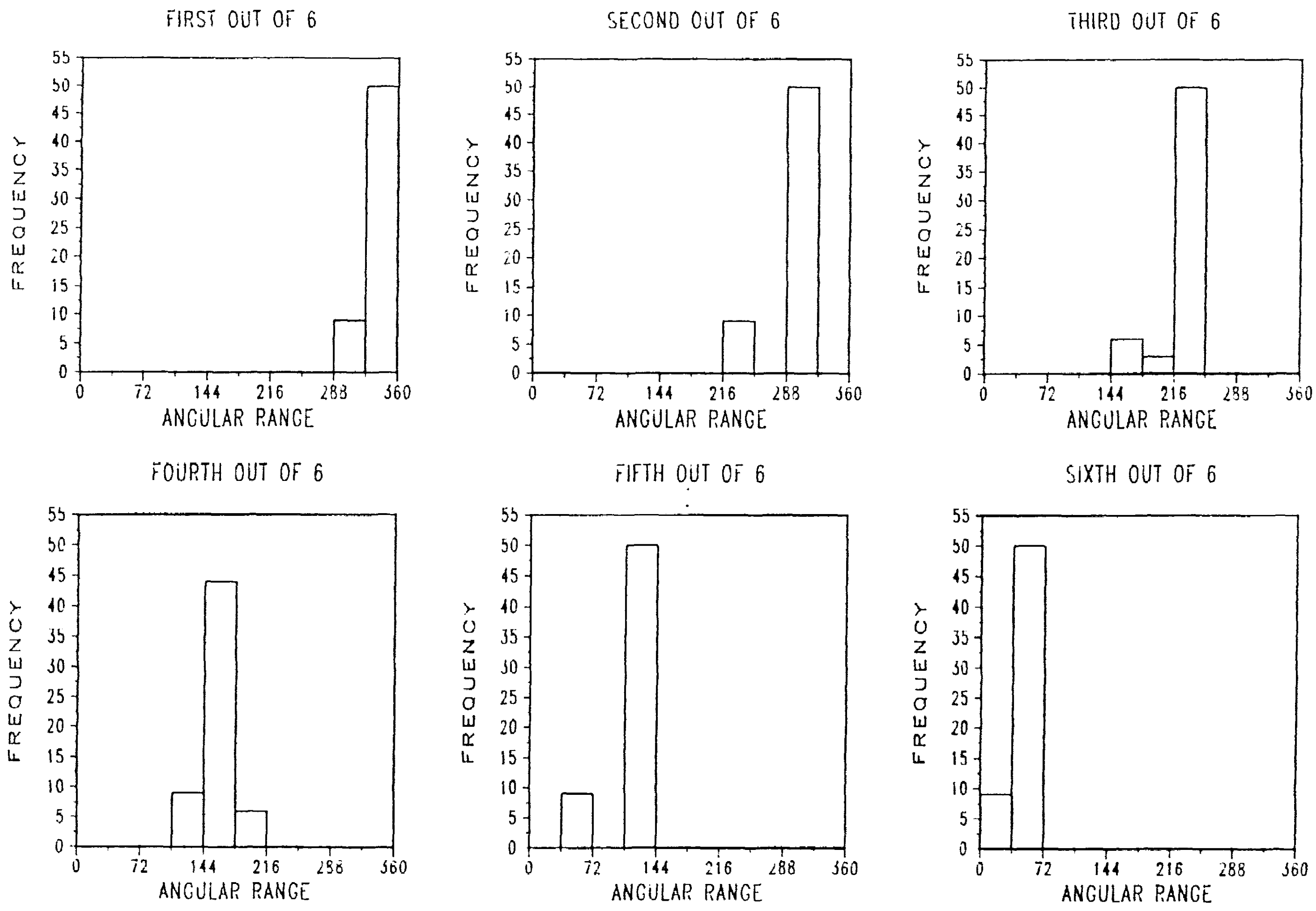


Figure 22: Angular distribution of each structural neighbour for disks possessing six structural neighbours.

Figures 23 and 24 show the decrease of the system energy versus shaking, while Figures 25 and 26 show the increase of the packing fraction versus shaking. In case study (1), the linear least square fit of the data in Figures 23 and 25 show that a 6.17% decrease in the system energy over 20 cycles resulted in a 6.96% increase in the packing fraction. Similarly, in case study (2), the linear least square fit of the data in Figures 24 and 26 show that a 6.13% decrease in the system energy over 20 cycles of shaking resulted in a 6.39% increase in the packing fraction. As the assemblies become more dense, the average coordination number also increases as discussed in Section 3.4.3. Figures 27 and 28 further illustrate the relationship between the packing fraction and the average coordination number. The fact that the packing fraction increases with average coordination number is in agreement with the results of D. N. Sutherland [52] although the coordination numbers presented here are greater. This may have been caused by the selection of Bernal's tolerance of 0.05 applied in three-dimensional spheres, which is an upper bound we selected in our study.

3.4.6 Rigid Wall Effect

Up to this point, the analyses were aimed at the overall characteristics of a configuration. The configuration with non-periodic boundaries, a finite configuration with constraining walls at both sides, has some interesting local characteristics in the vicinity of the wall, which are now discussed. Specifically, the variation of the packing

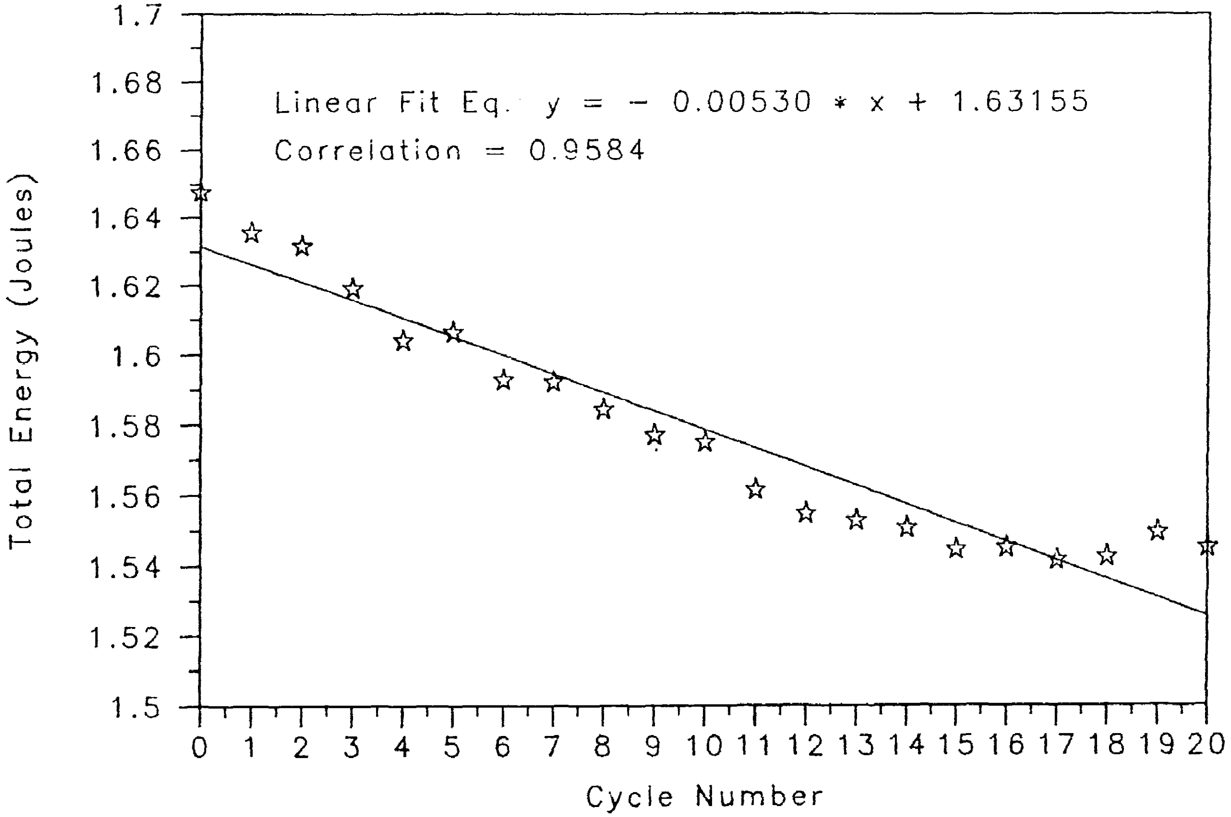


Figure 23: Energy variation versus shaking: 1,000 disks with periodic boundary conditions.

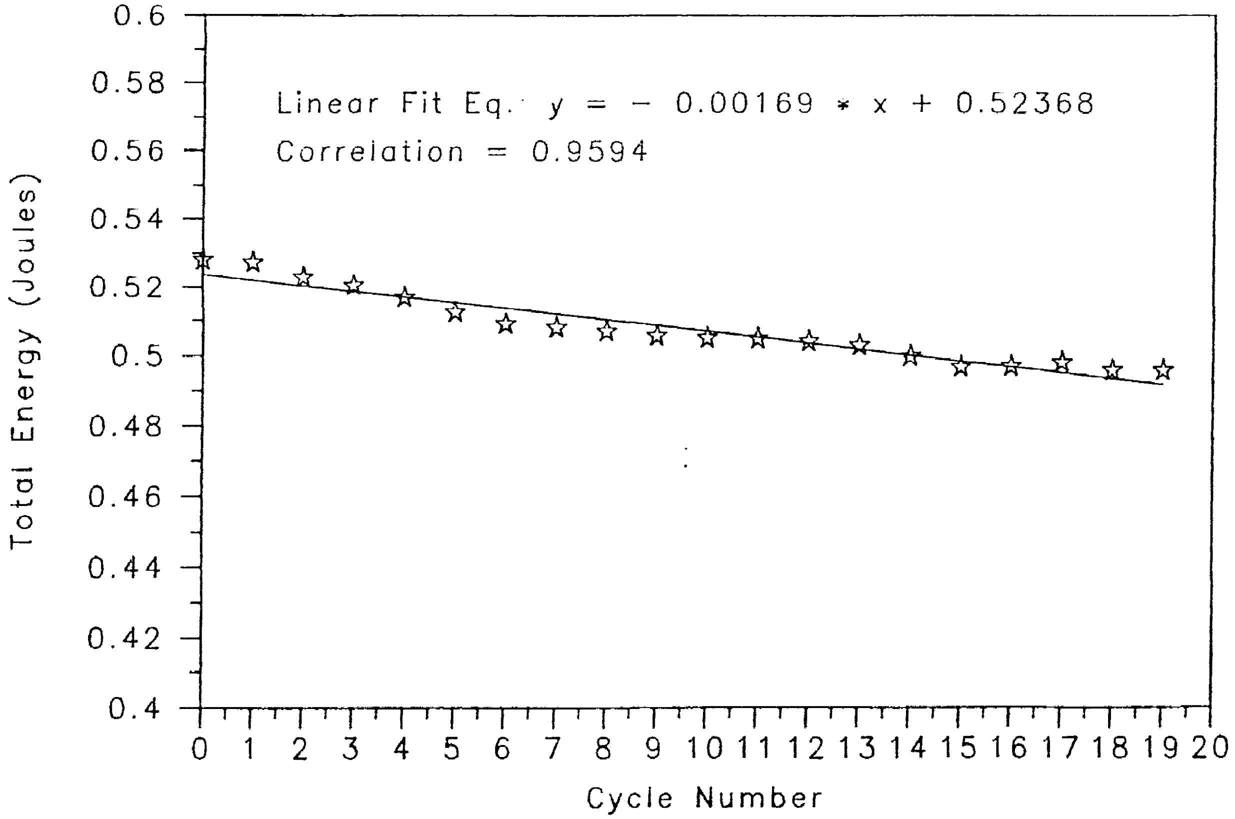


Figure 24: Energy variation versus shaking: 1,250 disks with non-periodic boundary conditions.

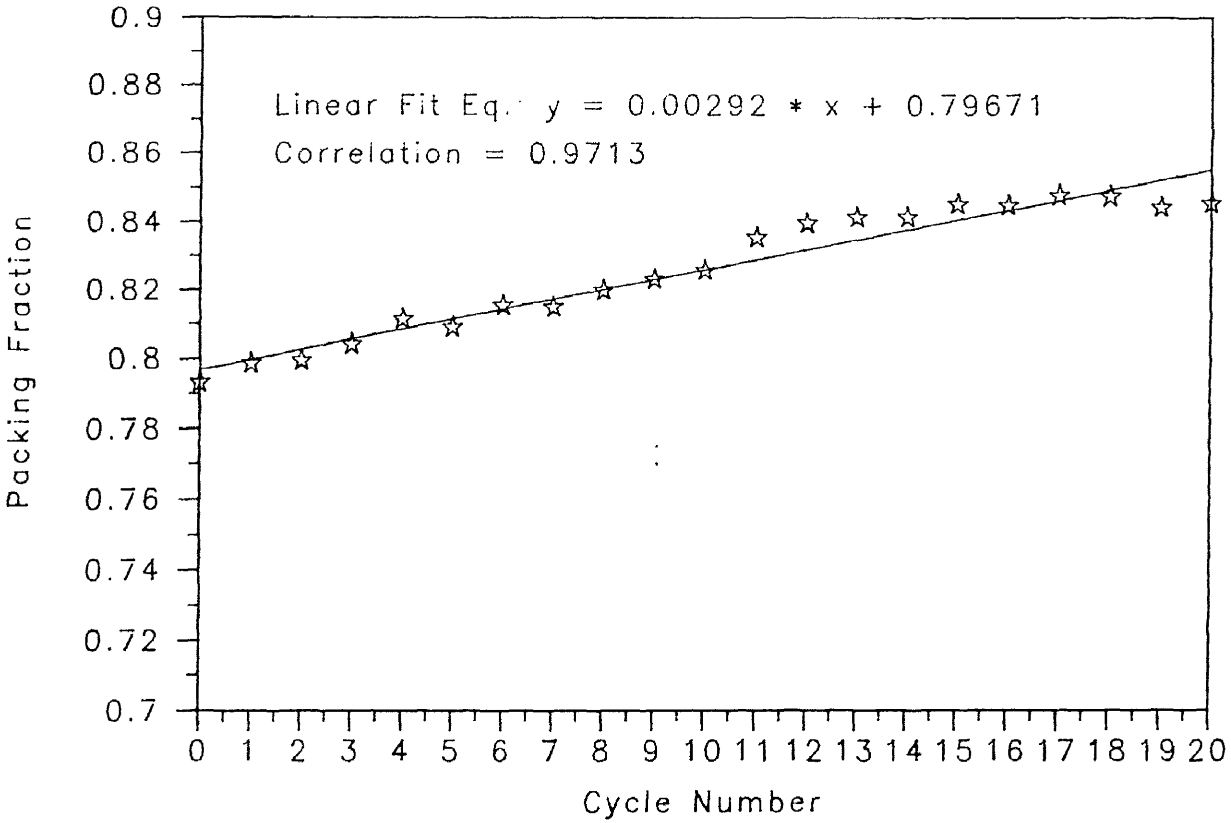


Figure 25: Packing fraction variation versus shaking: 1,000 disks with periodic boundary conditions.

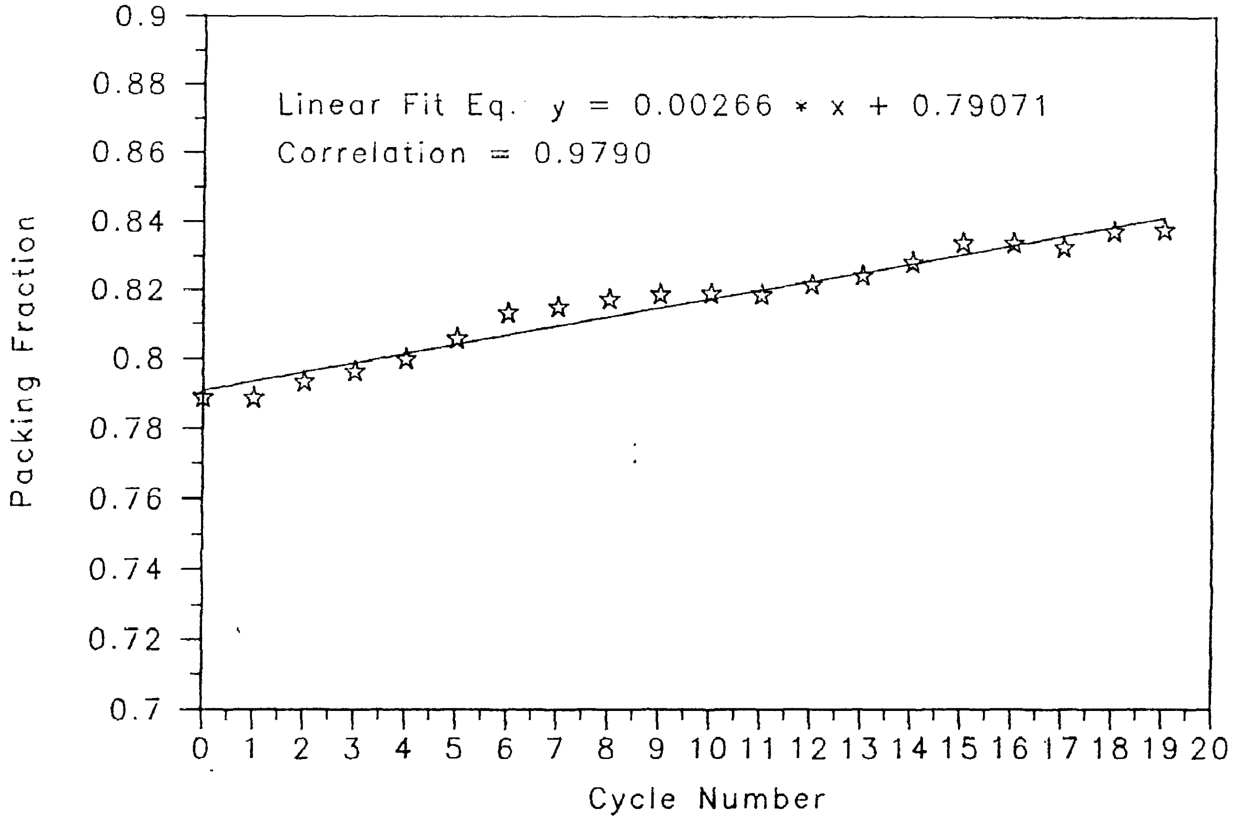


Figure 26: Packing fraction variation versus shaking: 1250 disks with non-periodic boundary conditions.

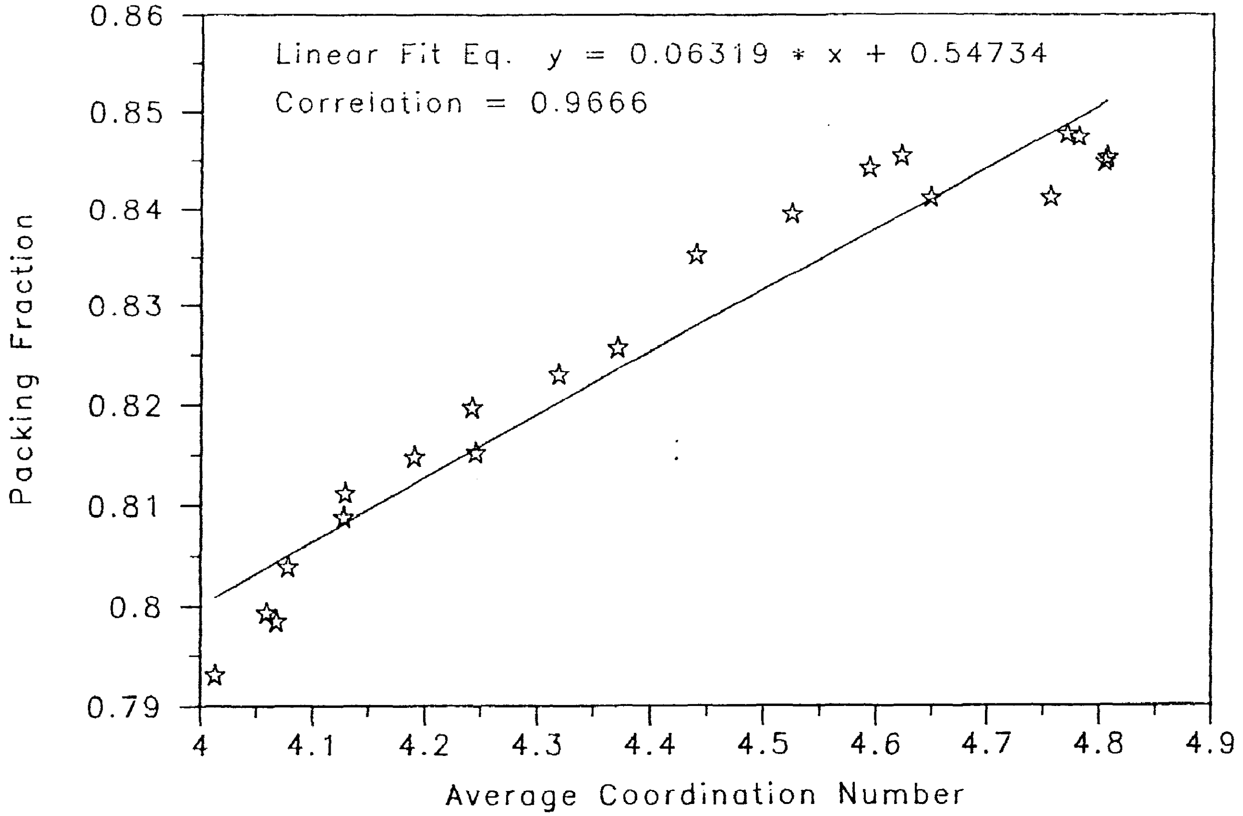


Figure 27: Packing fraction versus average coordination number: 1,000 disks with periodic boundary conditions.

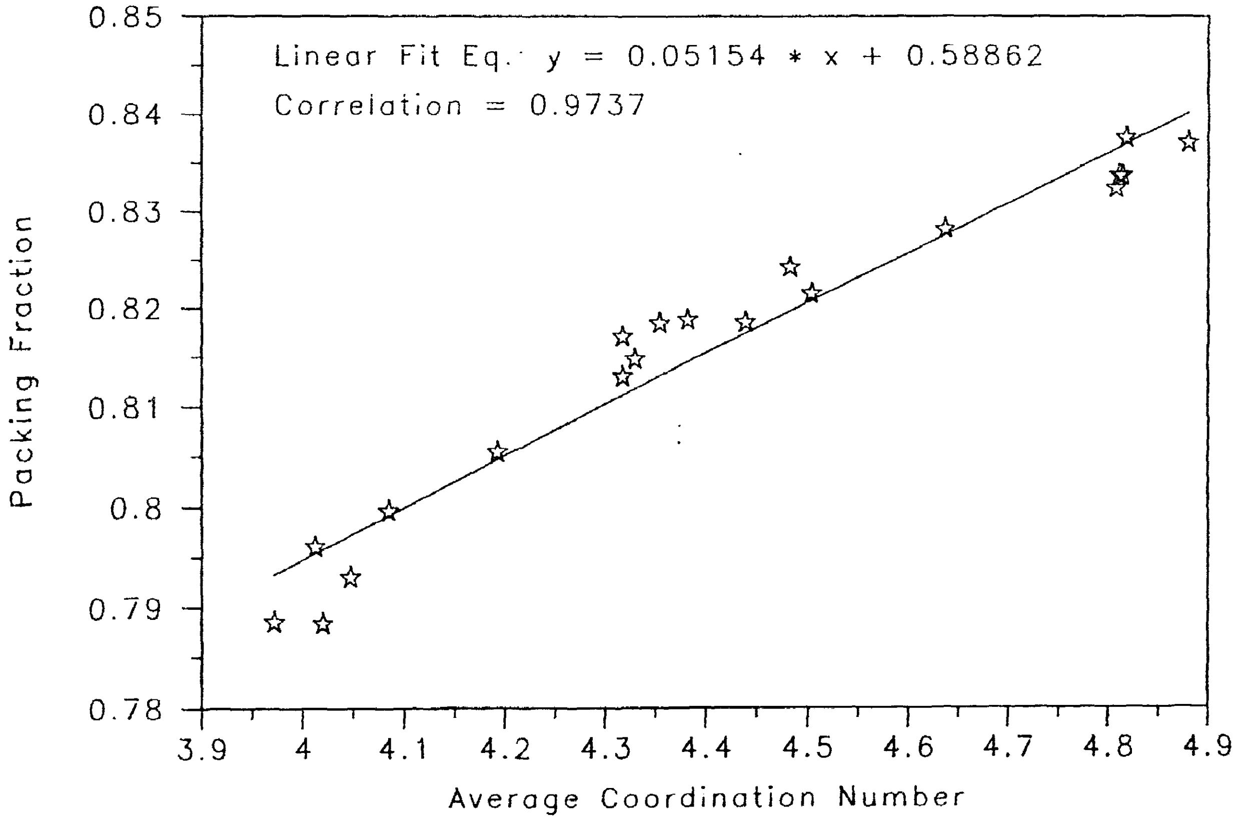


Figure 28: Packing fraction versus average coordination number: 1,250 disks with non-periodic boundary conditions.

fraction affected by walls is discussed.

Starting with an collection of 1,250 disks in a cell with hard vertical walls the poured configuration was obtained, and subsequently it was shaken for 19 cycles. To find the packing fraction variation near the wall, different *PF box*es were selected and the corresponding packing fractions were calculated.

The left edge of the *PF boxes* in which the packing fractions were determined, denoted PF_l, was fixed at the left wall of the configuration cell $x = 0$. The bottom edge, denoted PF_b, was fixed at the bottom of the cell $y = 0$. The top edge, denoted PF_t, was selected so that no top boundary disk would be included. Initially, the *PF box* had a width equal to one disk diameter. The right edge, denoted PF_r, was gradually moved until it coincided with the right wall of the cell. For any *PF box*, the packing fraction, η, is calculated as:

$$\eta = \frac{Sum\ of\ disk\ areas\ within\ the\ PF\ box}{PF\ box\ area} \tag{8}$$

Figure 29 shows the variation of η with respect to PF_r (normalized by the disk diameter). The packing fraction is smallest at the location of the wall and increases with the size of the $PFbox$. It reaches the average packing fraction discussed in Section 3.4.5 while PF_r moves to the right wall, which is far away from the left wall. The trend here is similar to that studied by Pillai [39] and Tory [23], in which the variation of cross sectional packing fraction of a monolayer with respect to the distance from the wall was of calculated.

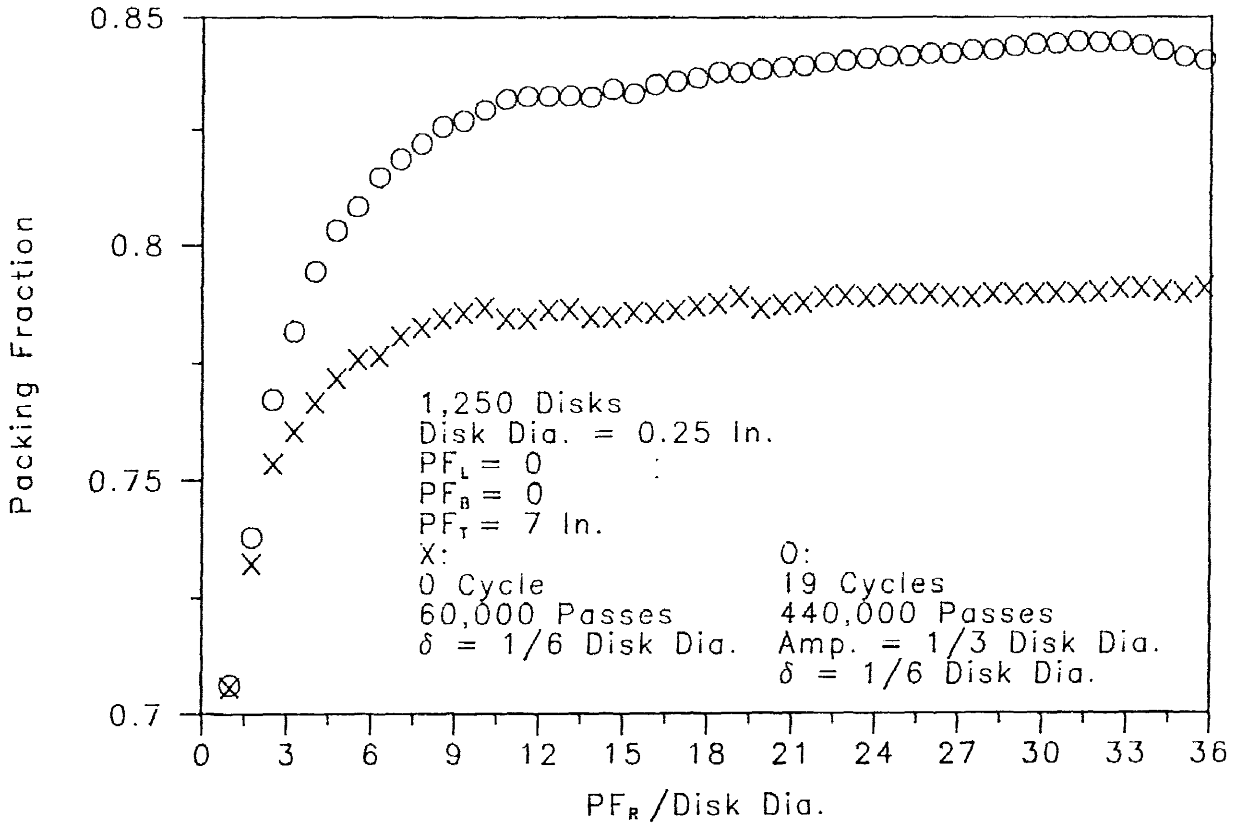


Figure 29: Influence of rigid walls on packing fraction for a 1,250 disk configuration.

4 Summary

The purpose of this work was to study the disk packing structure generated using a Monte Carlo technique, whereby disks slowly settle under gravity to the bottom of a container. This container of disks was then shaken, using a modification of the Monte Carlo code [42,43], and the resulting configurations were analyzed.

Two different types of boundary conditions were used: horizontal, periodic boundary conditions and rigid vertical walls. The former condition simulates a very large system by removing the restrictions imposed by hard vertical walls. In this way, the wall effects are eliminated. Imposition of hard vertical walls was done to study the effects of this type of boundary on the packing fraction. In order to analyze the configurations, an algorithm by Kurt E. Brassel and Douglas Reif [14] was chosen, modified and implemented to construct the Voronoi diagram. This permitted measurements of the distribution of coordination number, geometric and structural neighbors, distribution of structural neighbour angles, packing fraction and rigid wall effects. The Voronoi code was verified by checking that the average number of geometric neighbors, or the average number of sides of a Voronoi polygon, was equal to the mathematically proven value of six. In addition, the packing fraction for a hexagonally close-packed structure was computed as 0.906901, which agreed very well with the theoretically-computed value of 0.9068997. The structural neighbours of a disk (of diameter D) were defined as those disks whose centers were $(1+\epsilon)\cdot D$ away from the specific disk. The tolerance, ϵ, was chosen to be equal to Bernal's experimentally-determined value of 0.05. From the list of structural neighbours, the median nearest neighbor radius was computed. The cumulative probability of the median nearest neighbour radius was also computed. The upper bound value of r/D, for which the probability equaled unity, was 1.03. Therefore, the tolerance value of 0.03 may be considered a lower bound. Analyses on the sensitivity of the algorithm to the tolerance was not done. However, the variation of the coordination number versus tolerance gave an indication of this sensitivity over the range of tolerance values, from 0.0 to 0.2. A continuation of this curve past a tolerance of 0.2 would have resulted in an average coordination number of six, and hence all of the geometric neighbours would be captured.

After the pouring was completed, the assembly was shaken for a number of cycles. For both the periodic and non-periodic boundary conditions, this resulted in an increase of the coordination number after 19 cycles. Linear regressions on the coordination number versus cycle number resulted in a high correlation. The values predicted from the regression equation (in the case of periodic boundary conditions) agreed well with those calculated from the first peak of the radial distribution function for the poured and shaken assemblies. The increase of coordination number as shaking proceeds is physically reasonable and is a consequence of the densification of the assembly and an increase in the average number of contacts per disk. In fact, the structure was quite hexagonally close-packed and the packing fraction increased from its poured value of approximately 0.79 to 0.85. Linear regressions on the packing fraction versus cycle number yielded a high value of the correlation coefficient, indicating a good linear fit. A linear regression on the packing fraction against average coordination number also gave a very good linear fit.

The influence of the wall on the packing fraction was determined by using the hard vertical wall boundary conditions. A plot of the packing fraction versus normalized distance from the wall indicated that the wall had a strong influence up to approximately nine diameters away from the wall for the poured configuration. This influence extended somewhat further for the shaken assembly. The trend for both the poured and shaken assemblies were the same.

Two observations are made concerning the result of shaking the poured assembly of disks. The first of these deals with the coordination number, or the average number of structural neighbours. The simulated shaking has the effect of changing the poured, random configuration to a somewhat ordered, dense structure The average coordination number increased linearly with the cycle and this is physically realistic since shaking should cause an increase in the disk contacts. Secondly the packing fraction showed a six percent increase over its poured value. The structure became less random and appeared to more like an hexagonal close-packed crystal. This result is apparent from the actual disk configuration as well as from the fact that the peaks of the radial distribution function became more pronounced. The location of these peaks were in very good agreement with those of a hexagonal close-packed structure. In fact, the first three peaks are indicative of short-range order.

Extensions—the following is a listing of possible extensions to this research:

1. Study of the effect of the tolerance on the average coordination number.
2. Determination of the distribution of void space within the assembly.
3. Experimentation to verify the data with regard to the poured configuration.
4. Study of the angular distribution of geometric neighbours as the assembly densifies with shaking.
5. Extensions to three-dimensional systems of spheres.

Appendix:

A Definitions and Properties Regarding Voronoi Diagram

The Voronoi polygon[3], also termed *Thiessen polygon* [54] or *Dirichlet region* [17], is used to define the geometric neighbour. In any collection of points there is, about each point, a region containing all points of the plane closer to that point than to any other point. Dirichlet was first to describe these regions, hence the name Dirichlet region. It has been proven [49] that for any collection of points in the plane the Voronoi polygon has an average of six sides. If the perpendicular bisectors of all the lines connecting the point in question and all other points of the set are constructed, a set or polygons will result. The "closest" of these polygon, the one which is not truncated by any other line, is the one which satisfies the condition that it shall contain all points of plane closest to the point in question. With this understanding in mind, the following definitions quoted from D. T. Lee [30] are easier to understand:

Definition 5 *Given an ensemble S of points $\{p_1,\ p_2,\ \cdots,\ p_n\}$, the locus of points closer to p_i than to any other point is called the* Voronoi polygon, *denoted $V(p_i)$, associated with p_i.*

For an ensemble of n points, there are n Voronoi polygon associated with each and every point. A side of the Voronoi polygon is called a Voronoi Edge. A collection

[3] A Voronoi polygon corresponds to a two-dimensional point. However, a three-dimensional point will have a Voronoi polyhedron correspond to it.

of the n Voronoi polygon is called the Voronoi diagram $V(S)$.

Definition 6 *The points of the ensemble which contribute edges to the Voronoi polygon of a point are defined as the geometric neighbours of that point.*

Before applying the B-R Method, some properties of the Voronoi diagram are also needed to be discussed.

Definition 7 *A region R is star-shaped with nucleus p, where p is a point in R, if the line segment of p and any other point in R lies completely in R.*

Lemma 1 *Given an ensemble of points $\{p_1, p_2, \cdots, p_n\}$ and a point p, if the nearest neighbour of p is p_i, i.e., $p \in V(p_i)$, the Voronoi polygon associated with p_i, then the line segment $\overline{pp_i}$ lies entirely in $V(p_i)$.*

Proof: Referring to Figure 30 it is easy to demonstrate that the nearest neighbour of any point on the line segment $\overline{pp_i}$ is p_i if p_i is the nearest neighbour of p. Let $d(p, q)$ denote the distance between two points p and q. Suppose there exists a point q, $q \in \overline{pp_i}$ whose nearest neighbour is p_j, $j \neq i$; i.e.,

$$d(q, p_j) < d(q, p_i) \tag{9}$$

By the triangular inequality we have

$$d(p, p_j) \leq d(p, q) + d(q, p_j) \tag{10}$$

Further,

$$d(p, p_i) = d(p, q) + d(q, p_i) \tag{11}$$

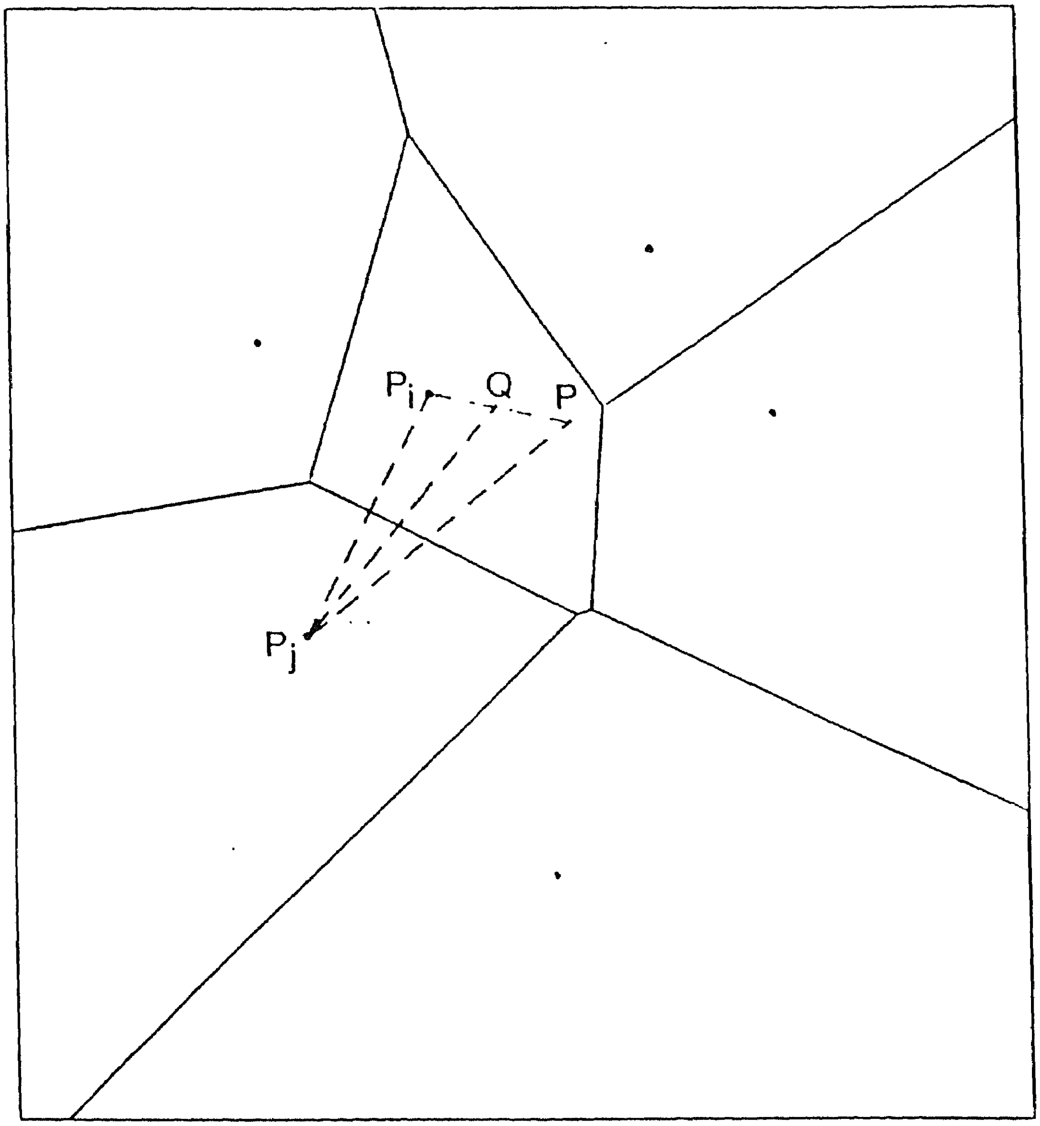


Figure 30: Lemma 1.

We thus have the following inequality from Eq. (9) – (11) above:

$$d(p, p_j) < d(p, p_i) \tag{12}$$

which contradicts the assertion that p_i is the nearest neighbour of p. Thus, for all points $q \in \overline{pp_i}$, p_i must be the one and only nearest neighbour of it, i.e., the line segment $\overline{pp_i}$ lies entirely in $V(p_i)$. ♯

From Definition 7 and Lemma 1, the following corollary is given:

Corollary 1 *Given an ensemble of points $\{p_1, p_2, \cdots, p_n\}$, the Voronoi polygon $V(p_i)$ is a star-shaped polygon with nucleus p_i.*

The angle extended from the nucleus to any two vertices in sequence of a *bounded* star-shaped polygon, $\angle AOB$ in Figure 31 for instance, must be less than π. The Voronoi polygon is a star-shaped polygon as of Corollary 1, it is thus followed:

Corollary 2 *Let point O and point A be the nucleus and one of the vertices of a bounded Voronoi polygon. Let $E_r(O, A)$ and $E_l(O, A)$ be the right and left half planes divided by vector $\overrightarrow{OA}$. Then, the next sequential vertex in clockwise direction to vertex A will lie in $E_r(O, A)$ and the next sequential vertex in counterclockwise direction to vertex A will lie in $E_l(O, A)$.*

This is a simple, while important property of Voronoi polygon.

Lemma 2 *Given an ensemble S of points $\{p_1, p_2, \cdots, p_n\}$, the Voronoi polygons $V(p_i)$ and $V(p_j)$ share an edge if and only if there exists a point q such that the circle*

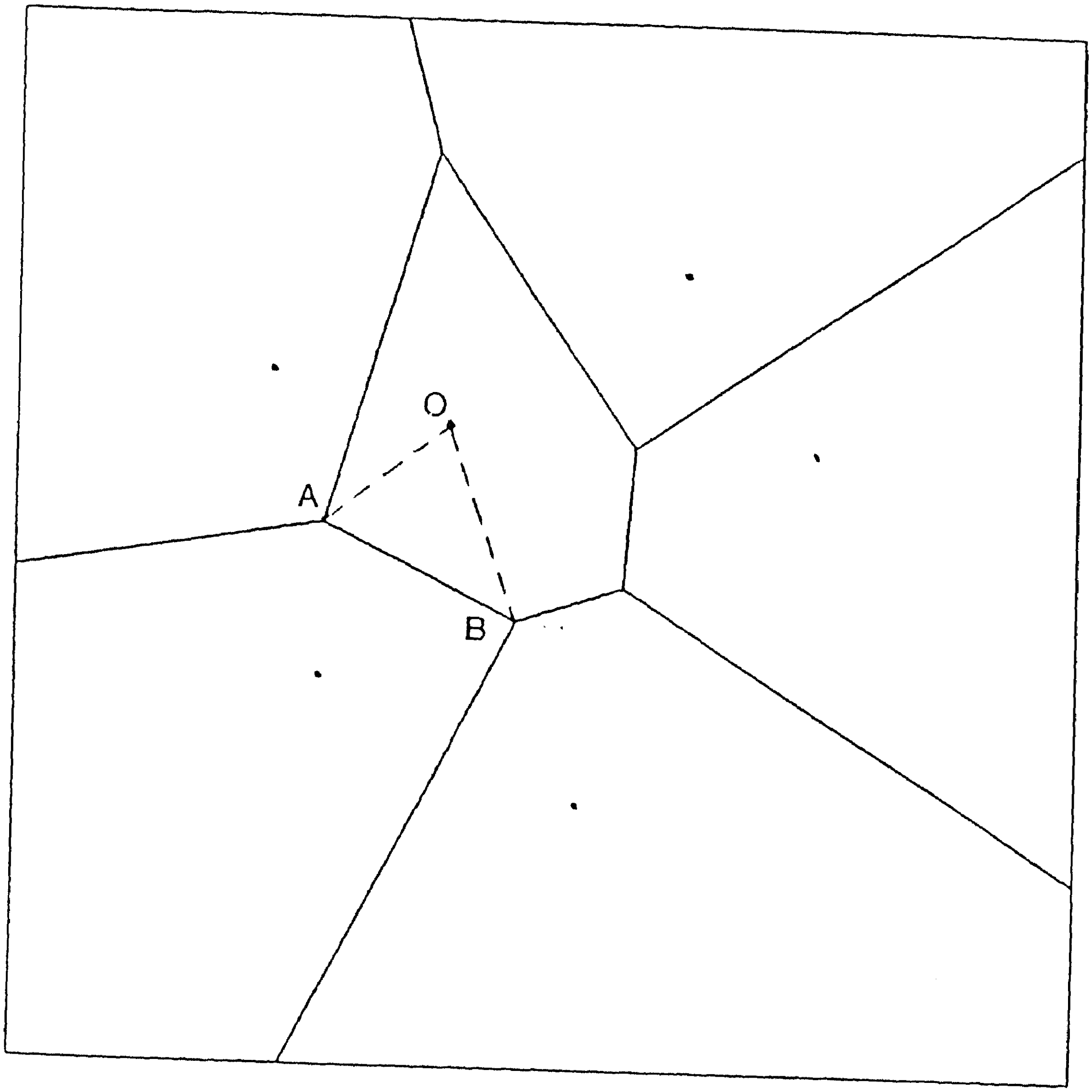


Figure 31: The extended angle AOB.

centered at q with radius $d(q, p_i)$ passing through points p_i and p_j does not include any other point of S in its interior or on its boundary.

Proof: Refer to Figure 32. Suppose there exists a point q satisfying this condition; the circle Q centered at q with radius $d(q, p_i)$ passing through points p_i and p_j does not include any other point of S. Then the point q must lie on the bisector $B(p_i, p_j)$ perpendicularly bisecting points p_i and p_j, and both p_i and p_j are its nearest neighbours. Since q is shared by $V(p_i)$ and $V(p_j)$, by continuity of the distance metric we can always find a portion of $B(p_i, p_j)$, denoted $\overline{B(p_i, p_j)}$, containing q such that every point on the line segment $\overline{B(p_i, p_j)}$ is shared only by $V(p_i)$ and $V(p_j)$. That is, some portion of $B(p_i, p_j)$ must be shared by $V(p_i)$ and $V(p_j)$.

To prove the converse, let us consider any point q on the edge shared by $V(p_i)$ and $V(p_j)$, but q is not an endpoint of the edge. Since both p_i and p_j are the nearest neighbours of q, the circle Q centered at q with radius $d(q, p_i)$ passes through p_i and p_j and will not contain any other point of S in its interior or on its boundary. $\sharp$

The two endpoints of $\overline{B(p_i, p_j)}$, if $\overline{B(p_i, p_j)}$ is bounded, are called Voronoi points. Each Voronoi point is equidistant from the points whose associated polygon have the Voronoi point in common. Thus, if $\overline{B(p_i, p_j)}$, $\overline{B(p_j, p_k)}$, and $\overline{B(p_k, p_i)}$ meet at a common point p, the point p is the circumcenter of the triangle $\Delta p_i p_j p_k$. If we assume that no more than three points are cocircular , then for each Voronoi point there are three Voronoi edges incident with it.

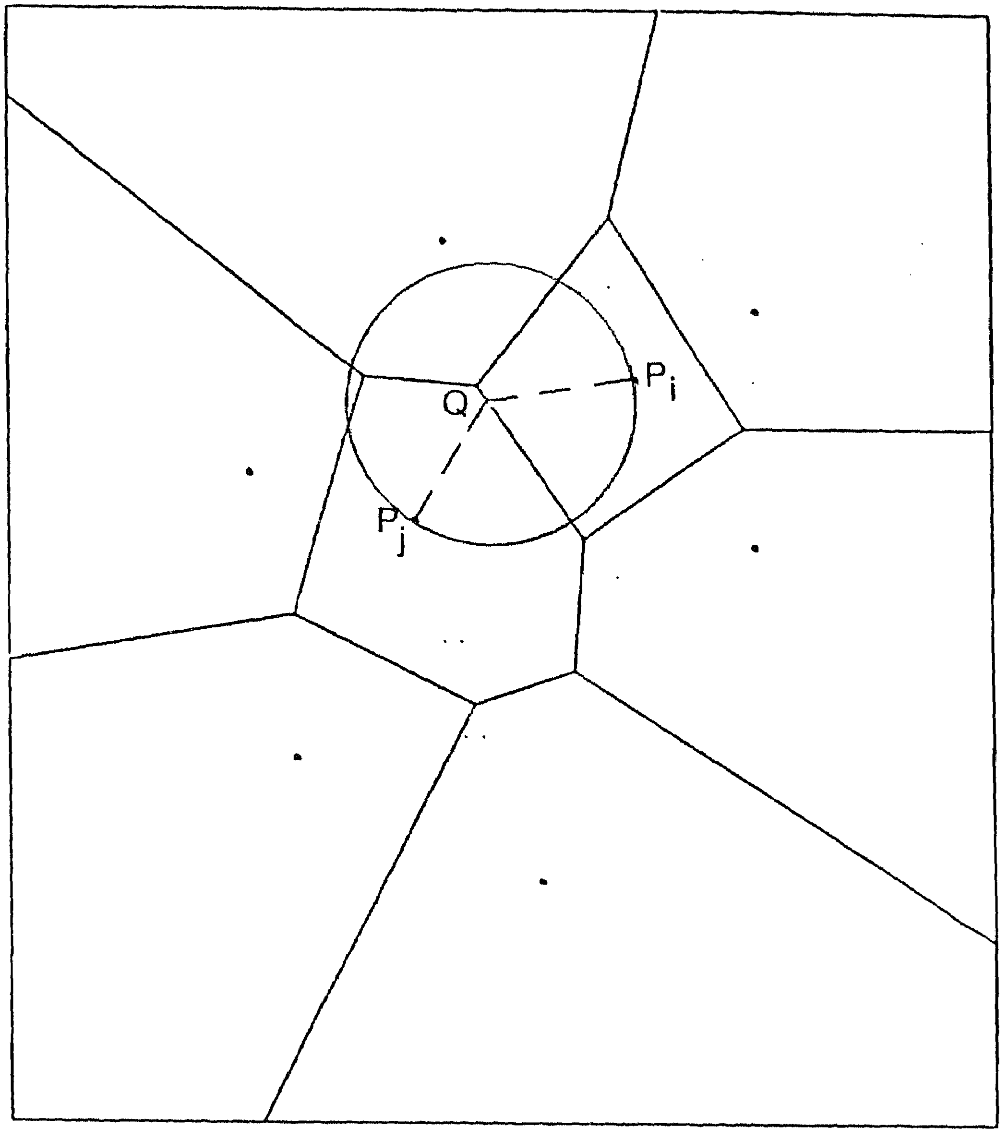


Figure 32: Lemma 2.

Lemma 3 *A point p equidistant to three points p_i, p_j, and p_k is a true Voronoi point if no other point is located within a circle centered at point p with radius the distance from point p to either one of the three points p_i, p_j, or p_k.*

Now, let us consider the *straight-line dual* of the Voronoi diagram $V(S)$, the Delaunay triangulation, denoted $D(S)$. $D(S)$ is a planar graph on the given set of points in which two points are connected if and only if their associated polygon share a Voronoi edge. $D(S)$ partitions the plane into a number of finite triangular regions and its complementary infinite region. The edges in $D(S)$ are called *Delaunay edges*. Since each Voronoi polygon $V(p_i)$ is star-shaped with nucleus p_i, the edges of the Voronoi polygon must occur in sequence, and the two corresponding Delaunay edges must appear in sorted angular order. In particular, the point p_i whose associated Voronoi polygon is unbounded will be on the boundary of $D(S)$, and the two boundary edges incident with p_i correspond to the two unbounded Voronoi edges. The Delaunay triangulations for a set of 1,000 points is shown in Figure 33. The corresponding configuration plot and Voronoi diagram are presented in Figures 34 to 36. The Delaunay triangulation can be said to be a byproduct of the Voronoi diagram. With some modifications, it can be applied for triangular mesh generation in finite element method. Knowledge on the Delaunay triangulation helps better understanding of the Voronoi diagram.

Definition 8 *Given two points p_i and p_j and a point p which lies to the left of the vector $\overrightarrow{p_ip_j}$ and on the bisector $B(p_i,p_j)$, the circle centered at p with radius $d(p,p_i)$*

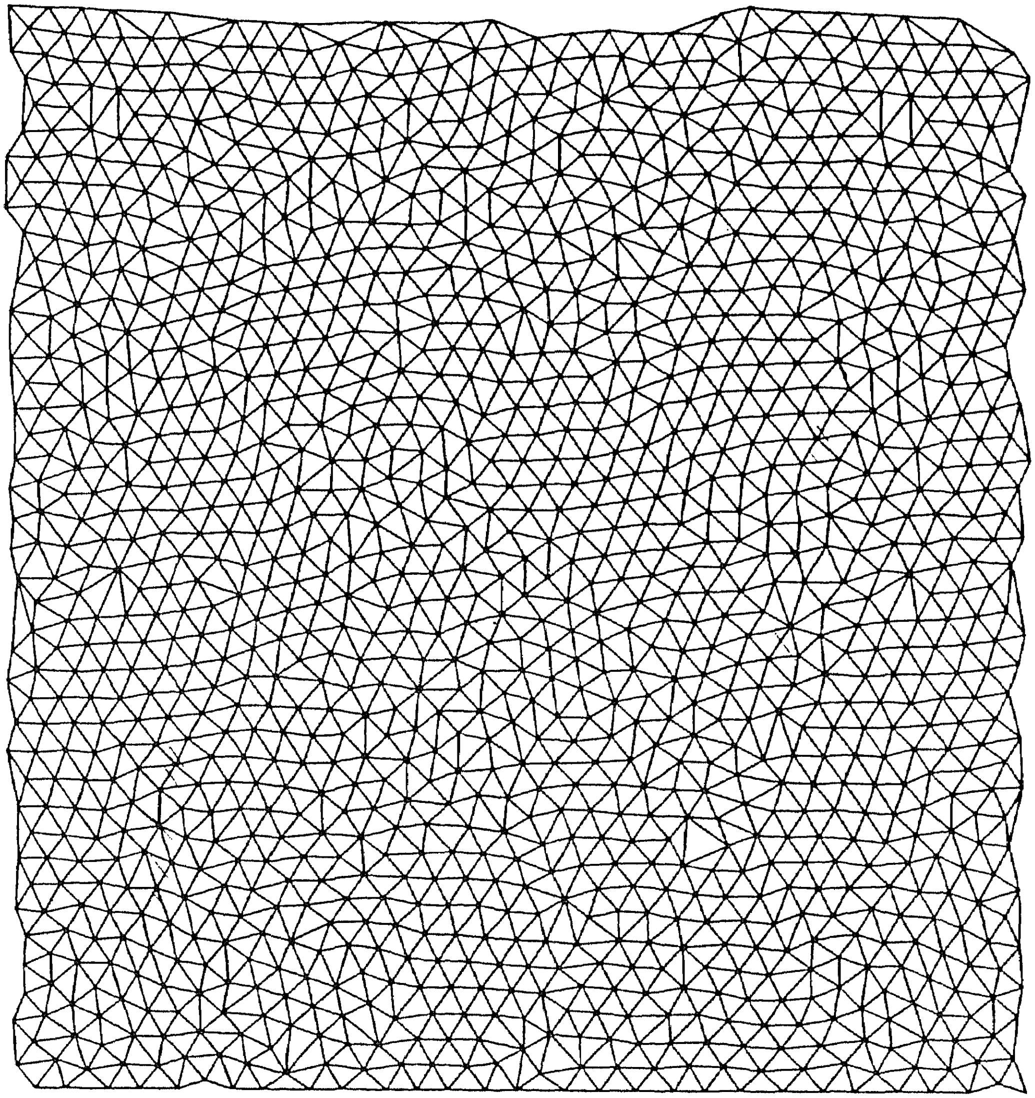
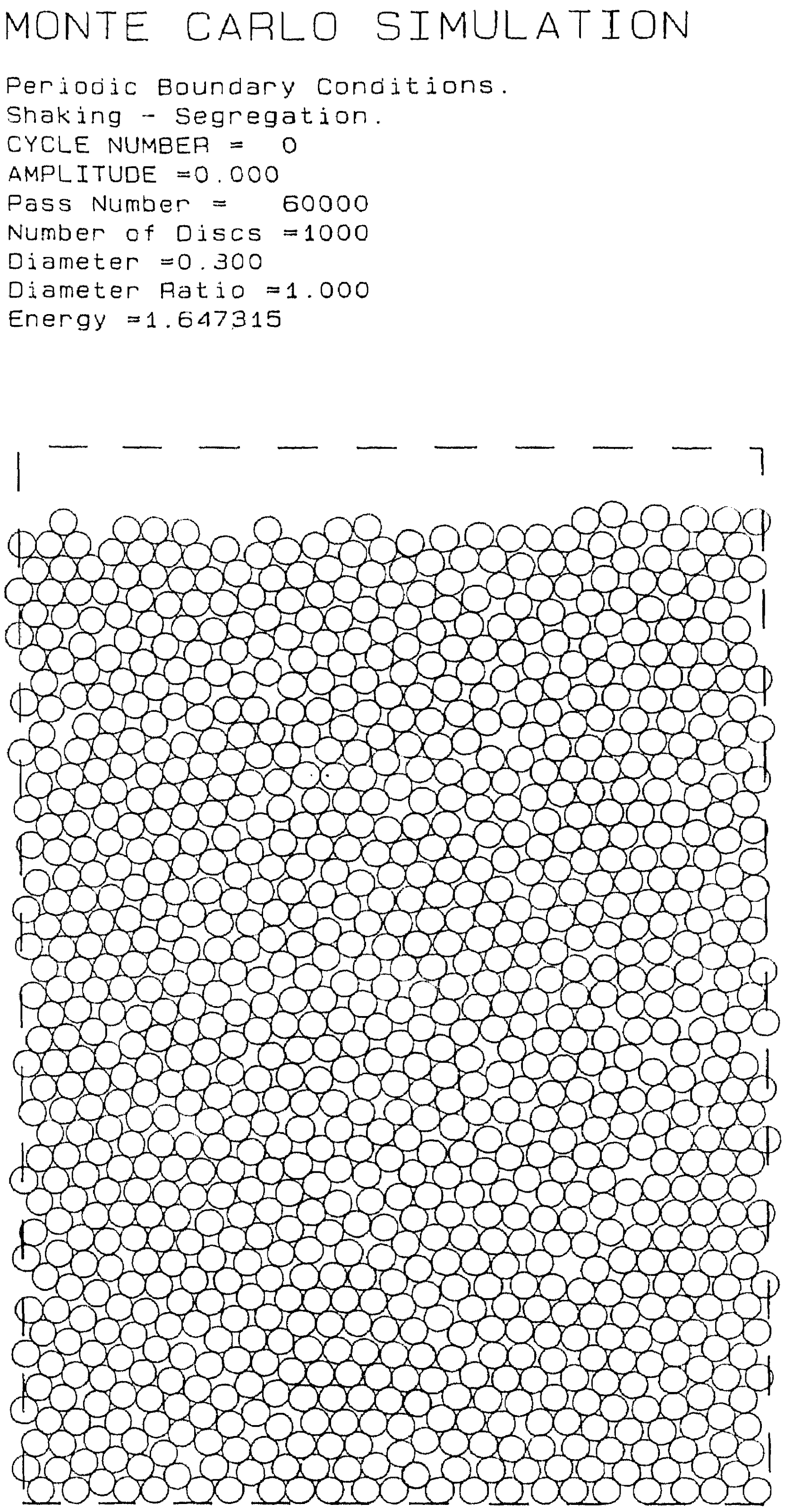


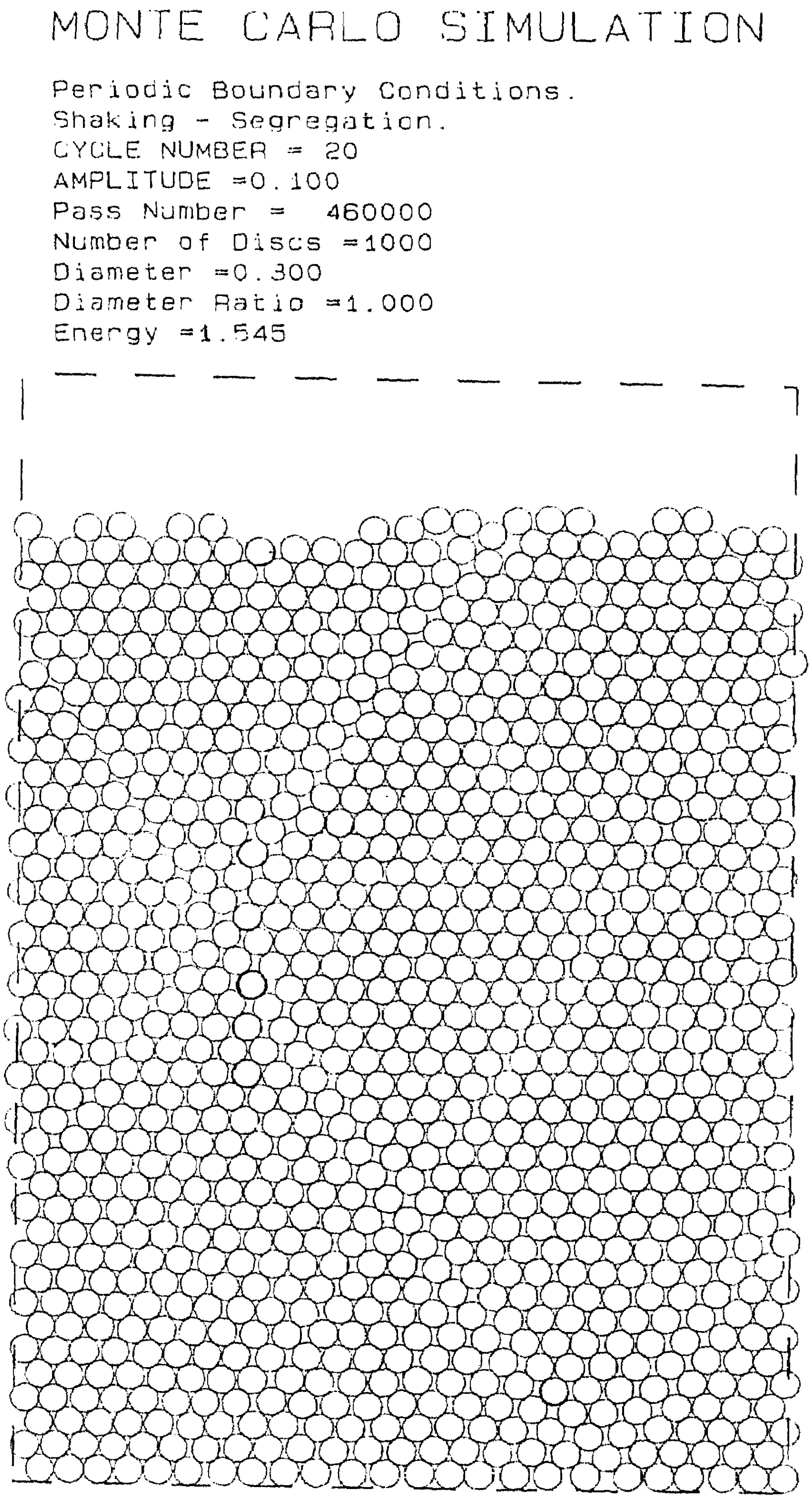
Figure 33: Delaunay traingulation of 1,000 disks after pouring.



```
MONTE CARLO SIMULATION

Periodic Boundary Conditions.
Shaking - Segregation.
CYCLE NUMBER =  0
AMPLITUDE =0.000
Pass Number =   60000
Number of Discs =1000
Diameter =0.300
Diameter Ratio =1.000
Energy =1.647315
```

Figure 34: The configuration of 1,000 disks after pouring —courtesy of A. Rosato, K. Reddy, and Y. Lan.



```
MONTE CARLO SIMULATION

Periodic Boundary Conditions.
Shaking - Segregation.
CYCLE NUMBER = 20
AMPLITUDE =0.100
Pass Number =  460000
Number of Discs =1000
Diameter =0.300
Diameter Ratio =1.000
Energy =1.545
```

Figure 35: The configuration of 1,000 disks after 20 cycles of shaking —courtesy of A. Rosato, K. Reddy, and Y. Lan.

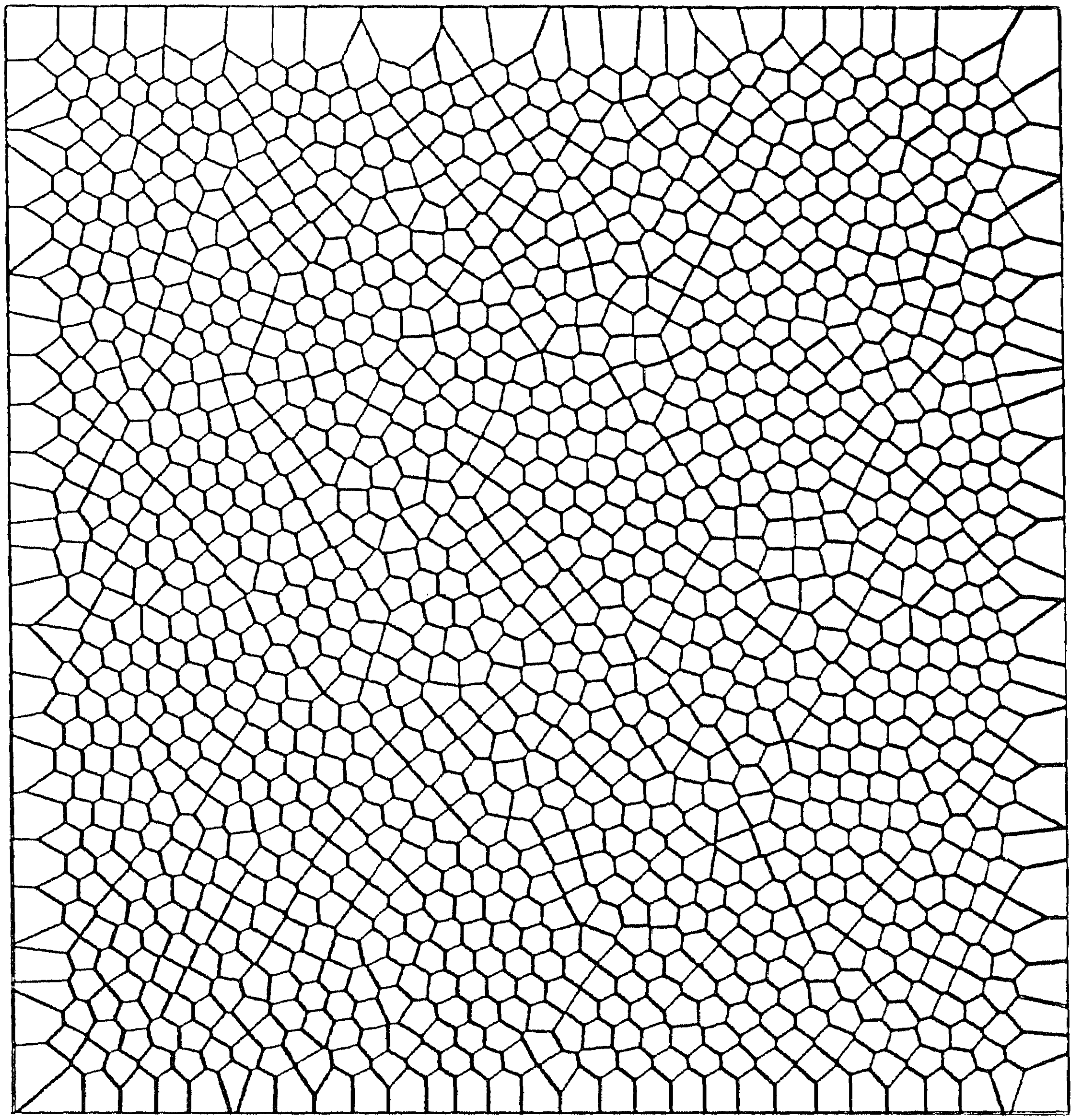


Figure 36: Voronoi diagram of 1,000 disks after pouring.

passes through p_i and p_j and is called the limiting circle $LC(p_i, p_j)$ of p_i and p_j when the radius approaches infinity. If p lies to the right of the vector $\overrightarrow{p_ip_j}$ (to the left of $\overrightarrow{p_jp_i}$), its corresponding limiting circle is denoted by $LC(p_j, p_i)$.

In L_2-Metric [30], the limiting circle $LC(p_i, p_j)$ and $LC(p_j, p_i)$ coincides and is the line $\overleftrightarrow{p_ip_j}$.

Theorem 1 *The boundary of the dual graph $D(S)$ of the Voronoi diagram $V(S)$ is the convex hull $CH(S)$ of the set S of points.*

Proof: Referring to Figure 37. Suppose $\overline{p_ip_j}$ is an edge of the convex hull $CH(S)$, shown in dashed line, of the set S of points. All the points of S must lie on one side of the line $\overleftrightarrow{p_ip_j}$ containing $\overline{p_ip_j}$. Suppose $S \subset E_r(p_i, p_j) \cup \overleftrightarrow{p_ip_j}$, i.e., the points of S lie to the right of $\overrightarrow{p_ip_j}$. Consider the limiting circle $LC(p_i, p_j)$, which is the straight line $\overleftrightarrow{p_ip_j}$ and hence does not contain any other point of S in its interior. From Lemma 2, the perpendicular bisector $B(p_i, p_j)$ must contain an unbounded Voronoi edge of $V(S)$, and so must $\overline{p_ip_j}$ be a Delaunay edge.

Now, suppose $\overline{p_ip_j}$ is a Delaunay edge on the boundary of $D(S)$. Since it corresponds to an unbounded Voronoi edge on $B(p_i, p_j)$, the limiting circle centered at the unbounded end of $B(p_i, p_j)$ does not contain any other point in its interior. That is, all the points lie on one side of the line containing $\overline{p_ip_j}$. Therefore $\overline{p_ip_j}$ is an edge on the convex hull $CH(S)$. This completes the proof. $\natural$

In other words, $\overline{p_ip_j}$ is a boundary edge of $D(S)$ if and only if one of the limiting circles of p_i and p_j does not contain any other point of S in its interior. Each boundary

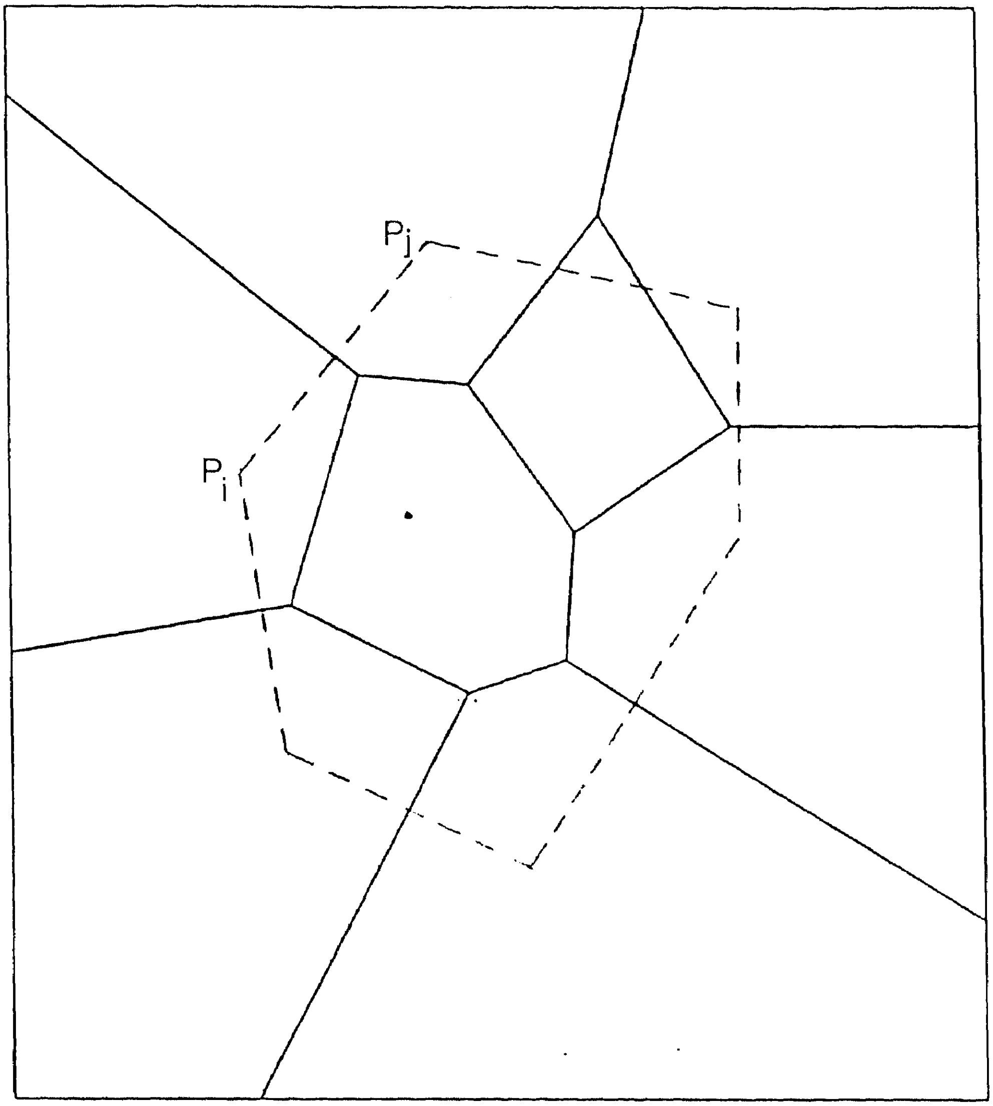


Figure 37: Theorem 1.

edge of $D(S)$ has an unbounded Voronoi edge corresponding to it. This can be extended to another statement:

> The number of points on the convex hull of the ensemble S is the same as the number of unbounded Voronoi polygon in the Voronoi diagram $V(S)$.

Theorem 2 *Given an set S of points $\{p_1, p_2, \cdots, p_n\}$, let $D_i(S)$ denote the subset of points of S which are connected to p_i in the Delaunay triangulation. Then $D_i(S)$ contains the nearest neighbour of p_i, i.e., there exists a point $p_j \in D_i(S)$ such that*

$$d(p_i, p_j) = min_{q \in S - p_i} d(q, p_i)$$

Proof: Referring to Figure 38, $D_i(S)$ is composed of $\{p_r, p_s, p_t, p_u, p_v\}$. Suppose the nearest neighbours of p_i are not contained in $D_i(S)$. Let p_k be the nearest neighbour of p_i. Then $d(p_k, p_i) < d(q, p_i)$ for all $q \in D_i(S)$.

Consider the line segment $\overline{p_k p_i}$, it must intersect some Voronoi edge of the Voronoi polygon, say point z on $\overline{B(p_i, p_s)}$. By definition, $p_s \in D_i(S)$ and

$$d(z, p_s) = d(z, p_i) \tag{13}$$

Also, the circle centered at z with radius $d(z, p_i)$ does not contain any other point of S. So,

$$d(z, pi) < d(z, p_k) \tag{14}$$

From Eq. (13) and (14) and the triangular inequality:

$$d(p_s, p_i) \leq d(z, p_s) + d(z, p_i) < d(z, p_k) + d(z, p_i) = d(p_k, p_i) \tag{15}$$

This is a contradiction of the assumption. therefore $D_i(S)$ contains the nearest neighbour of p_i. $\sharp$

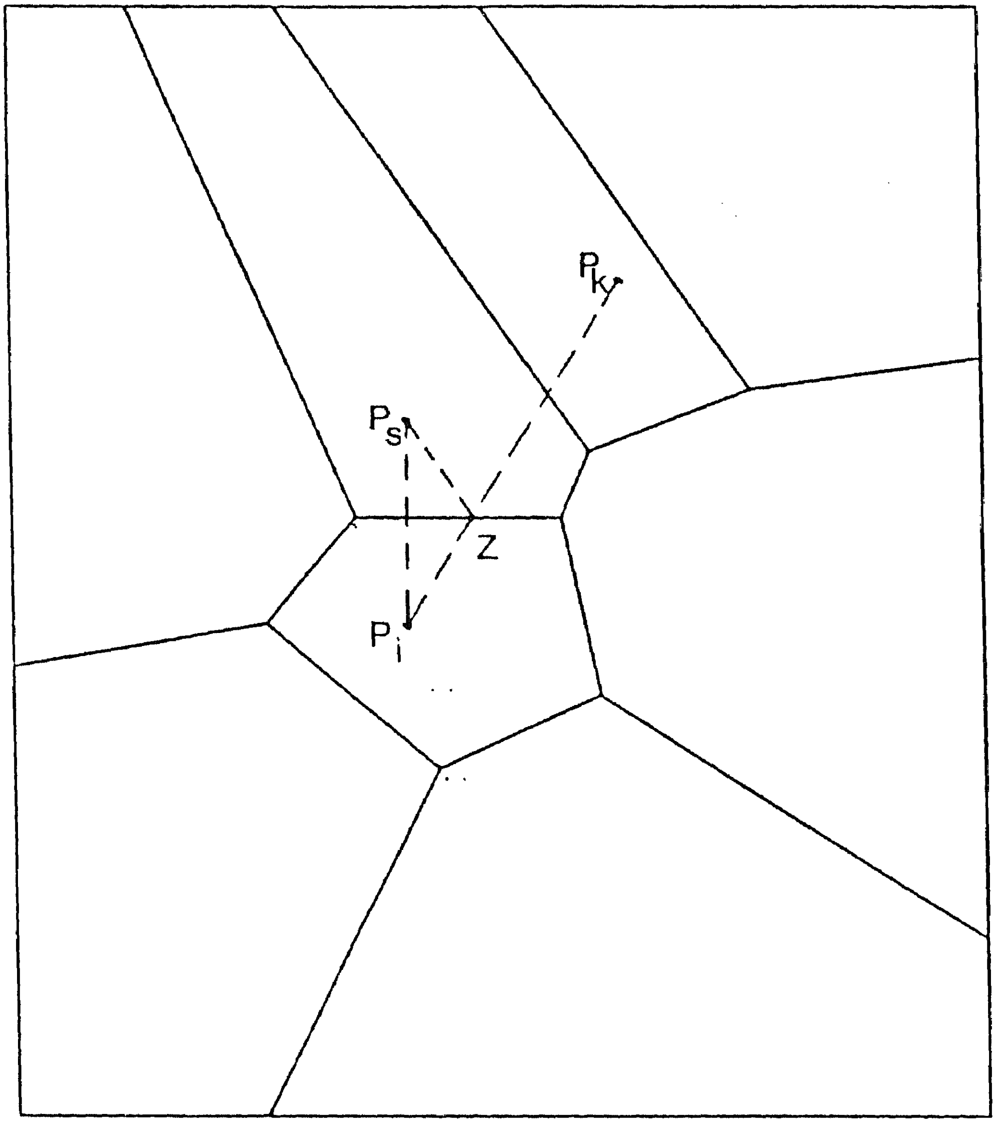
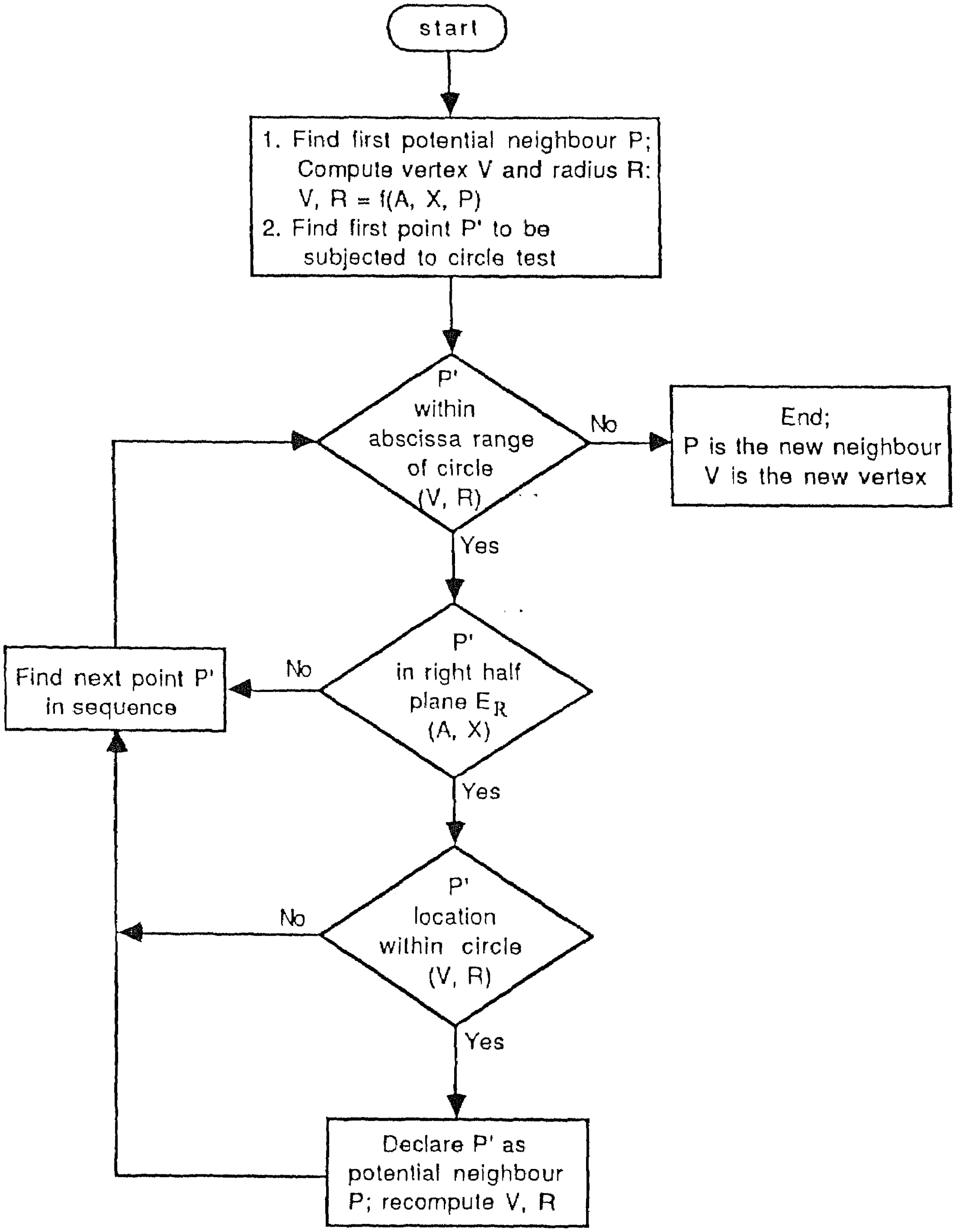
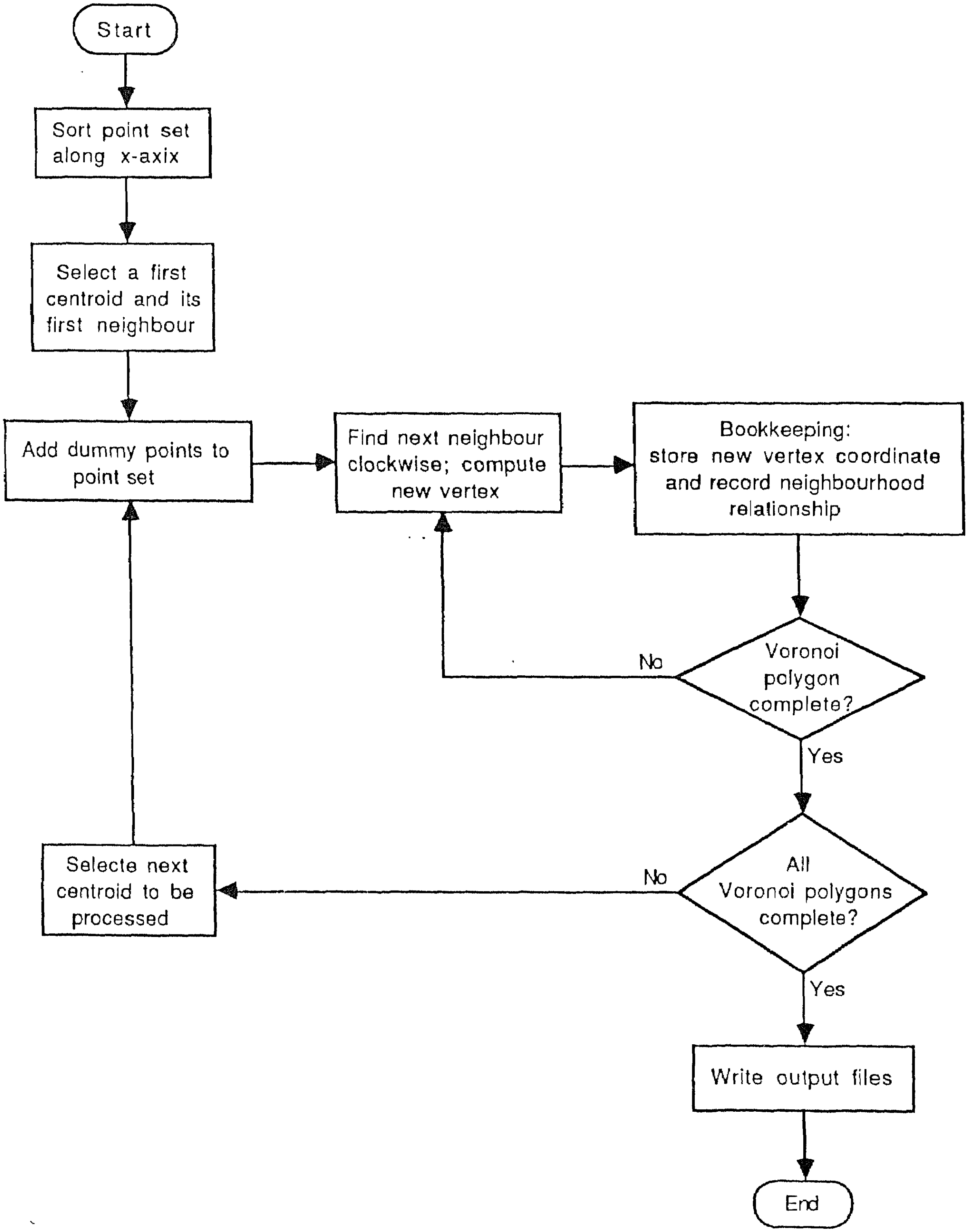


Figure 38: Theorem 2.

B Algorithm Finding Next Clockwise Geometric Neighbour


start
1. Find first potential neighbour P;
Compute vertex V and radius R:
V, R = f(A, X, P)
2. Find first point P' to be
subjected to circle test
P' within abscissa range of circle (V, R)
No
End;
P is the new neighbour
V is the new vertex
Yes
P' in right half plane E_R (A, X)
No
Find next point P' in sequence
Yes
P' location within circle (V, R)
No
Yes
Declare P' as potential neighbour P; recompute V, R

C Strategy on Completing the Voronoi Diagram


Start
Sort point set along x-axix
Select a first centroid and its first neighbour
Add dummy points to point set
Find next neighbour clockwise; compute new vertex
Bookkeeping: store new vertex coordinate and record neighbourhood relationship
Voronoi polygon complete?
No
Yes
All Voronoi polygons complete?
No
Yes
Selecte next centroid to be processed
Write output files
End

D Program disk.pas

```
(******************************************************************************)
(*                                                                            *)
(*                          INTRODUCTION                                      *)
(*                                                                            *)
(*          -------------------------------------------------------           *)
(*                                                                            *)
(*      THE CODE ANALYZES AN ENSEMBLE OF DISKS, EITHER IN THE SAME  SIZE  OR  *)
(*  IN DIFFERENT SIZES, WITH OR WITHOUT  PERIODICAL  BOUNDARY  CONDITION  IN  *)
(*  THE HORIZONTAL DIRECTION.                                                 *)
(*                                                                            *)
(*      FIRST, A LINKED LIST 'RANDOM' IS CREATED.  IT CONTAINS THE INDEX AND  *)
(*  THE DIAMETER OF THE DISK, AND THE COORDINATES OF  THE  CENTROID.  BEFORE  *)
(*  PROCESSING, WE SORT THE LINKED LIST IN LEXICOGRAPHICAL  ORDER  AND  NAME  *)
(*  THE SORTED LINKED LIST 'SORT'.  A SORTED TWO-DIMENSIONAL COORDINATES  IN  *)
(*  LEXICOGRAPHICAL ORDER IS INTERPRETED AS: P1  (X1,  Y1)  IS  SAID  TO  BE  *)
(*  LEXICOGRAPHICALLY LESS THAN P2 (X2, Y2), IF AND ONLY  IF  X1  <  X2,  OR  *)
(*  X1 = X2 AND Y1 < Y2.                                                      *)
(*                                                                            *)
(*      SECOND, THE VORONOI  DIAGRAM  IS  GENERATED  ACCORDING  TO  THE  B-R  *)
(*  METHOD, WHICH IS CONSTRUCTED BY KURT E. BRASSEL AND DOUGLAS  REIF.   THE  *)
(*  GEOMETRIC NEIGHBOURS ARE THUS FOUND.  IN VIEWING THE VORONOI DIAGRAM, WE  *)
(*  FIXED A BOX WHICH IS EXPRESSED EXPLICITLY:                                *)
(*                                                                            *)
(*  BOX = (X, Y) | XMIN - BOX_C * DMAX <= X <= XMAX + BOX_C * DMAX;           *)
(*                 YMIN - BOX_C * DMAX <= Y <= YMAX + BOX_C * DMAX            *)
(*                                                                            *)
(*  WHERE XMIN,  XMAX,  YMIN  AND  YMAX  ARE  THE  EXTREMUM  COORDINATES  OF  *)
(*  CENTROIDS OF THE DISKS, DMAX IS THE MAXIMUM DIAMETER OF THE  DISKS,  AND  *)
(*  BOX_C IS A CONSTANT WHICH DETERMINES THE SIZE OF THE BOX.                 *)
(*                                                                            *)
(*      FROM THE GEOMETRIC NEIGHBOURS WE CHOOSE THE  NEAREST  NEIGHBOUR  AND  *)
(*  COMPUTE MEDIAN NEAREST NEIGHBOUR RADIUS.  FOR DISKS OF SAME SIZE, IF THE  *)
(*  MEDIAN NEAREST NEIGHBOUR RADIUS IS GREATER  THEN  THE  DIAMETER  OF  THE  *)
(*  DISKS (OR (1 + TOLERANCE) * DIAMETER)), THE ENSEMBLE IS TOO THIN TO BE A  *)
(*  RANDOM CLOSE PACKING.  NO FURTHER ANALYSIS IS GOING TO BE MADE  IN  THIS  *)
(*  CASE OTHERWISE, WE PROCEDE AND PERFORME THE FOLLOWING ANALYSIS.           *)
(*                                                                            *)
(*      TO BEGIN WITH, WE FIX ANOTHER INNER BOX, AND DELETE ALL THOSE  DISKS  *)
(*  COMPLETELY OUT OF THE INNER BOX.  THE REMAINING LINKED  LIST,  WHICH  IS  *)
(*  CALLED 'INNER', CONTAINS ONLY DISKS IN OR ON THE BOUNDARY OF  THE  INNER  *)
(*  BOX AND WITH BOUNDED VORONOI POLYGONS.  THE  STATICS  WILL  BE  MADE  ON  *)
(*  THESE DISKS.                                                              *)
(*                                                                            *)
(*      THE  STRUCTURAL  NEIGHBOURS  ARE  PICKED  OUT  FROM  THE   GEOMETRIC  *)
(*  NEIGHBOURS.  AGAIN, THE SAME TOLERANCE FOR DETERMINING THE RANDOM  CLOSE  *)
(*  PACKING IS  APPLIED  TO  DECIDE  WHETHER  A  GEOMETRIC  NEIGHBOUR  IS  A  *)
(*  STRUCTURAL NEIGHBOUR OR NOT.  A TOLERANCE 0.05 IS SELECTED IN OUR  CASE,  *)
(*  WHICH WAS THE TOLERANCE J. D. BERNAL USED IN HIS 3-D MODEL.               *)
(*                                                                            *)
(*      ANGLES FROM THE POSITIVE X-DIRECTION TO A LINE FROM THE CENTROID  OF  *)
(*  THE CENTER DISK  TO  THE  CENTROID  OF  EACH  STRUCTURAL  NEIGHBOUR  ARE  *)
(*  CALCULATED.  THE STATISTICS IS THEN CARRIED OUT, WHICH INCLUDS:           *)
(*                                                                            *)
(*      1. THE MEAN VALUE  AND  DISTRIBUTION  OF  THE  NUMBER  OF  GEOMETRIC  *)
(*         NEIGHBOUR.                                                         *)
(*      2. THE MEAN VALUE AND  DISTRIBUTION  OF  THE  NUMBER  OF  STRUCTURAL  *)
(*         NEIGHBOUR.                                                         *)
(*      3. CATEGOERISE INNER  DISKS  WITH  THE  SAME  NUMBER  OF  STRUCTURAL  *)
(*         NEIGHBOURS IN GROUPS.  THEN, FOR EACH GROUP, FIND:                 *)
(*         THE MEAN VALUE, THE STANDARD DEVIATION, AND THE DISTRIBUTION  FOR  *)
(*         THE ANGLE ASSOCIATED WITH THE FIRST, THE SECOND,..., DOWN TO  THE  *)
(*         LAST STRUCTURAL NEIGHBOUR.                                         *)
(*      4. PACKING FRACTION, WHICH IS DEFINED AS:                             *)
(*                                                                            *)
(*                     DISK AREA WITHIN THE INNER BOX                         *)
(*              ETA = -------------------------------                         *)
(*                             INNER BOX AREA                                 *)
(*                                                                            *)
(*      IF THE CONFIGURATION IS CONSTRAINED BY TWO VERTICAL WALLS, THE RIGID  *)
(*  WALL EFFECT MAY BE CALCULATED IF DESIRED.  THIS CONCLUDES THE CODE.       *)
(*  ************************************************************************  *)
(*                                                                            *)
(*                           INPUT AND OUTPUT                                 *)
(*                                                                            *)
(*                ---------------------------------------                     *)
(*                                                                            *)
(*      TO RUN THE CODE, A INPUT FILE DISKIN.DAT IS FIRST CREATED.  THE DATA  *)
(*      PROVIDED IN DISKIN.DAT ARE LISTED BELOW:                              *)
(*                                                                            *)
(*      LINE #    DATA                                                        *)
(*  ----------------------------------------------------------------------    *)
(*        1       # OF DISKS                                                  *)
(*        2       BOOLEAN VARIABLE IF ALL DISKS ARE OF SAME SIZE              *)
(*        3       BOOLEAN VARIABLE IF GIVEN ENSEMBLE IS KNOWN TO BE A RANDOM  *)
(*                CLOSE PACKING                                               *)
(*        4       DISTANCE BETWEEN VERTICAL PERIODICAL BOUNDARIES OR WALLS    *)
(*        5       BOOLEAN VARIBLE IF THE PERIODICAL BOUNDARY CONDITION IS TO  *)
(*                BE IMPLEMENTED                                              *)
(*        6       BOOLEAN VARIABLE IF THE WALL EFFECT IS TO BE CALCULATED     *)
(*        7       HEIGHT OF THE INNER BOX AND WIDTH OF THE INNER BOX          *)
(*        8       BOOLEAN  VARIABLE  IF  THE  BOX  FOR  CALCULATING  PACKING  *)
(*                FRACTION IS TO BE DEFINED DIFFERENT FROM THE INNER BOX      *)
(*        8'      IF 8 IS TRUE, GIVE  PF_L,  PF_R,  PF_B,  PF_T,  SUCH  THAT  *)
(*                X = PF_L, X = PF_R, Y = PF_B, AND Y = PF_T CONSTITUTE  THE  *)
(*                BOX FOR CALCULATING PACKING FRACTION                        *)
(*        9       TOLERANCE FOR DETERMINING STRUCTURAL NEIGHBOUR              *)
(*       10       NUMBER OF ANGULAR DIVISION                                  *)
(*    10 TO EOF   INDEX, X-COORDINATE, Y-COORDINATE, DIAMETER OF A DISK       *)
(*                                                                            *)
(*      THE CODE  THEN  GIVES  SIX  OUTPUT  FILES:  NBRFILE,  VTXFILE,  BOX,  *)
(*  SNBRFILE, DELAUNAY, AND TABLE AFTER  BEING   RUN.    EACH   OUTPUT  FILE  *)
(*  CONTAINS THE FOLLOWING INFORMATIONS:                                      *)
(*                                                                            *)
(*     1) NBRFILE: 'NUM_LOOP' (NUMBER OF DISKS TO BE  PROCESSED  AFTER  THE  *)
(*                 IMPLEMENTATION OF PERIODICAL BOUNDARY CONDITION; SAME AS  *)
(*                 NUMBER OF DISK  IF  PERIODICAL  BOUNDARY  CONDITION  NOT  *)
(*                 REQUIRED) OF LINKED LIST OF NEIGHBOURS; THE  FIRST  NODE  *)
(*                 IN THE LIST BE THE CENTER DISK.                           *)
(*     2) VTXFILE: 'NUM_LOOP' OF LINKED LIST OF VERTICES.  THIS  FILE  WILL  *)
(*                 BE   USED   AS   THE   INPUT   FILE   OF   THE   PROGRAM  *)
(*                 'VORONOIFILE.FOR', WHICH TRANSFORM  'VTXFILE'  INTO  THE  *)
(*                 FORMAT HP7580_A PLOTTER CAN READ.                         *)
(*     3) BOX: GIVES THE COORDINATES OF THE VIEWING BOX AND THE INNER  BOX,  *)
(*             'NUM_LOOP', AND 'NUM_IN' (NUMBER OF DISKS IN OR ON THE INNER  *)
(*             BOX), AND ERROR MESSAGES IF ANY, ETC.                         *)
(*     4) SNBRFILE: 'NUM_IN' OF LINKED LIST OF  STRUCTURAL  NEIGHBOURS  FOR  *)
(*                  INNER DISKS; THE FIRST NODE BE THE CENTER DISK.          *)
(*     5) DELAUNAY: END POINTS OF EDGES  OF  DELAUNAY  TRINAGULATION.  THIS  *)
(*                  FILE WILL BE USED AS THE  INPUT  FILE  OF  THE  PROGRAM  *)
(*                  'DELAUNAYFILE.FOR', WHICH TRANSFORM 'DELAUNAY.DAT' INTO  *)
(*                  THE FORMAT HP7580_A PLOTTER CAN READ.                    *)
(*     6) TABLE: GIVES THE FOLLOWING INFORMATION FOR EACH INNER DISK:        *)
(*       A) THE NUMBER OF GEOMETRIC NEIGHBOUR AND STRUCTRUAL NEIGHBOUR.      *)
(*       B) THE INDEX OF EACH GEOMETRIC NEIGHBOUR AND STRUCTRUAL NEIGHBOUR.  *)
(*       C) THE ANGLE ASSOCIATED WITH EACH STRUCTRUAL NEIGHBOUR.             *)
(*       D) THE MEAN  VALUE  OF  THE  NUMBER  OF  GEOMETRIC  NEIGHBOUR  AND  *)
(*          STRUCTURAL NEIGHBOUR.                                            *)
(*       E) THE CUMULATIVE PROBABILITY OF THE NEAREST NEIGHBOUR RADIUS.      *)
(*       F) THE DISTRIBUTION OF  THE  NUMBER  OF  GEOMETRIC  NEIGHBOUR  AND  *)
(*          STRUCTURAL NEIGHBOUR.                                            *)
(*       G) FOR EACH CATEGORISED GROUP WITH THE SAME NUMBER  OF  STRUCTURAL  *)
(*          NEIGHBOURS,                                                      *)
(*         a) THE MEAN VALUE OF THE ANGLE ASSOCIATED WITH  THE  FIRST,  THE  *)
(*            SECOND,..., DOWN TO THE LAST STRUCTURAL NEIGHBOUR.             *)
(*         b) THE STANDARD DEVIATION  OF  THE  ANGLE  ASSOCIATED  WITH  THE  *)
(*            THE FIRST,  THE  SECOND,...,  DOWN  TO  THE  LAST  STRUCTURAL  *)
(*            NEIGHBOUR.                                                     *)
(*         c) THE DISTRIBUTION OF THE ANGLE ASSOCIATED WITH THE FIRST,  THE  *)
(*            SECOND,..., DOWN TO THE LAST STRUCTURAL NEIGHBOUR.             *)
(*       H) THE PACKING FRACTION.                                            *)
(*       AND IF WALL EFFECT IS TO BE FOUND:                                  *)
(*       I) PACKING FRACTION VARIATION.                                      *)
(* ************************************************************************ *)
(*                                                                          *)
(*                            NOMENCLATURE                                  *)
(*                                                                          *)
(*          ------------------------------------------------------          *)
(*                                                                          *)
(* NUM_DISK     : NUMBER OF DISKS TO BE HANDELED.                           *)
(* NUM_LOOP     : NUMBER OF DISKS TO BE HANDELED AFTER  THE  IMPLEMENTATION *)
(*                OF THE PERIODICAL BOUNDARY CONDITION.                     *)
(* NUM_IN       : NUMBER OF DISKS IN OR ON THE BUNDARY OF  THE  INNER  BOX; *)
(*                NUMBER OF INNER DISKS.                                    *)
(* NUM_ANG_DIV  : NUMBER OF ANGULAR DIVISION FOR THE STATICS ON THE ANGULAR *)
(*                DISTRIBUTION.                                             *)
(* Z            : DUMMY TAIL OF A LINKED LIST.                              *)
(*  RANDOM          : RANDOM LINKED LIST OF DISKS.                            *)
(*  SORT            : SORTED LINKED LIST OF DISKS.                            *)
(*  INNER           : LINKED LIST OF DISKS IN OR ON THE INNER BOX.            *)
(*  LAST            : MOVING POINTER IN THE LINKED LIST.                      *)
(*  NBR [K]         : ELEMENT OF ARRAY OF LINKED LIST OF GEOMETRIC  NEIGHBOURS, *)
(*                    WITH THE CENTER DISK AS THE LIST HEAD.                  *)
(*  NBR_LAST [K] : MOVING POINTER IN THE LINKED LIST 'NBR [K]'.               *)
(*  GNBR [K]        : ELEMENT OF SORTED  ARRAY  OF  LINKED  LIST  OF  GEOMETRIC  *)
(*                    NEIGHBOURS.                                             *)
(*  INNERG [K]      : ELEMENT OF ARRAY OF LINKED LIST OF GEOMETRICAL NEIGHBOURS  *)
(*                    FOR INNER DISKS.                                        *)
(*  SNBR [K]        : ELEMENT OF SORTED ARRAY  OF  LINKED  LIST  OF  STRUCTURAL  *)
(*                    NEIGHBOURS.                                             *)
(*  SNBR_LAST [K]: MOVING POINTER IN THE LINKED LIST 'SNBR [K]'.              *)
(*  INNERS [K]      : ELEMENT OF ARRAY OF LINKED LIST OF STRUCTRUAL  NEIGHBOURS  *)
(*                    FOR INNER DISKS.                                        *)
(*  NEW_NBR         : NEWLY FOUND (POTENTIAL) NEIGHBOUR.                      *)
(*  NBR_TEMP        : TEMPERARY MEMORY LOCATION OF 'NEW_NBR' TO  BE  LINKED  TO  *)
(*                    THE LINKED LIST NBR [K]'s                               *)
(*  VTX [K]         : ARRAAY OF LINKED LIST OF VORONOI POINTS WITH  THE  CENTER  *)
(*                    DISK AS THE LIST HEAD.                                  *)
(*  VTX_LAST [K] : MOVING POINTER IN THE LINKED LIST 'VTX [K]'.               *)
(*  NEW_VTX         : NEWLY FOUND (POTENTIAL) VORONOI POINT.                  *)
(*  VTX_TEMP        : TEMPERARY MEMORY LOCATION OF 'NEW_VTX' TO  BE  LINKED  TO  *)
(*                    LINKED LIST VTX [K]'S.                                  *)
(*  NVTX [K]        : ELEMENT OF SORTED ARRAY OF LINKED LIST OF VERTICES.     *)
(*  INNERV [K]      : ELEMENT OF ARRAY OF LINKED LIST  OF  VERTICES  FOR  INNER  *)
(*                    DISKS.                                                  *)
(*  INDEX           : THE UNIQUE INTEGER REPRESENTING A CERTAIN DISK.         *)
(*  X, Y            : THE COORDINATE OF A CENTROID OF A DISK.                 *)
(*  DIA             : THE DIAMETER OF A DISK.                                 *)
(*  ANGLE           : THE ANGLE ASSOCIATED WITH A STRUCTURAL NEIGHBOUR.       *)
(*  XMAX            : MAXIMUM X COORDINATE OF THE CENTROIDS OF THE DISKS HANDLED.*)
(*  XMIN            : MINIMUM X COORDINATE OF THE CENTROIDS OF THE DISKS HANDLED.*)
(*  YMAX            : MAXIMUM Y COORDINATE OF THE CENTROIDS OF THE DISKS HANDLED.*)
(*  YMIN            : MINIMUM Y COORDINATE OF THE CENTROIDS OF THE DISKS HANDLED.*)
(*  DMAX            : THE MAXIMUM DIAMETER OF THE DISKS.                      *)
(*  WIDE            : THE DISTANCE BETWEEN TWO VERTICAL PERIODICAL BOUNDARIES.  *)
(*  HEIGHT          : THE HEIGHT OF THE INNER BOX.                            *)
(*  WIDTH           : THE WIDTH OF THE INNER BOX.                             *)
(*  DUMMY1, 2       : COORDINATES OF THE  DUMMY  POINTS  WITH  RESPECT  TO  THE  *)
(*       3, 4         CENTROID BEING PROCESSED.                               *)
(*  CORNER1, 2      : DISKS NEAREST TO FOUR CORNERS OF THE BOX RESPECTIVELY.  *)
(*        3, 4                                                                *)
(*  FIRST, SECOND: THE FIRST  AND  THE  SECOND  DUMMY  POINTS  IN  CLOCKWISE  *)
(*                    DIRECTION WITH RESPECT TO THE LINE FROM THE  CENTROID  TO  *)
(*                    THE LAST NBR FOUND.                                     *)
(*  NBR_FIRST       : THE FIRST GEOMETRIC NEIGHBOUR IN A LINKED LIST NBR [K].  *)
(*  AVG_GN          : THE MEAN VALUE OF THE NUMBER OF GEOMETRIC NEIGHBOUR.    *)
(*  AVG_SN          : THE MEAN VALUE OF THE NUMBER OF STRUCTURAL NEIGHBOUR.   *)
(*  NUM_GN [K]      : ELEMENT OF  ARRAY  OF  INTEGER  OF  NUMBER  OF  GEOMETRIC  *)
(*                    NEIGHBOUR FOR THE Kth INNER DISK.                       *)
(*  NUM_SN [K]      : ELEMENT OF ARRAY  OF  INTEGER  OF  NUMBER  OF  STRUCTRUAL  *)
(*                NEIGHBOUR  FOR THE Kth INNER DISK.                          *)
(*  NUM_DST_GN[K]: ELEMENT OF ARRAY OF INTEGER OF NUMBER  OF  DISKS  WITH  K  *)
(*                GEOMETRICAL NEIGHBOURS.                                     *)
(*  NUM_DST_SN[K]: ELEMENT OF ARRAY OF INTEGER OF NUMBER  OF  DISKS  WITH  K  *)
(*                STRUCTURAL NEIGHBOURS.                                      *)
(*  NNR [K]      : ELEMENT OF ARRAY OF REAL OF NEAREST  NEIGHBOUR  RADIUS OF  *)
(*                THE Kth DISK.                                               *)
(*  GROUP_SN [K, J]: THE Jth ELEMENT OF ARRAY OF LINKED LIST  OF  STRUCTURAL  *)
(*                  NEIGHBOUR FOR DISKS WITH K STRUCTURAL NEIGHBOURS.         *)
(*  GROUP_SUM [K]: ELEMENT OF ARRAY OF INTEGER OF NUMBER  OF  DISKS  WITH  K  *)
(*                STRUCTURAL NEIGHBOURS.                                      *)
(*  NMIN, NMAX   : MINIMUM AND MAXIMUM NUMBER OF GEOMETRIC NEIGHBOUR A  DISK  *)
(*                IN THE GIVEN ENSEMBLE HAS.                                  *)
(*  SMIN, SMAX   : MINIMUM AND MAXIMUM NUMBER OF STRUCTURAL NEIGHBOUR A DISK  *)
(*                IN THE GIVEN ENSEMBLE HAS.                                  *)
(*  ANG_DST_SN [K, J, I]: ELEMENT OF ARRAY OF INTEGER  OF  NUMBER  OF  DISKS  *)
(*                       WITH THE Jth STRUCTURAL NEIGHBOUR OF IT  LYING  IN   *)
(*                       THE  Ith  ANGULAR  DIVISION.   THE   STATICS   IS   *)
(*                       PERFORMED FOR  EACH  CATAGORISED  GROUP  OF  DISKS   *)
(*                       CONTAINING  THE  SAME  NUMBER,  K,  OF  STRUCTURAL   *)
(*                       NEIGHBOURS.                                          *)
(*  MEAN_NNR     : MEAN NEAREST NEIGHBOUR RADIUS.                             *)
(*  MEDIAN_NNR   : MEDIAN NEAREST NEIGHBOUR RADIUS.                           *)
(*  CP_NNR [K]   : ELEMENT OF ARRAY OF REAL OF  CUMULATIVE  PROBABILITY  FOR  *)
(*                THE RADIAL DISTRIBUTION OF NEAREST NEIGHBOUR RADIUS.        *)
(*  ETA          : THE PACKING FRACTION.                                      *)
(*  PLUS         : BOOLEAN VARIABLE, WHICH IS TRUE IF                         *)
(*                1) THE NEWLY FOUND NBR IS NOT A DUMMY POINT.                *)
(*                2) THE NEWLY FOUND NBR IS NOT THE FIRST NBR.                *)
(*                3) THERE IS STILL NOT A LINKED LIST OF  NBR'S  AND  VTX'S   *)
(*                   FORMED CORRESPONDING TO THE NEWLY FOUND NBR.             *)
(*                AND, WHICH IS UNCHANGED IF THE NEWLY  FOUND  NBR  IS  THE   *)
(*                FIRST NBR.                                                  *)
(*  ADD          : BOOLEAN VARIABLE, WHICH IS TRUE  IF  THE  PREVIOUS  NEWLY  *)
(*                FOUND NBR (TO THE CENTROID THEN UNDER PROCESS) PRODUCES A   *)
(*                TRUE 'PLUS'.                                                *)
(*  EQ_DISKS     : BOOLEAN VARIABLE, WHICH IS TRUE IF ALL DISKS IN THE GIVEN  *)
(*                ENSEMBLE ARE OF EQUAL SIZE.                                 *)
(*  PERIODICAL_REQUIRED: BOOLEAN VARIABLE, WHICH IS TRUE IF  THE  PERIODICAL  *)
(*                      BOUNDARY CONDITION IS TO BE IMPLEMENTED.              *)
(*  KNOWN_TO_BE_RCP: BOOLEAN VARIABLE, WHICH IS TRUE  IF  IT  IS  KNOWN  THE  *)
(*                  GIVEN DISK ENSEMBLE IS A RANDOM CLOSE PACKING.            *)
(*  DEFINE_PF_BOX: BOOLEAN  VARIABLE,  WHICH  IS  TRUE  IF   THE  BOX   FOR  *)
(*                CALCULATING THE PACKING IS TO BE DEFINED  DIFFERENT  FROM   *)
(*                THE INNER BOX.                                              *)
(*  FIND_WALL_EFFECT: BOOLEAN VARIABLE, WHICH IS TRUE IF THE WALL EFFECT  IS  *)
(*                   TO BE FOUND.                                             *)
(*                                                                            *)
(*                            AUTHOR: JIRYIH TSAUR                            *)
(*                                    MECHANICAL ENGINEERING DEPARTMENT       *)
(*                                    NEW JERSEY INSTITUTE OF TECHNOLOGY      *)
(*                                                                            *)
(******************************************************************************)
```

```
PROGRAM DISK (INPUT, OUTPUT, DISKIN, NBRFILE, VTXFILE, BOX, SNBRFILE,
              TABLE, DELAUNAY);
   LABEL 100;
   CONST PI = 3.141592654;
         N = 1250;
         SUB_L = - ROUND (0.3 * N);
         SUB_R = ROUND (1.3 * N);
         BOX_C = 1;
   TYPE INFO = RECORD
                  INDEX: INTEGER;
                  X, Y, DIA, ANGLE: REAL
               END;
        LIST = ^NODE;
        NODE = RECORD
                  DATA: INFO;
                  NEXT: LIST
               END;
        DOUBLE_ARRAY = ARRAY [SUB_L..SUB_R] OF LIST;
        LIST_ARRAY = ARRAY [1..N] OF LIST;
        GROUP = ARRAY [1..6,1..N] OF LIST;
        SMALL_ARRAY = ARRAY [0..10] OF INTEGER;
        SMALL_REAL_ARRAY = ARRAY [0..100] OF REAL;
        NUM_ARRAY = ARRAY [0..SUB_R] OF INTEGER;
        REAL_ARRAY = ARRAY [SUB_L..SUB_R] OF REAL;
        ARRAY_3D = ARRAY [1..6,1..6,0..SUB_R] OF INTEGER;

   VAR STRING30: PACKED ARRAY [1..30] OF CHAR;

       Z, RANDOM, SORT, SORT_COPY, LAST, NEW_NBR, NBR_TEMP, NEW_VTX, VTX_TEMP,
       INNER, PF_INNER: LIST;

       NBR, NBR_LAST, GNBR, VTX, VTX_LAST: DOUBLE_ARRAY;

       SNBR, SNBR_LAST, INNERG, INNERV, INNERS: LIST_ARRAY;

       GROUP_SN: GROUP;

       GROUP_SUM, NUM_DST_GN, NUM_DST_SN, DST: SMALL_ARRAY;

       NNR: REAL_ARRAY;

       CP_NNR: SMALL_REAL_ARRAY;

       EXPECT_ANGLE, STD_DVA: ARRAY [1..6,1..6] OF REAL;

       ANG_DST_SN, DST_SN: ARRAY_3D;

       DUMMY1, DUMMY2, DUMMY3, DUMMY4,
       NBR_FIRST, FIRST, SECOND, VERTEX_TEMP,
       CORNER1, CORNER2, CORNER3, CORNER4: INFO;

       INDEX, NUM_DISK, NUM_IN, NUM_LOOP,
       NMIN, NMAX, SMIN, SMAX, NUM_RAD_DIV, NUM_ANG_DIV,
       I, J, K, L: INTEGER;

       XC, YC, XC_TEMP, YC_TEMP, X1, Y1, X2, Y2, X3, Y3, X4, Y4, XL, XR,
       XMAX, XMIN, YMAX, YMIN,
       R, NEW_R, R_TEMP, DMAX, AVG_GN, AVG_SN, DIA1, DIA2, MIN, DIVISION,
       ALFA, BETA, GAMMA, AREA, ETA, SUM, SUMS, MEAN_NNR, MEDIAN_NNR,
       LEFT, RIGHT, BOTTOM, TOP, PF_L, PF_R, PF_B, PF_T,
       TOLERANCE, WIDE, HEIGHT, WIDTH: REAL;

       NUM_GN, NUM_SN: NUM_ARRAY;

       STOP, ADD, PLUS, EQ_DISKS, PERIODICAL_REQUIRED, KNOWN_TO_BE_RCP,
       DEFINE_PF_BOX, FIND_WALL_EFFECT: BOOLEAN;

       DISKIN, NBRFILE, VTXFILE, BOX, SNBRFILE, TABLE, DELAUNAY: TEXT;
(*****************************************************************************)
(*                                                                           *)
(*                      PROCEDURES AND FUNCTIONS                             *)
(*                                                                           *)
(*****************************************************************************)

   (**************************************************************************)
   (*       CREATE A LINKED LIST CONTAINING ONLY ONE CENTROID                *)
   (**************************************************************************)
   FUNCTION NODE_CREATE: LIST;
      VAR CENTROID: LIST;
      BEGIN
         NEW (CENTROID);
         WITH CENTROID^.DATA DO
            BEGIN
               READLN (DISKIN, INDEX, X, Y, DIA);
               CENTROID^.NEXT := Z
            END;   {END WITH CONTROID^.DATA}
         NODE_CREATE := CENTROID
      END;   {END FUNCTION NODE_CREATE}

   (**************************************************************************)
   (*            CREATE A LINKED LIST CONTAINING ALL CENTROIDS               *)
   (**************************************************************************)
   FUNCTION LIST_CREATE: LIST;
      VAR LISTHEAD, NEWNODE: LIST;
      BEGIN
         NEW (LISTHEAD);
         LISTHEAD^.NEXT := Z;
         LAST := LISTHEAD;
         WHILE NOT EOF (DISKIN) DO
            BEGIN
               NEWNODE := NODE_CREATE;
               LAST^.NEXT := NEWNODE;
               LAST := LAST^.NEXT
            END;   {END WHILE NOT EOF (DISKIN)}
         LIST_CREATE := LISTHEAD^.NEXT
      END;   {END FUNCTION LIST_CREATE}
```

```
(****************************************************************************)
(*    MERGE TWO SORTED LIST TO FORM ONE SORTED LIST, SUCH THAT             *)
(*    EITHER 1) LIST^.DATA.X < LIST^.NEXT.DATA.X                           *)
(*    OR     2) LIST^.DATA.X = LIST^.NEXT.DATA.X AND                       *)
(*              LIST^.DATA.Y < LIST^.NEXT.DATA.Y                           *)
(****************************************************************************)
FUNCTION LEXICO_MERGE (A, B: LIST): LIST;
   VAR LISTHEAD: LIST;
   BEGIN
      NEW (LISTHEAD);
      LISTHEAD^.NEXT := Z;
      LAST := LISTHEAD;

      WHILE LAST <> Z DO

         IF A^.DATA.X < B^.DATA.X THEN
            BEGIN LAST^.NEXT := A; LAST := LAST^.NEXT; A := A^.NEXT END
         ELSE IF B^.DATA.X < A^.DATA.X THEN
            BEGIN LAST^.NEXT := B; LAST := LAST^.NEXT; B := B^.NEXT END
         ELSE IF A^.DATA.Y <= B^.DATA.Y THEN
            BEGIN LAST^.NEXT := A; LAST := LAST^.NEXT; A := A^.NEXT END
         ELSE
            BEGIN LAST^.NEXT := B; LAST := LAST^.NEXT; B := B^.NEXT END;

      LEXICO_MERGE := LISTHEAD^.NEXT
   END;   {END FUNCTION LEXICO_MERGE}

(****************************************************************************)
(*                      SORT A LIST BY MERGE                               *)
(****************************************************************************)
FUNCTION MERGESORT (A: LIST;
                    NUM_DISK: INTEGER): LIST;
   VAR B, C, LEXICO_B, LEXICO_C: LIST;
   BEGIN
      IF A^.NEXT = Z THEN
         MERGESORT := A

      ELSE
         BEGIN
            B := A;
            FOR K := 2 TO ( NUM_DISK DIV 2 ) DO A := A^.NEXT;
            C := A^.NEXT; A^.NEXT := Z;
            IF B^.NEXT <> Z THEN
               LEXICO_B := MERGESORT ( B, ( NUM_DISK DIV 2 ) )
            ELSE
               LEXICO_B := B;
            IF C^.NEXT <> Z THEN
               LEXICO_C := MERGESORT ( C, NUM_DISK - ( NUM_DISK DIV 2 ) )
            ELSE
               LEXICO_C := C;
            MERGESORT := LEXICO_MERGE (LEXICO_B, LEXICO_C)
         END   {END ELSE - A^.NEXT <> Z}
   END;   {END FUNCTION MERGESORT}
```

```
(****************************************************************************)
(*      FIND THE DISK WITH THE CENTROID NEAREST TO A POINT (XC, YC)        *)
(****************************************************************************)
FUNCTION NEAREST (XC, YC: REAL;
                  SORT: LIST): INFO;
   BEGIN
      LAST := SORT;
      NEW_NBR^.DATA := LAST^.DATA;
      WITH NEW_NBR^.DATA DO
         BEGIN
            X1 := X; Y1 := Y
         END;   {END WITH NEW_NBR^.DATA}
      R := SQRT ( SQR ( X1 - XC ) + SQR ( Y1 - YC ) );
      REPEAT
         STOP := TRUE;
         XL := XC - R;
         XR := XC + R;
         LAST := LAST^.NEXT;
         WITH LAST^.DATA DO
            BEGIN
               X2 := X;  Y2 := Y
            END;   {END WITH LAST^.DATA}
         NEW_R := SQRT ( SQR ( X2 - XC ) + SQR ( Y2 - YC ) );
         IF ( XL <= X2 ) AND ( X2 <= XR ) THEN
            BEGIN
               STOP := FALSE;
               IF NEW_R < R THEN
                  BEGIN
                     NEW_NBR^.DATA := LAST^.DATA;
                     X1 := X2;
                     Y1 := Y2;
                     R := NEW_R
                  END   {END IF NEW_R <R}
            END   {END IF (XL <= X2) AND (X2 <= XR)}
      UNTIL
         STOP;
      NEAREST := NEW_NBR^.DATA
   END;   {END FUNCTION NEAREST}
(****************************************************************************)
(* FIND THE FOUR DUMMY POINTS WITH RESPECT TO A PARTICULAR POINT (XC, YC)  *)
(****************************************************************************)
PROCEDURE DUMMY_CREATE (XC, YC, XMAX, XMIN, YMAX, YMIN: REAL;
                        VAR DUMMY1, DUMMY2, DUMMY3, DUMMY4: INFO);
   BEGIN
      WITH DUMMY1 DO
         BEGIN INDEX := 0; X := 2 * XMIN - XC; Y := YC END;
      WITH DUMMY2 DO
         BEGIN INDEX := 0; X := XC; Y := 2 * YMAX - YC END;
      WITH DUMMY3 DO
         BEGIN INDEX := 0; X := 2 * XMAX - XC; Y := YC END;
      WITH DUMMY4 DO
         BEGIN INDEX := 0; X := XC; Y := 2 * YMIN - YC END
   END;   {END PROCEDURE DUMMY_CREATE}
```

```
(****************************************************************************)
(*       FIND 'FIRST' AND 'SECOND', WHICH ARE THE FIRST AND THE SECOND     *)
(*       DUMMY POINTS IN CLOCKWISE DIRECTION WITH RESPECT TO THE  LINE     *)
(*       FROM THE CENTROID BEING PROCESSED TO THE PREVIOUS NBR             *)
(****************************************************************************)
PROCEDURE DUMMY_FIND (X1, Y1, X2, Y2: REAL;
                      DUMMY1, DUMMY2, DUMMY3, DUMMY4: INFO;
                      VAR FIRST, SECOND: INFO);
   BEGIN
      IF ( X2 <= X1 ) AND ( Y2 < Y1 ) THEN
         BEGIN FIRST := DUMMY1; SECOND := DUMMY2 END;
      IF ( X2 < X1 ) AND ( Y2 >= Y1 ) THEN
         BEGIN FIRST := DUMMY2; SECOND := DUMMY3 END;
      IF ( X2 >= X1 ) AND ( Y2 > Y1 ) THEN
         BEGIN FIRST := DUMMY3; SECOND := DUMMY4 END;
      IF ( X2 > X1 ) AND ( Y2 <= Y1 ) THEN
         BEGIN FIRST := DUMMY4; SECOND := DUMMY1 END
   END;   {END PROCEDURE DUMMY_FIND}

(****************************************************************************)
(*     FIND THE POINT EQUIDISTANT TO (X1, Y1), (X2, Y2), AND (X3, Y3)      *)
(****************************************************************************)
FUNCTION VTX_FIND (X1, Y1, X2, Y2, X3, Y3: REAL): INFO;
   VAR XC, YC, MC, A1, B1, C1, A2, B2, C2: REAL;
       VERTEX: INFO;
   BEGIN
      XC := ( X1 + X2 ) / 2;
      YC := ( Y1 + Y2 ) / 2;

      IF X1 = X2 THEN
         BEGIN
            A1 := 0;
            B1 := 1;
            C1 := YC
         END   {END IF X1 = X2}

      ELSE
         BEGIN
            MC := ( Y1 - Y2 ) / ( X1 - X2 );
            A1 := 1;
            B1 := MC;
            C1 := XC + MC * YC
         END;   {END ELSE - X1 <> X2}

      XC := ( X1 + X3 ) / 2;
      YC := ( Y1 + Y3 ) / 2;

      IF X1 = X3 THEN
         BEGIN
            A2 := 0;
            B2 := 1;
            C2 := YC
         END   {END IF X1 = X3}
      ELSE
         BEGIN
            MC := ( Y1 - Y3 ) / ( X1 -X3 );
            A2 := 1;
            B2 := MC;
            C2 := XC + MC * YC
         END;  {END ELSE - X1 <> X3}
      WITH VERTEX DO
         BEGIN
            X := ( C1 * B2 - C2 * B1 ) / ( A1 * B2 - A2 * B1);
            Y := ( A1 * C2 - A2 * C1 ) / ( A1 * B2 - A2 * B1)
         END;  {END WITH VERTEX}
      VTX_FIND := VERTEX;
   END;  {END FUNCTION VTX_FIND}

(***************************************************************************)
(*       IMPLEMENT THE PERIODICAL BOUNDARY CONDITION.                      *)
(*       1) LINK NODES IN THE ORIGINAL LINKED LIST 'SORT' AND WITHIN 'DMAX'*)
(*          FROM THE LEFT MARGIN OF THE BOX TO THE REAR OF 'SORT'.         *)
(*       2) LINK NODES IN THE ORIGINAL LINKED LIST 'SORT' AND WITHIN 'DMAX'*)
(*          FROM THE RIGHT MARGIN OF THE BOX IN FRONT OF 'SORT'.           *)
(***************************************************************************)
PROCEDURE PERIODICAL (VAR SORT: LIST;
                      NUM_DISK: INTEGER;
                      VAR NUM_LOOP: INTEGER;
                      DMAX, WIDE: REAL);
   VAR TAIL, SORT_HEAD, HEAD: LIST;
   BEGIN
      (*                             *)
      (*LINK NODES IN FRONT OF 'SORT'*)
      (*                             *)
      NEW (SORT_HEAD);
      SORT_HEAD^.NEXT := Z;
      HEAD := SORT_HEAD;
      LAST := SORT;

      REPEAT
         LAST := LAST^.NEXT
      UNTIL
         LAST^.DATA.X >= WIDE - 4 * DMAX;

      K := 0;
      WHILE LAST <> Z DO
         BEGIN
            NEW (NBR_TEMP);
            NBR_TEMP^.NEXT := Z;
            WITH NBR_TEMP^.DATA DO
               BEGIN
                  INDEX := LAST^.DATA.INDEX - ( NUM_DISK + 1 );
                  X := LAST^.DATA.X - WIDE;
                  Y := LAST^.DATA.Y;
                  DIA := LAST^.DATA.DIA
               END;  {END WITH NBR_TEMP^.DATA}
            HEAD^.NEXT := NBR_TEMP;
            HEAD := HEAD^.NEXT;
            LAST := LAST^.NEXT;
            K := K + 1
         END;   {END WHILE LAST <> Z}
      HEAD^.NEXT := SORT;
      (*                                *)
      (*LINK NODES TO THE REAR OF 'SORT'*)
      (*                                *)
      LAST := SORT;
      FOR I := 1 TO NUM_DISK - 1 DO
         LAST := LAST^.NEXT;
      TAIL := SORT;
      J := 0;
      WHILE TAIL^.DATA.X <= 4 * DMAX DO
         BEGIN
            NEW (NBR_TEMP);
            NBR_TEMP^.NEXT := Z;
            WITH NBR_TEMP^.DATA DO
               BEGIN
                  INDEX := TAIL^.DATA.INDEX + NUM_DISK;
                  X := TAIL^.DATA.X + WIDE;
                  Y := TAIL^.DATA.Y;
                  DIA := TAIL^.DATA.DIA
               END;   {END WITH NBR_TEMP^.DATA}
            LAST^.NEXT := NBR_TEMP;
            LAST := LAST^.NEXT;
            TAIL := TAIL^.NEXT;
            J := J + 1
         END;   {END WHILE TAIL^.DATA.X <= 3 * DMAX}
      SORT := SORT_HEAD^.NEXT;
      NUM_LOOP := NUM_DISK + K + J
   END;   {END PROCEDURE PERIODICAL}

(****************************************************************************)
(*       FIND THE ANGLE SWEEPING FROM THE POSITIVE X-DIRECTION TO           *)
(*       THE LINE EXTENDED FROM (X1, Y1) TO (X2, Y2)                        *)
(****************************************************************************)
FUNCTION THETA  (X1, Y1, X2, Y2: REAL): REAL;
   BEGIN
      IF X2 = X1 THEN
         BEGIN
            IF Y2 > Y1 THEN THETA  := 90
            ELSE THETA  := 270
         END   {END IF X2 = X1}
      ELSE
         BEGIN
            ALFA := 180 * ARCTAN ( ( Y2 - Y1 ) / ( X2 - X1 ) ) / PI;
            IF X2 < X1 THEN
               BEGIN
                  ALFA := ALFA + 180;
                  THETA  := ALFA
               END   {END IF X2 < X1}
            ELSE IF Y2 < Y1 THEN
               BEGIN
                  ALFA := ALFA + 360;
                  THETA  := ALFA
               END   {END IF Y2 < Y1}
            ELSE
               THETA  := ALFA
         END   {END ELSE - X2 <> X1}
   END;   {END FUNCTION THETA }

(***************************************************************************)
(*                 MAKE A COPY OF A LINKED LIST                            *)
(***************************************************************************)
PROCEDURE MAKE_COPY (SORT: LIST; VAR SORT_COPY: LIST);
   VAR COPY_LAST: LIST;
BEGIN
   NEW (SORT_COPY);
   SORT_COPY^.NEXT := Z;
   COPY_LAST := SORT_COPY;

   LAST := SORT;
   WHILE LAST <> Z DO
      BEGIN
         NEW (NBR_TEMP);
         NBR_TEMP^.NEXT := Z;
         NBR_TEMP^.DATA := LAST^.DATA;
         COPY_LAST^.NEXT := NBR_TEMP;
         LAST := LAST^.NEXT;
         COPY_LAST := COPY_LAST^.NEXT
      END;   {END WHILE LAST <> Z}
   SORT_COPY := SORT_COPY^.NEXT
END;   {END PROCEDURE MAKE_COPY}

(***************************************************************************)
(*                                                                         *)
(*          GIVEN A BOX DEFINED BY:                                        *)
(*                                                                         *)
(*          X = LEFT, X = RIGHT, Y = BOTTOM, AND Y = TOP                   *)
(*                                                                         *)
(*          AND A SORTED LINKED LIST WITH EACH NODE A TWO DIMENTIONAL      *)
(*          POINT.  ELIMINATE OUTER DISKS FROM THE LINKED LIST 'SORT'      *)
(*          NAME THE NEW LINKED LIST 'INNER'                               *)
(*                                                                         *)
(***************************************************************************)
PROCEDURE FIND_INNER (SORT_COPY: LIST;
                      LEFT, RIGHT, BOTTOM, TOP: REAL;
                      VAR INNER: LIST);
   VAR X1, Y1, R: REAL;
       STOP: BOOLEAN;
   BEGIN
      LAST := SORT_COPY;
      REPEAT
         STOP := TRUE;
   WHILE (LAST^.DATA.X <= LEFT - LAST^.DATA.DIA / 2) OR
         (LAST^.DATA.Y <= BOTTOM - LAST^.DATA.DIA  / 2) OR
         (LAST^.DATA.Y >= TOP + LAST^.DATA.DIA / 2 ) DO
      BEGIN
         NBR_TEMP := LAST;
         LAST := LAST^.NEXT;
         DISPOSE (NBR_TEMP)
      END;   {END WHILE}
   WITH LAST^.DATA DO
      BEGIN
         X1 := X;
         Y1 := Y;
         R := DIA / 2
      END;   {END WITH LAST^.DATA}

   IF X1 < LEFT THEN
      BEGIN
         IF Y1 < BOTTOM THEN
            BEGIN
               IF SQR (R) <= SQR (X1 - LEFT) + SQR (Y1 - BOTTOM) THEN
                  BEGIN
                     STOP := FALSE;
                     NBR_TEMP := LAST;
                     LAST := LAST^.NEXT;
                     DISPOSE (NBR_TEMP)
                  END
            END   {END IF Y1 < BOTTOM}

         ELSE IF Y1 > TOP THEN
            BEGIN
               IF SQR (R) <= SQR (X1 - LEFT) + SQR (Y1 - TOP) THEN
                  BEGIN
                     STOP := FALSE;
                     NBR_TEMP := LAST;
                     LAST := LAST^.NEXT;
                     DISPOSE (NBR_TEMP)
                  END
            END   {END ELSE IF Y1 > TOP}
      END   {END IF X1 < LEFT}
UNTIL
   STOP;

INNER := LAST;
WHILE LAST^.NEXT^.DATA.X < LEFT DO
   BEGIN
      REPEAT
         STOP := TRUE;
         WITH LAST^.NEXT^.DATA DO
            BEGIN
               X1 := X;
               Y1 := Y;
               R := DIA / 2
            END;   {END WITH LAST^.NEXT^.DATA}
         IF X1 <= LEFT - R THEN
            BEGIN
               STOP := FALSE;
               NBR_TEMP := LAST^.NEXT;
               LAST^.NEXT := LAST^.NEXT^.NEXT;
               DISPOSE (NBR_TEMP)
            END   {END IF X1 <= LEFT - R}
         ELSE IF ( Y1 <= BOTTOM - R ) OR ( Y1 >= TOP + R ) THEN
            BEGIN
               STOP := FALSE;
               NBR_TEMP := LAST^.NEXT;
               LAST^.NEXT := LAST^.NEXT^.NEXT;
               DISPOSE (NBR_TEMP)
            END
         ELSE IF Y1 < BOTTOM THEN
            BEGIN
               IF SQR (R) <= SQR (X1 - LEFT) + SQR (Y1 - BOTTOM) THEN
                  BEGIN
                     STOP := FALSE;
                     NBR_TEMP := LAST^.NEXT;
                     LAST^.NEXT := LAST^.NEXT^.NEXT;
                     DISPOSE (NBR_TEMP)
                  END
            END   {END IF Y1 < BOTTOM}
         ELSE IF Y1 > TOP THEN
            BEGIN
               IF SQR (R) <= SQR (X1 - LEFT) + SQR (Y1 - TOP) THEN
                  BEGIN
                     STOP := FALSE;
                     NBR_TEMP := LAST^.NEXT;
                     LAST^.NEXT := LAST^.NEXT^.NEXT;
                     DISPOSE (NBR_TEMP)
                  END
            END   {END ELSE IF Y1 > TOP}
      UNTIL
         ( STOP ) OR ( LAST^.NEXT^.DATA.X >= LEFT );
      IF STOP THEN
         LAST := LAST^.NEXT
   END;   {END WHILE LAST^.NEXT^.DATA.X < LEFT}
WHILE LAST^.NEXT^.DATA.X <= RIGHT DO
   BEGIN
      REPEAT
         STOP := TRUE;
         IF (LAST^.NEXT^.DATA.Y<=BOTTOM - LAST^.NEXT^.DATA.DIA / 2) OR
            (LAST^.NEXT^.DATA.Y>=TOP + LAST^.NEXT^.DATA.DIA / 2) THEN
            BEGIN
               STOP := FALSE;
               NBR_TEMP := LAST^.NEXT;
               LAST^.NEXT := LAST^.NEXT^.NEXT;
               DISPOSE (NBR_TEMP)
            END
      UNTIL
         ( STOP ) OR ( LAST^.NEXT^.DATA.X > RIGHT );
         IF STOP THEN
            LAST := LAST^.NEXT
      END;   {END WHILE LAST^.NEXT^.DATA.X <= RIGHT}

   WHILE LAST^.NEXT <> Z DO
      BEGIN
         REPEAT
            STOP := TRUE;
            WITH LAST^.NEXT^.DATA DO
               BEGIN
                  X1 := X;
                  Y1 := Y;
                  R := DIA / 2
               END;   {END WITH LAST^.NEXT^.DATA}
            IF X1 >= RIGHT + R THEN
               BEGIN
                  STOP := FALSE;
                  NBR_TEMP := LAST^.NEXT;
                  LAST^.NEXT := LAST^.NEXT^.NEXT;
                  DISPOSE (NBR_TEMP)
               END   {END IF X1 >= RIGHT + R}
            ELSE IF ( Y1 <= BOTTOM - R ) OR ( Y1 >= TOP + R ) THEN
               BEGIN
                  STOP := FALSE;
                  NBR_TEMP := LAST^.NEXT;
                  LAST^.NEXT := LAST^.NEXT^.NEXT;
                  DISPOSE (NBR_TEMP)
               END
            ELSE IF Y1 < BOTTOM THEN
               BEGIN
                  IF SQR (R) <= SQR (X1 - RIGHT) + SQR (Y1 - BOTTOM) THEN
                     BEGIN
                        STOP := FALSE;
                        NBR_TEMP := LAST^.NEXT;
                        LAST^.NEXT := LAST^.NEXT^.NEXT;
                        DISPOSE (NBR_TEMP)
                     END
               END   {END IF Y1 < BOTTOM}
            ELSE IF Y1 > TOP THEN
               BEGIN
                  IF SQR (R) <= SQR (X1 - RIGHT) + SQR (Y1 - TOP) THEN
                     BEGIN
                        STOP := FALSE;
                        NBR_TEMP := LAST^.NEXT;
                        LAST^.NEXT := LAST^.NEXT^.NEXT;
                        DISPOSE (NBR_TEMP)
                     END
               END   {END ELSE IF Y1 > TOP}
         UNTIL
            ( STOP ) OR ( LAST^.NEXT = Z );
         LAST := LAST^.NEXT
      END   {END WHILE LAST^.NEXT <> Z}
END;   {END PROCEDURE FIND_INNER}
```

```
(***************************************************************************)
(*           FIND THE NUMBER DISTRIBUTION                                  *)
(***************************************************************************)
PROCEDURE NUM_DST (NUM: NUM_ARRAY;
                   NUM_IN: INTEGER;
                   VAR NMIN, NMAX: INTEGER;
                   VAR DST: SMALL_ARRAY);
   VAR J, K: INTEGER;
   BEGIN
      NMIN := 100;
      NMAX := 0;
      FOR J := 0 TO 10
         DO DST [J] := 0;
      FOR K := 1 TO NUM_IN DO
         BEGIN
            J := NUM [K];
            IF J < NMIN THEN NMIN := J;
            IF J > NMAX THEN NMAX := J;
            DST [J] := DST [J] + 1
         END   {END FOR K := 1 TO NUM_IN}
   END;   {END PROCEDURE NUM_DST}

(***************************************************************************)
(*         FIND THE ANGULAR DISTRIBUTION OF STRUCTURAL NEIGHBOURS          *)
(***************************************************************************)
PROCEDURE ANG_DST (GROUP_SN: GROUP;
                   GROUP_SUM: SMALL_ARRAY;
                   SMIN, SMAX, NUM_ANG_DIV: INTEGER;
                   VAR DST: ARRAY_3D);
   VAR I, J, K, N, Q: INTEGER;
       GAMMA: REAL;
   BEGIN
      GAMMA := 360 / NUM_ANG_DIV;
      FOR K := SMIN TO SMAX DO
         BEGIN
            IF K > 0 THEN
               BEGIN
                  FOR N := 1 TO GROUP_SUM [K] DO
                     NBR_LAST [N] := GROUP_SN [K, N]^.NEXT;
                  FOR J := 1 TO K DO
                     BEGIN
                        FOR I := 0 TO NUM_ANG_DIV - 1 DO DST [K, J, I] := 0;
                        FOR N := 1 TO GROUP_SUM [K] DO
                           BEGIN
                              Q :=
                                 TRUNC ( NBR_LAST [N]^.DATA.ANGLE / GAMMA );
                              DST [K, J, Q] := DST [K, J, Q] + 1;
                              NBR_LAST [N] := NBR_LAST [N]^.NEXT
                           END   {END FOR N := 1 TO GROUP_SUM [K]}
                     END   {END FOR J := 1 TO K}
               END   {END IF K > 0}
         END   {END FOR K := SMIN TO SMAX}
   END;   {END PROCEDURE ANG_DST}
```

```
(****************************************************************************)
(*        FIND THE NEAREST NEIGHBOUR RADII, STORE THEM IN A                *)
(*        ONE-DIMENSIONAL ARRAY 'NNR'.                                      *)
(****************************************************************************)
PROCEDURE FIND_NNR (INNERS: LIST_ARRAY;
                    GNBR: DOUBLE_ARRAY;
                    NUM_IN: INTEGER;
                    VAR NNR: REAL_ARRAY);
   VAR NBR_TEMP: LIST;
       K, J: INTEGER;
       X1, Y1, X2, Y2: REAL;
BEGIN
   FOR K := 1 TO NUM_IN DO
      BEGIN
         (*                                                         *)
         (* IF INNERS[K] IS NOT EMPTY.  THERE IS SOME STRUCTURAL    *)
         (* NEIGHBOURS IN THE LINKED LIST INNERS[K].  THEN, SEARCH *)
         (* FOF THE NEAREST NEIGHBOUR AMONG THE STRUCTURAL         *)
         (* NEIGHBOURS.                                             *)
         (*                                                         *)
         IF INNERS[K]^.NEXT <> Z THEN
            NBR_TEMP := INNERS[K]
         (*                                                       *)
         (* IF INNERS [K] IS EMPTY.  THEN SEARCH FOR THE NEAREST *)
         (* NEIGHBOUR AMONG THE GEOMETRIC NEIGHBOURS.             *)
         (*                                                       *)
         ELSE
            BEGIN
               J := INNERS[K]^.DATA.INDEX;
               NBR_TEMP := GNBR[J]
            END;   {END ELSE - INNERS[K] IS NOT EMPTY}
         WITH NBR_TEMP^.DATA DO
            BEGIN
               X1 := X; Y1 := Y
            END;   {END WITH NBR_TEMP^.DATA}

         NBR_TEMP := NBR_TEMP^.NEXT;
         WITH NBR_TEMP^.DATA DO
            BEGIN
               X2 := X; Y2 := Y
            END;   {END WITH NBR_TEMP^.DATA}
         NNR [K] := SQRT (SQR (X1 - X2) + SQR (Y1 - Y2));

         NBR_TEMP := NBR_TEMP^.NEXT;
         WHILE NBR_TEMP <> Z DO
            BEGIN
               WITH NBR_TEMP^.DATA DO
                  BEGIN
                     X2 := X; Y2 := Y
                  END;   {END WITH NBR_TEMP^.DATA}
               R := SQRT (SQR (X1 - X2) + SQR (Y1 - Y2));
               IF R < NNR [K] THEN
                  NNR [K] := R;
               NBR_TEMP := NBR_TEMP^.NEXT
            END;   {END WHILE NBR_TEMP <> Z}
      END   {END FOR K := 1 TO NUM_LOOP}
   END;   {END PROCEDURE FIND_NNR}
(***************************************************************************)
(*                    SORT A ONE-DIMENSIONAL ARRAY                         *)
(***************************************************************************)
PROCEDURE ARRAY_SORT (VAR NNR: REAL_ARRAY; NUM_IN: INTEGER);
   VAR I, J: INTEGER;
       TEMP: REAL;
   BEGIN
      FOR I := 1 TO NUM_IN - 1 DO
         FOR J := I + 1 TO NUM_IN DO
            IF NNR[J] < NNR[I] THEN
               BEGIN
                  TEMP := NNR[I];
                  NNR[I] := NNR[J];
                  NNR[J] := TEMP
               END   {END IF}
   END;   {END PROCEDURE ARRAY_SORT}
(***************************************************************************)
(*                                                                         *)
(*          GIVEN A BOX DEFINED BY:                                        *)
(*                                                                         *)
(*          X = LEFT, X = RIGHT, Y = BOTTOM, AND Y = TOP                   *)
(*                                                                         *)
(*          AND A SORT LINKED LIST 'INNER' WITH EACH NODE A POINT WITHIN   *)
(*          OR ON THE BOUNDARY OF THE BOX.  FIND THE PACKING FRACTION:     *)
(*                      SUM OF DISK AREA INSIDE THE BOX                    *)
(*          P.F. =   --------------------------------------                *)
(*                                 BOX AREA                                *)
(*                                                                         *)
(***************************************************************************)
PROCEDURE FIND_PF (INNER: LIST;
                   LEFT, RIGHT, BOTTOM, TOP: REAL;
                   VAR ETA, SUM: REAL);
   VAR AREA: REAL;
       ALFA, BETA, GAMMA: REAL;
       X1, X2, Y1, Y2, R: REAL;
       LAST: LIST;
BEGIN
SUM := 0;
LAST := INNER;
WHILE (LAST^.DATA.X < LEFT + DMAX / 2) AND (LAST <> Z) DO
   BEGIN
      WITH LAST^.DATA DO
         BEGIN
            X1 := X - LEFT;
            X2 := RIGHT - X;
            Y1 := Y - BOTTOM;
            Y2 := TOP - Y;
            R := DIA / 2
         END;   {END WITH LAST^.DATA}
```

```
IF X1 < 0 THEN
BEGIN
   IF Y1 < 0 THEN
      BEGIN
         ALFA := 2 * ARCTAN ( SQRT ( R * R - X1 * X1 ) / ( - X1 ) );
         BETA := 2 * ARCTAN ( SQRT ( R * R - Y1 * Y1 ) / ( - Y1 ) );
         GAMMA := 0.5 * PI + ( ALFA + BETA) / 2;
         AREA := X1 * Y1 + R * R * ( ALFA - SIN ( ALFA ) / 2 +
                                     BETA - SIN ( BETA ) / 2 -
                                     GAMMA ) / 2
      END   {END IF Y1 < 0}
   ELSE IF Y2 < 0 THEN
      BEGIN
         ALFA := 2 * ARCTAN ( SQRT ( R * R - X1 * X1 ) / ( - X1 ) );
         BETA := 2 * ARCTAN ( SQRT ( R * R - Y2 * Y2 ) / ( - Y2 ) );
         GAMMA := 0.5 * PI + ( ALFA + BETA) / 2;
         AREA := X1 * Y2 + R * R * ( ALFA - SIN ( ALFA ) / 2 +
                                     BETA - SIN ( BETA ) / 2 -
                                     GAMMA ) / 2
      END   {END ELSE IF Y2 < 0}
   ELSE IF ( Y1 = 0 ) OR ( Y2 = 0 ) THEN
      BEGIN
         ALFA := 2 * ARCTAN ( SQRT ( R * R - X1 * X1 ) / ( - X1 ) );
         AREA := R * R * ( ALFA - SIN ( ALFA ) ) / 4
      END   {END ELSE IF (Y1 = 0) OR (Y2 = 0)}

   ELSE IF Y1 < R THEN
   BEGIN
      IF R * R > X1 * X1 + Y1 * Y1 THEN
         BEGIN
            ALFA := 2 * ARCTAN ( SQRT ( R * R - X1 * X1 ) / ( - X1 ) );
            BETA := 2 * ARCTAN ( SQRT ( R * R - Y1 * Y1 ) / Y1 );
            GAMMA := 0.5 * PI + ( ALFA + BETA ) / 2;
            AREA := R * R * ( GAMMA - BETA + SIN ( BETA ) / 2 -
                              SIN ( ALFA ) / 2 ) / 2 + X1 * Y1
         END   {END IF R * R > X1 * X1 + Y1 * Y1}
      ELSE
         BEGIN
            ALFA := 2 * ARCTAN ( SQRT ( R * R - X1 * X1 ) / ( - X1 ) );
            AREA := R * R * ( ALFA - SIN ( ALFA ) ) / 2
         END   {END ELSE - R * R <= X1 * X1 + Y1 * Y1}
   END   {END ELSE IF Y1 < R}

   ELSE IF Y2 < R THEN
   BEGIN
      IF R * R > X1 * X1 + Y2 * Y2 THEN
         BEGIN
            ALFA := 2 * ARCTAN ( SQRT ( R * R - X1 * X1 ) / ( - X1 ) );
            BETA := 2 * ARCTAN ( SQRT ( R * R - Y2 * Y2 ) / Y2 );
            GAMMA := 0.5 * PI + ( ALFA + BETA ) / 2;
            AREA := R * R * ( GAMMA - BETA + SIN ( BETA ) / 2 -
                              SIN ( ALFA ) / 2 ) / 2 + X1 * Y2
         END   {END IF R * R > X1 * X1 + Y2 * Y2}
```

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    ELSE
      BEGIN
        ALFA := 2 * ARCTAN ( SQRT ( R * R - X1 * X1 ) / ( - X1 ) );
        AREA := R * R * ( ALFA - SIN ( ALFA ) ) / 2
      END   {END ELSE - R * R <= X1 * X1 + Y2 * Y2}
  END   {END ELSE IF Y2 < R}
  ELSE
    BEGIN
      ALFA := 2 * ARCTAN ( SQRT ( R * R - X1 * X1 ) / ( - X1 ) );
      AREA := R * R * ( ALFA - SIN ( ALFA ) ) / 2
    END   {END ELSE}
END   {END IF X1 < 0}
ELSE IF X1 = 0 THEN
BEGIN
  IF Y1 < 0 THEN
    BEGIN
      BETA := 2 * ARCTAN ( SQRT ( R * R - Y1 * Y1 ) / ( - Y1 ) );
      AREA := R * R * ( BETA - SIN ( BETA ) ) / 4
    END   {END IF Y1 < 0}
  ELSE IF Y2 < 0 THEN
    BEGIN
      ALFA := 2 * ARCTAN ( SQRT ( R * R - Y2 * Y2 ) / ( - Y2 ) );
      AREA := R * R * ( ALFA - SIN ( ALFA ) ) / 4
    END   {END ELSE IF Y2 < 0}
  ELSE IF ( Y1 = 0 ) OR ( Y2 = 0 ) THEN
    BEGIN
      AREA := R * R * PI / 4
    END   {END ELSE IF ( Y1 = 0 ) OR ( Y2 = 0 )}
  ELSE IF Y1 < R THEN
    BEGIN
      ALFA := 2 * ARCTAN ( SQRT ( R * R - Y1 * Y1 ) / Y1 );
      GAMMA := PI - ALFA / 2;
      AREA := R * R * ( SIN ( ALFA ) / 2 + GAMMA ) / 2
    END   {END ELSE IF Y1 < R}
  ELSE IF Y2 < R THEN
    BEGIN
      ALFA := 2 * ARCTAN ( SQRT ( R * R - Y2 * Y2 ) / Y2 );
      GAMMA := PI - ALFA / 2;
      AREA := R * R * ( SIN ( ALFA ) / 2 + GAMMA ) / 2
    END   {END ELSE IF Y2 < R}
  ELSE
    AREA := R * R * PI / 2
END   {END ELSE IF X1 = 0}

ELSE IF X1 < R THEN
BEGIN
  IF Y1 < 0 THEN
  BEGIN
    IF R * R > X1 * X1 + Y1 * Y1 THEN
      BEGIN
        ALFA := 2 * ARCTAN ( SQRT ( R * R - X1 * X1 ) / X1 );
        BETA := 2 * ARCTAN ( SQRT ( R * R - Y1 * Y1 ) / ( - Y1 ) );
        GAMMA := 0.5 * PI + ( ALFA + BETA ) / 2;
```

```
         AREA := R * R * ( GAMMA - ALFA + SIN ( ALFA ) / 2 -
                           SIN ( BETA ) / 2 ) / 2 + X1 * Y1
      END   {END IF R * R > X1 * X1 + Y1 * Y1}
   ELSE
      BEGIN
         ALFA := 2 * ARCTAN ( SQRT ( R * R - Y1 * Y1 ) / ( - Y1 ) );
         AREA := R * R * ( ALFA - SIN ( ALFA ) ) / 2
      END   {END ELSE - R * R <= X1 * X1 + Y1 * Y1}
END   {END IF Y1 < 0}
ELSE IF Y2 < 0 THEN
BEGIN
   IF R * R > X1 * X1 + Y2 * Y2 THEN
      BEGIN
         ALFA := 2 * ARCTAN ( SQRT ( R * R - X1 * X1 ) / X1 );
         BETA := 2 * ARCTAN ( SQRT ( R * R - Y2 * Y2 ) / ( - Y2 ) );
         GAMMA := 0.5 * PI + ( ALFA + BETA ) / 2;
         AREA := R * R * ( GAMMA - ALFA + SIN ( ALFA ) / 2 -
                           SIN ( BETA ) / 2 ) / 2 + X1 * Y2
      END   {END IF R * R > X1 * X1 + Y2 * Y2}
   ELSE
      BEGIN
         ALFA := 2 * ARCTAN ( SQRT ( R * R - Y2 * Y2 ) / ( - Y2 ) );
         AREA := R * R * ( ALFA - SIN ( ALFA ) ) / 2
      END   {END ELSE - R * R <= X1 * X1 + Y2 * Y2}
END   {END ELSE IF Y2 < 0}
ELSE IF ( Y1 = 0 ) OR ( Y2 = 0 ) THEN
   BEGIN
      ALFA := 2 * ARCTAN ( SQRT ( R * R - X1 * X1 ) / X1 );
      GAMMA := PI - ALFA / 2;
      AREA := R * R * ( SIN ( ALFA ) / 2 + GAMMA ) / 2
   END   {END ELSE IF (Y1 = 0) OR (Y2 = 0)}

ELSE IF Y1 < R THEN
BEGIN
   IF R * R > X1 * X1 + Y1 * Y1 THEN
      BEGIN
         ALFA := 2 * ARCTAN ( SQRT ( R * R - X1 * X1 ) / X1 );
         BETA := 2 * ARCTAN ( SQRT ( R * R - Y1 * Y1 ) / Y1 );
         GAMMA := 1.5 * PI - ( ALFA + BETA ) / 2;
         AREA := X1 * Y1 + R * R * ( SIN ( ALFA ) / 2 +
                                     SIN ( BETA ) / 2 + GAMMA ) / 2
      END   {END IF R * R > X1 * X1 + Y1 * Y1}
   ELSE
      BEGIN
         ALFA := 2 * ARCTAN ( SQRT ( R * R - X1 * X1 ) / X1 );
         BETA := 2 * ARCTAN ( SQRT ( R * R - Y1 * Y1 ) / Y1 );
         AREA := R * R * ( 2 * PI - ALFA + SIN ( ALFA ) -
                                    BETA + SIN ( BETA ) ) / 2
      END   {END ELSE - R * R <= X1 * X1 + Y1 * Y1}
END   {END ELSE IF Y1 < R}

ELSE IF Y2 < R THEN
BEGIN
```

```
      IF R * R > X1 * X1 + Y2 * Y2 THEN
         BEGIN
            ALFA := 2 * ARCTAN ( SQRT ( R * R - X1 * X1 ) / X1 );
            BETA := 2 * ARCTAN ( SQRT ( R * R - Y2 * Y2 ) / Y2 );
            GAMMA := 1.5 * PI - ( ALFA + BETA ) / 2;
            AREA := X1 * Y2 + R * R * ( SIN ( ALFA ) / 2 +
                                        SIN ( BETA ) / 2 + GAMMA ) / 2
         END   {END IF R * R > X1 * X1 + Y2 * Y2}
      ELSE
         BEGIN
            ALFA := 2 * ARCTAN ( SQRT ( R * R - X1 * X1 ) / X1 );
            BETA := 2 * ARCTAN ( SQRT ( R * R - Y2 * Y2 ) / Y2 );
            AREA := R * R * ( 2 * PI - ALFA + SIN ( ALFA ) -
                                       BETA + SIN ( BETA ) ) / 2
         END   {END ELSE - R * R <= X1 * X1 + Y2 * Y2}
   END   {END ELSE IF Y2 < R}
   ELSE
      BEGIN
         ALFA := 2 * ARCTAN ( SQRT ( R * R - X1 * X1 ) / X1 );
         AREA := R * R * ( 2 * PI - ALFA + SIN ( ALFA ) ) / 2
      END   {END ELSE}
END   {END ELSE IF X1 < R}
(*                   *)
(*R <= X1 < DMAX / 2 *)
(*                   *)
ELSE
BEGIN
   IF Y1 < 0 THEN
      BEGIN
         BETA := 2 * ARCTAN ( SQRT ( R * R - Y1 * Y1 ) / ( - Y1 ) );
         AREA := R * R * ( BETA - SIN ( BETA ) ) / 2
      END   {END IF Y1 < 0}
   ELSE IF Y2 < 0 THEN
      BEGIN
         BETA := 2 * ARCTAN ( SQRT ( R * R - Y2 * Y2 ) / ( - Y2 ) );
         AREA := R * R * ( BETA - SIN ( BETA ) ) / 2
      END   {END ELSE IF Y2 < 0}
   ELSE IF ( Y1 = 0 ) OR ( Y2 = 0 ) THEN
      BEGIN
         AREA := R * R * PI / 2
      END   {END ELSE IF (Y1 = 0) OR (Y2 = 0)}

   ELSE IF Y1 < R THEN
      BEGIN
         BETA := 2 * ARCTAN ( SQRT ( R * R - Y1 * Y1 ) / Y1 );
         AREA := R * R * ( 2 * PI - BETA + SIN ( BETA ) ) / 2
      END   {END ELSE IF Y1 < R}

   ELSE IF Y2 < R THEN
      BEGIN
         BETA := 2 * ARCTAN ( SQRT ( R * R - Y2 * Y2 ) / Y2 );
         AREA := R * R * ( 2 * PI - BETA + SIN ( BETA ) ) / 2
      END   {END ELSE IF Y2 < R}
```

```
         ELSE
            AREA := R * R * PI
      END;   {END ELSE - R <= X1 < DMAX / 2}
      SUM := SUM + AREA;
      LAST := LAST^.NEXT
   END;   {END WHILE LAST^.DATA.X < LEFT + DMAX / 2}
WHILE (LAST^.DATA.X <= RIGHT - DMAX / 2) AND (LAST <> Z) DO
   BEGIN
      WITH LAST^.DATA DO
         BEGIN
            X1 := X - LEFT;
            X2 := RIGHT - X;
            Y1 := Y - BOTTOM;
            Y2 := TOP - Y;
            R := DIA / 2
         END;   {END WITH LAST^.DATA}
      IF Y1 < 0 THEN
         BEGIN
            BETA := 2 * ARCTAN ( SQRT ( R * R - Y1 * Y1 ) / ( - Y1 ) );
            AREA := R * R * ( BETA - SIN ( BETA ) ) / 2
         END   {END IF Y1 < 0}
      ELSE IF Y2 < 0 THEN
         BEGIN
            BETA := 2 * ARCTAN ( SQRT ( R * R - Y2 * Y2 ) / ( - Y2 ) );
            AREA := R * R * ( BETA - SIN ( BETA ) ) / 2
         END   {END ELSE IF Y2 < 0}
      ELSE IF (Y1 = 0 ) OR ( Y2 = 0 ) THEN
         BEGIN
            AREA := R * R * PI / 2
         END   {END ELSE IF (Y1 = 0) OR (Y2 = 0)}
      ELSE IF Y1 < R THEN
         BEGIN
            BETA := 2 * ARCTAN ( SQRT ( R * R - Y1 * Y1 ) / Y1 );
            AREA := R * R * ( 2 * PI - BETA + SIN ( BETA ) ) / 2
         END   {END ELSE IF Y1 < R}
      ELSE IF Y2 < R THEN
         BEGIN
            BETA := 2 * ARCTAN ( SQRT ( R * R - Y2 * Y2 ) / Y2 );
            AREA := R * R * ( 2 * PI - BETA + SIN ( BETA ) ) / 2
         END   {END ELSE IF Y2 < R}
      ELSE
         BEGIN
         AREA := R * R * PI
         END;   {END ELSE}
      SUM := SUM + AREA;
      LAST := LAST^.NEXT
   END;   {END WHILE LAST^.DATA.X <= RIGHT - DMAX / 2}
WHILE LAST <> Z DO
   BEGIN
      WITH LAST^.DATA DO
         BEGIN
            X1 := X - LEFT;
            X2 := RIGHT - X;
      Y1 := Y - BOTTOM;
      Y2 := TOP - Y;
      R := DIA / 2
   END;   {END WITH LAST^.DATA}

IF X2 >= R THEN
BEGIN
   IF Y1 < 0 THEN
      BEGIN
         BETA := 2 * ARCTAN ( SQRT ( R * R - Y1 * Y1 ) / ( - Y1 ) );
         AREA := R * R * ( BETA - SIN ( BETA ) ) / 2
      END   {END IF Y1 < 0}
   ELSE IF Y2 < 0 THEN
      BEGIN
         BETA := 2 * ARCTAN ( SQRT ( R * R - Y2 * Y2 ) / ( - Y2 ) );
         AREA := R * R * ( BETA - SIN ( BETA ) ) / 2
      END   {END ELSE IF Y2 < 0}
   ELSE IF ( Y1 = 0 ) OR ( Y2 = 0 ) THEN
      BEGIN
         AREA := R * R * PI / 2
      END   {END ELSE IF (Y1 = 0) OF (Y2 = 0)}
   ELSE IF Y1 < R THEN
      BEGIN
         BETA := 2 * ARCTAN ( SQRT ( R * R - Y1 * Y1 ) / Y1 );
         AREA := R * R * ( 2 * PI - BETA + SIN ( BETA ) ) / 2
      END   {END ELSE IF Y1 < R}
   ELSE IF Y2 < R THEN
      BEGIN
         BETA := 2 * ARCTAN ( SQRT ( R * R - Y2 * Y2 ) / Y2 );
         AREA := R * R * ( 2 * PI - BETA + SIN ( BETA ) ) / 2
      END   {END ELSE IF Y2 < R}
   ELSE
      AREA := R * R * PI
END   {END IF X2 >= R}

ELSE IF X2 > 0 THEN
BEGIN
   IF Y1 < 0 THEN
   BEGIN
      IF R * R > X2 * X2 + Y1 * Y1 THEN
         BEGIN
            ALFA := 2 * ARCTAN ( SQRT ( R * R - X2 * X2 ) / X2 );
            BETA := 2 * ARCTAN ( SQRT ( R * R - Y1 * Y1 ) / ( - Y1 ) );
            GAMMA := 0.5 * PI + ( ALFA + BETA ) / 2;
            AREA := R * R * ( GAMMA - ALFA + SIN ( ALFA ) / 2 -
                                      SIN ( BETA ) / 2 ) / 2 + X2 * Y1
         END   {END IF R * R > X2 * X2 + Y1 * Y1}

      ELSE
         BEGIN
            BETA := 2 * ARCTAN ( SQRT ( R * R - Y1 * Y1 ) / ( - Y1 ) );
            AREA := R * R * ( BETA - SIN ( BETA ) ) / 2
         END   {END ELSE - R * R <= X2 * X2 + Y1 * Y1}
END   {END IF Y1 < 0}
ELSE IF Y2 < 0 THEN
BEGIN
   IF R * R > X2 * X2 + Y2 * Y2 THEN
      BEGIN
         ALFA := 2 * ARCTAN ( SQRT ( R * R - X2 * X2 ) / X2 );
         BETA := 2 * ARCTAN ( SQRT ( R * R - Y2 * Y2 ) / ( - Y2 ) );
         GAMMA := 0.5 * PI + ( ALFA + BETA ) / 2;
         AREA := R * R * ( GAMMA - ALFA + SIN ( ALFA ) / 2 -
                           SIN ( BETA ) / 2 ) / 2 + X2 * Y2
      END   {END IF R * R < X2 * X2 + Y2 * Y2}
   ELSE
      BEGIN
         BETA := 2 * ARCTAN ( SQRT ( R * R - Y2 * Y2 ) / ( - Y2 ) );
         AREA := R * R * ( BETA - SIN ( BETA ) ) / 2
      END   {END ELSE - R * R <= X2 * X2 + Y2 * Y2}
END   {END ELSE IF Y2 < 0}
ELSE IF ( Y1 = 0 ) OR ( Y2 = 0 ) THEN
   BEGIN
      ALFA := 2 * ARCTAN ( SQRT ( R * R - X2 * X2 ) / X2 );
      GAMMA := PI - ALFA / 2;
      AREA := R * R * ( GAMMA + SIN ( ALFA ) / 2 ) / 2
   END   {END ELSE IF (Y1 = 0) OR (Y2 = 0)}
ELSE IF Y1 < R THEN
BEGIN
   IF R * R > X2 * X2 + Y1 * Y1 THEN
      BEGIN
         ALFA := 2 * ARCTAN ( SQRT ( R * R - X2 * X2 ) / X2 );
         BETA := 2 * ARCTAN ( SQRT ( R * R - Y1 * Y1 ) / Y1 );
         GAMMA := 1.5 * PI - ( ALFA + BETA ) / 2;
         AREA := X2 * Y1 + R * R * ( GAMMA + SIN ( ALFA ) / 2 +
                                     SIN ( BETA ) / 2 ) / 2
      END   {END IF R * R > X2 * X2 + Y1 * Y1}
   ELSE
      BEGIN
         ALFA := 2 * ARCTAN ( SQRT ( R * R - X2 * X2 ) / X2 );
         BETA := 2 * ARCTAN ( SQRT ( R * R - Y1 * Y1 ) / Y1 );
         AREA := R * R * ( 2 * PI - ALFA + SIN ( ALFA ) -
                                    BETA + SIN ( BETA ) ) / 2
      END   {END ELSE - R * R <= X2 * X2 + Y1 * Y1}
END   {END ELSE IF Y1 < R}
ELSE IF Y2 < R THEN
BEGIN
   IF R * R > X2 * X2 + Y2 * Y2 THEN
      BEGIN
         ALFA := 2 * ARCTAN ( SQRT ( R * R - X2 * X2 ) / X2 );
         BETA := 2 * ARCTAN ( SQRT ( R * R - Y2 * Y2 ) / Y2 );
         GAMMA := 1.5 * PI - ( ALFA + BETA ) / 2;
         AREA := X2 * Y2 + R * R * ( GAMMA + SIN ( ALFA ) / 2 +
                                      SIN ( BETA ) / 2 ) / 2
      END   {END IF R * R > X2 * X2 + Y2 * Y2}
   ELSE
      BEGIN
```

```
            ALFA := 2 * ARCTAN ( SQRT ( R * R - X2 * X2 ) / X2 );
            BETA := 2 * ARCTAN ( SQRT ( R * R - Y2 * Y2 ) / Y2 );
            AREA := R * R * ( 2 * PI - ALFA + SIN ( ALFA ) -
                                       BETA + SIN ( BETA ) ) / 2
         END   {END ELSE - R * R <= X2 * X2 + Y2 * Y2}
   END   {END ELSE IF Y2 < R}
   ELSE
      BEGIN
         ALFA := 2 * ARCTAN ( SQRT ( R * R - X2 * X2 ) / X2 );
         AREA := R * R * ( 2 * PI - ALFA + SIN ( ALFA ) ) / 2
      END   {END ELSE}
END   {END ELSE IF X2 > 0}
ELSE IF X2 = 0 THEN
BEGIN
   IF Y1 < 0 THEN
      BEGIN
         BETA := 2 * ARCTAN ( SQRT ( R * R - Y1 * Y1 ) / ( - Y1 ) );
         AREA := R * R * ( BETA - SIN ( BETA ) ) / 4
      END   {END IF Y1 < 0}
   ELSE IF Y2 < 0 THEN
      BEGIN
         BETA := 2 * ARCTAN ( SQRT ( R * R - Y2 * Y2 ) / ( - Y2 ) );
         AREA := R * R * ( BETA - SIN ( BETA ) ) / 4
      END   {END ELSE IF Y2 < 0}
   ELSE IF ( Y1 = 0 ) OR ( Y2 = 0 ) THEN
      BEGIN
         AREA := R * R * PI / 4
      END   {END ELSE IF (Y1 = 0) OR (Y2 = 0)}
   ELSE IF Y1 < R THEN
      BEGIN
         BETA := 2 * ARCTAN ( SQRT ( R * R - Y1 * Y1 ) / Y1 );
         GAMMA := PI - BETA / 2;
         AREA := R * R * ( GAMMA + SIN ( BETA ) / 2 ) / 2
      END   {END ELSE IF Y1 < R}
   ELSE IF Y2 < R THEN
      BEGIN
         BETA := 2 * ARCTAN ( SQRT ( R * R - Y2 * Y2 ) / Y2 );
         GAMMA := PI - BETA / 2;
         AREA := R * R * ( GAMMA + SIN ( BETA ) / 2 ) / 2
      END   {END ELSE IF Y2 < R}
   ELSE
      AREA := R * R * PI / 2
END   {END ELSE IF X2 = 0}
(*      *)
(*X2 < 0*)
(*      *)
ELSE
BEGIN
   IF Y1 < 0 THEN
      BEGIN
         ALFA := 2 * ARCTAN ( SQRT ( R * R - X2 * X2 ) / ( - X2 ) );
         BETA := 2 * ARCTAN ( SQRT ( R * R - Y1 * Y1 ) / ( - Y1 ) );
         GAMMA := 0.5 * PI + ( ALFA + BETA ) / 2;
      AREA := R * R * ( ALFA - SIN ( ALFA ) / 2 +
              BETA - SIN ( BETA ) / 2 - GAMMA ) / 2 + X2 * Y1
   END   {END IF Y1 < 0}
ELSE IF Y2 < 0 THEN
   BEGIN
      ALFA := 2 * ARCTAN ( SQRT ( R * R - X2 * X2 ) / ( - X2 ) );
      BETA := 2 * ARCTAN ( SQRT ( R * R - Y2 * Y2 ) / ( - Y2 ) );
      GAMMA := 0.5 * PI + ( ALFA + BETA ) / 2;
      AREA := R * R * ( ALFA  - SIN ( ALFA ) / 2 +
              BETA - SIN ( BETA ) / 2 - GAMMA ) / 2 + X2 * Y2
   END   {END ELSE IF Y2 < 0}

ELSE IF ( Y1 = 0 ) OR ( Y2 = 0 ) THEN
   BEGIN
      ALFA := 2 * ARCTAN ( SQRT ( R * R - X2 * X2 ) / ( - X2 ) );
      AREA := R * R * ( ALFA - SIN ( ALFA ) ) / 4
   END   {END ELSE IF (Y1 = 0) OR (Y2 = 0)}

ELSE IF Y1 < R THEN
BEGIN
   IF R * R > X2 * X2 + Y1 * Y1 THEN
      BEGIN
         ALFA := 2 * ARCTAN ( SQRT ( R * R - X2 * X2 ) / ( - X2 ) );
         BETA := 2 * ARCTAN ( SQRT ( R * R - Y1 * Y1 ) / Y1 );
         GAMMA := 0.5 * PI + ( ALFA + BETA ) / 2;
         AREA := R * R * ( GAMMA - BETA + SIN ( BETA ) / 2
                 - SIN ( ALFA ) / 2 ) / 2 + X2 * Y1
      END   {END IF R * R > X2 * X2 + Y1 * Y1}

   ELSE
      BEGIN
         ALFA := 2 * ARCTAN ( SQRT ( R * R - X2 * X2 ) / ( - X2 ) );
         AREA := R * R * ( ALFA - SIN ( ALFA ) ) / 2
      END   {END ELSE - R * R <= X2 * X2 + Y1 * Y1}
END   {END ELSE IF Y1 < R}

ELSE IF Y2 < R THEN
BEGIN
   IF R * R > X2 * X2 + Y2 * Y2 THEN
      BEGIN
         ALFA := 2 * ARCTAN ( SQRT ( R * R - X2 * X2 ) / ( - X2 ) );
         BETA := 2 * ARCTAN ( SQRT ( R * R - Y2 * Y2 ) / Y2 );
         GAMMA := 0.5 * PI + ( ALFA + BETA ) / 2;
         AREA := R * R * ( GAMMA - BETA + SIN ( BETA ) / 2
                 - SIN ( ALFA ) / 2 ) / 2 + X2 * Y2
      END   {END IF R * R > X2 * X2 + Y2 * Y2}

   ELSE
      BEGIN
         ALFA := 2 * ARCTAN ( SQRT ( R * R - X2 * X2 ) / ( - X2 ) );
         AREA := R * R * ( ALFA - SIN ( ALFA ) ) / 2
      END   {END ELSE - R * R <= X2 * X2 + Y2 * Y2}
END   {END ESLE IF Y2 < R}
```

```
            ELSE
               BEGIN
                  ALFA := 2 * ARCTAN ( SQRT ( R * R - X2 * X2 ) / ( - X2 ) );
                  AREA := R * R * ( ALFA - SIN ( ALFA ) ) / 2
               END   {END ELSE}
         END;   {END ELSE - X2 < 0}
         SUM := SUM + AREA;
         LAST := LAST^.NEXT
      END;   {END WHILE LAST <> Z}

   ETA := SUM / ((RIGHT - LEFT) * (TOP - BOTTOM))
   END;   {END PROCEDURE FIND_PF}

(********************************************************************************)
(*                                                                              *)
(*                THE MAIN PROGRAM STARTS FROM HERE                             *)
(*                                                                              *)
(********************************************************************************)
BEGIN
   RESET (DISKIN);
   REWRITE (NBRFILE);
   REWRITE (VTXFILE);
   REWRITE (BOX);
   REWRITE (DELAUNAY);
   REWRITE (SNBRFILE);
   REWRITE (TABLE);
   READLN (DISKIN, STRING30, NUM_DISK);
   READLN (DISKIN, STRING30, EQ_DISKS);
   READLN (DISKIN, STRING30, KNOWN_TO_BE_RCP);
   READLN (DISKIN, STRING30, WIDE);
   READLN (DISKIN, STRING30, PERIODICAL_REQUIRED);
   READLN (DISKIN, STRING30, FIND_WALL_EFFECT);
   READLN (DISKIN, STRING30, HEIGHT, WIDTH);
   READLN (DISKIN, STRING30, DEFINE_PF_BOX);
   IF DEFINE_PF_BOX THEN
      READLN (DISKIN, PF_L, PF_R, PF_B, PF_T);
   READLN (DISKIN, STRING30, TOLERANCE);
   READLN (DISKIN, STRING30, NUM_ANG_DIV);
   (*                                      *)
   (*FORM A DUMMY END NODE FOR LINKED LISTS*)
   (*                                      *)
   NEW (Z);
   Z^.NEXT := Z;
   WITH Z^.DATA DO
      BEGIN
         X := 1000;
         Y := 1000
      END;   {END WITH Z^.DATA}

   (*                                                           *)
   (*CALL LIST_CREATE TO FORM A LINKED LIST OF POINTS NOT SORTED*)
   (*                                                           *)
   RANDOM := LIST_CREATE;
```

```
(*                                                      *)
(*CALL MERGESORT TO FORM A LINKED LIST OF POINTS SORTED*)
(*                                                      *)
SORT := MERGESORT (RANDOM, NUM_DISK);
(*                         *)
(*FIND THE MAXIMUM DIAMETER*)
(*                         *)
IF NOT EQ_DISKS THEN
   BEGIN
      LAST := SORT;
      DMAX := LAST^.DATA.DIA;

      LAST := LAST^.NEXT;
      FOR I := 2 TO NUM_DISK DO
         BEGIN
            IF DMAX < LAST^.DATA.DIA THEN
               DMAX := LAST^.DATA.DIA;
            LAST := LAST^.NEXT
         END  {END FOR I := 2 TO NUM_DISK}
   END   {END IF NOT EQ_DISKS}
ELSE
   BEGIN
      DMAX := SORT^.DATA.DIA
   END;   {END ELSE - EQ_DISKS}

WRITELN (BOX);
WRITELN (BOX, '  $MAXIMUM DISK DIAMETER:', DMAX);
(*                                                        *)
(*IMPLEMENT THE PERIODICAL BOUNDARY CONDITION IF REQUIRED.*)
(*OTHERWISE, KEEP THE ORIGINAL LINKED LIST OF DISK 'SORT'.*)
(*                                                        *)
IF PERIODICAL_REQUIRED THEN
   BEGIN
      PERIODICAL (SORT, NUM_DISK, NUM_LOOP, DMAX, WIDE);
      WRITELN (BOX);
      WRITELN(BOX,'  $NUMBER OF DISKS TO BE PROCESSED AFTER IMPLEMENTATION');
      WRITELN (BOX, '  OF THE PERIODICAL BOUNDARY CONDITION: ', NUM_LOOP);
   END   {END IF PERIODICAL_REQUIRED}
ELSE
   BEGIN
      NUM_LOOP := NUM_DISK;
      WRITELN (BOX);
      WRITELN (BOX, '  $NO PERIODICAL BOUNDARY CONDITION REQUIRED.');
      WRITELN (BOX, '  NUMBER OF DISKS TO BE HANDLED IS EXACTLY THE SAME');
      WRITELN (BOX, '  AS NUMBER OF DISKS IN THE ENSEMBLE: ', NUM_LOOP)
   END;   {END ELSE - NOT PERIODICAL_QUIRED}
(*                                                                      *)
(*FIND THE EXTREMA OF THE COORDINATES OF THE BOX, XMAX, XMIN, YMAX, YMIN*)
(*                                                                      *)
LAST := SORT;
WITH LAST^.DATA DO
   BEGIN
      XMAX := X;
      XMIN := X;
      YMAX := Y;
      YMIN := Y
   END;  {END WITH LAST^.DATA}
LAST := LAST^.NEXT;
WHILE LAST <> Z DO
   BEGIN
      IF XMAX < LAST^.DATA.X THEN XMAX := LAST^.DATA.X;
      IF XMIN > LAST^.DATA.X THEN XMIN := LAST^.DATA.X;
      IF YMAX < LAST^.DATA.Y THEN YMAX := LAST^.DATA.Y;
      IF YMIN > LAST^.DATA.Y THEN YMIN := LAST^.DATA.Y;
      LAST := LAST^.NEXT
   END;  {END WHILE LAST <> Z}
XMAX := XMAX + BOX_C * DMAX; XMIN := XMIN - BOX_C * DMAX;
YMAX := YMAX + BOX_C * DMAX; YMIN := YMIN - BOX_C * DMAX;
WRITELN (BOX);
WRITELN (BOX, '  $THE EXTREMA OF THE BOX:');
WRITELN (BOX);
WRITELN (BOX, '  XMIN = ', XMIN, ' XMAX = ', XMAX);
WRITELN (BOX, '  YMIN = ', YMIN, ' YMAX = ', YMAX);
(*          *)
(*INITIALIZE*)
(*          *)
FOR K := 1 TO NUM_LOOP DO
   BEGIN
      NEW (NBR [K]);
      NBR [K]^.NEXT := Z;
      NBR_LAST [K] := NBR [K];

      NEW (VTX [K]);
      VTX [K]^.NEXT := Z;
      VTX_LAST [K] := VTX [K];

      NEW (NEW_NBR);
      NEW_NBR^.NEXT := Z;

      NEW (NEW_VTX);
      NEW_VTX^.NEXT := Z
   END;  {END FOR K := 1 TO NUM_LOOP}
(*                                                                   *)
(*1) FIND THE DISKS WITH CENTROIDS NEAREST TO FOUR CORNERS OF THE BOX*)
(*                                                                   *)
CORNER1 := NEAREST (XMIN, YMIN, SORT);
CORNER2 := NEAREST (XMIN, YMAX, SORT);
CORNER3 := NEAREST (XMAX, YMAX, SORT);
CORNER4 := NEAREST (XMAX, YMIN, SORT);

(*                                       *)
(*FORM THE LISTHEAD OF NBR [1] BY CORNER1*)
(*                                       *)
NEW (NBR_TEMP);
NBR_TEMP^.NEXT := Z;
NBR_TEMP^.DATA := CORNER1;
```

```
NBR_LAST [1]^.NEXT := NBR_TEMP;
NBR_LAST [1] := NBR_LAST [1]^.NEXT;
(*                            *)
(*FORM THE LISTHEAD OF VTX [1]*)
(*                            *)
NEW (VTX_TEMP);
VTX_TEMP^.NEXT := Z;
VTX_TEMP^.DATA := CORNER1;

VTX_LAST [1]^.NEXT := VTX_TEMP;
VTX_LAST [1] := VTX_LAST [1]^.NEXT;

NEW (VTX_TEMP);
VTX_TEMP^.NEXT := Z;
WITH VTX_TEMP^.DATA DO
   BEGIN
      X := XMIN;
      Y := YMIN
   END;   {END WITH VTX_TEMP^.DATA}
VTX_LAST [1]^.NEXT := VTX_TEMP;
VTX_LAST [1] := VTX_LAST [1]^.NEXT;
(***************************************************************************)
(*              FIND NEW NBR'S AND NEW VTX'S                               *)
(***************************************************************************)
K := 1; J := 0;
DUMMY_CREATE (CORNER1.X, CORNER1.Y, XMAX, XMIN, YMAX, YMIN,
              DUMMY1, DUMMY2, DUMMY3, DUMMY4);
NBR_FIRST := DUMMY4;
NEW_NBR^.DATA := DUMMY1;
ADD := FALSE;
REPEAT
   WITH NBR [K]^.NEXT^.DATA DO
      BEGIN
         X1 := X; Y1 := Y
      END;   {END WITH NBR [K]^.NEXT^.DATA}
   WITH NEW_NBR^.DATA DO
      BEGIN
         X2 := X; Y2 := Y
      END;   {END WITH NEW_NBR^.DATA}
   DUMMY_CREATE (X1, Y1, XMAX, XMIN, YMAX, YMIN,
                 DUMMY1, DUMMY2, DUMMY3, DUMMY4);
   REPEAT
         DUMMY_FIND (X1, Y1, X2, Y2,
                     DUMMY1, DUMMY2, DUMMY3, DUMMY4,
                     FIRST, SECOND);
         (*                                                            *)
         (*ASSIGN THE FIRST DUMMY POINT AS THE FIRST POTENTIAL NEW NBR*)
         (*                                                            *)
         NEW_NBR^.DATA := FIRST;
         WITH NEW_NBR^.DATA DO
            BEGIN
               X3 := X; Y3 := Y
            END;   {END WITH NEW_NBR^.DATA}
```

```
NEW_VTX^.DATA := VTX_FIND (X1, Y1, X2, Y2, X3, Y3);
WITH NEW_VTX^.DATA DO
   BEGIN
      XC := X; YC := Y
   END;   {END WITH NEW_VTX^.DATA}
R := SQRT ( SQR ( X3 - XC ) + SQR ( Y3 - YC ) );
XL := XC - R;
XR := XC + R;
LAST := SORT;

(*                                                 *)
(*VERIFY IF THE POTENTIAL NEW NBR IS A REAL NBR  BY*)
(*TESTING IN SEQUENCE FROM THE FIRST CENTROID AMONG*)
(*CENTROIDS IN THE LINKED LIST 'SORT'              *)
(*                                                 *)
REPEAT
   WITH LAST^.DATA DO
      BEGIN
         X4 := X; Y4 := Y;
         NEW_R := SQRT (SQR (X4 - XC) + SQR (Y4 - YC))
      END;   {END WTIH LAST^.DATA}
   (*                                                             *)
   (*IF X4, THE X-COORDINATE OF THE POINT UNDER TEST,  IS  IN  THE*)
   (*INTERVAL  (XL, XR):  THE  LEFT  MOST  AND  THE  RIGHT MOST X-*)
   (*COORDINATE OF THE CIRCLE DETERMINED BY (X1, Y1), THE CENTROID*)
   (*BEING  PROCESSED, (X2,  Y2), THE PREVIOUS  NBR, AND (X3, Y3),*)
   (*THE PRESENT POTENTIAL NEW NBR...                             *)
   (*                                                             *)
   IF ( XL <= X4 ) AND ( X4 <= XR ) THEN
         (*                                                      *)
         (*IF 1) X4 IS IN THE INTERVAL (XL, XR)                  *)
         (*   2) (X4, Y4) IS IN THE RIGHT HALF PLANE WITH RESPECT*)
         (*      TO THE LINE FROM (X1, Y1) TO (X2, Y2)...        *)
         (*                                                      *)
         IF ( X2 - X1 ) * ( Y4 - Y1 ) <
            ( X4 - X1 ) * ( Y2 - Y1 ) THEN
            (*                                                    *)
            (*IF 1) X4 IS IN THE INTERVAL (XL, XR)                *)
            (*   2) (X4, Y4) IS IN THE RIGHT HALF PLANE WITH      *)
            (*      RESPECT TO THE LINE FROM (X1, Y1) TO (X2, Y2) *)
            (*   3) (X4, Y4) IS IN THE RIGHT HALF PLANE WITH      *)
            (*      RESPECT TO THE LINE FROM (X1, Y1) TO (X3, Y3) *)
            (*   4) (X4, Y4) IS IN THE CIRCLE                     *)
            (*THEN (X4, Y4) REPLACES (X3, Y3) AS THE POTENTIAL NEW*)
            (*NBR. THE POTENTIAL NEW VTX IS TO BE CALCULATED AGAIN*)
            (*                                                    *)
            IF (X3 - X1) * (Y4 - Y1) <
               (X4 - X1) * (Y3 - Y1) THEN
               BEGIN
                  IF R > NEW_R THEN
                     BEGIN
                        NEW_NBR^.DATA := LAST^.DATA;
                        X3 := X4; Y3 := Y4;
            NEW_VTX^.DATA :=
                VTX_FIND (X1, Y1, X2, Y2, X3, Y3);
            WITH NEW_VTX^.DATA DO
               BEGIN
                  XC := X; YC := Y
               END;   {END WITH NEW_VTX^.DATA}
            R := SQRT (SQR (X3 - XC) + SQR (Y3 - YC));
            XL := XC - R; XR := XC + R;
            LAST := SORT
         END   {END IF R > NEW_R}
      (*                                              *)
      (* IF 1), 2), AND 3) ARE SATISFIED,             *)
      (* WHILE (X4, Y4) IS OUT OF THE CIRCLE          *)
      (* THEN KEEP (X3, Y3) AS THE POTENTIAL NEW      *)
      (* NEIGHBOUR.  GO TO THE NEXT NODE ON THE LINKED*)
      (* LIST 'SORT' AND KEEP ON TESTING.             *)
      (*                                              *)
      ELSE
         LAST := LAST^.NEXT
   END
(*                                                    *)
(* IF 1), 2) ARE SATISFIED,                           *)
(* WHILE 1) (X4, Y4) IS IN THE LEFT HALF PLANE WITH   *)
(*          RESPECT TO THE LINE FROM (X1, Y1) TO      *)
(*          (X3, Y3)                                  *)
(*       2) NEW_R IS CLOSE TO OR SIGINFICANTLY LESS   *)
(*          THAN R                                    *)
(* THEN REDEFINE THE CIRCLE USING (X1, Y1), (X2, Y2), *)
(* AND (X3, Y3)                                       *)
(*                                                    *)
ELSE IF NEW_R - R < 0.00001 THEN
   BEGIN
      VERTEX_TEMP := VTX_FIND (X1, Y1, X2, Y2, X4, Y4);
      WITH VERTEX_TEMP DO
         BEGIN
            XC_TEMP := X; YC_TEMP := Y
         END;   {END WITH VERTEX_TEMP}
      R_TEMP := SQRT (SQR (X3 - XC_TEMP) +
                      SQR (Y3 - YC_TEMP));
      NEW_R := SQRT (SQR (X4 - XC_TEMP) +
                     SQR (Y4 - YC_TEMP));
      (*                            *)
      (* (X4, Y4) IS IN THE CIRCLE  *)
      (*                            *)
      IF R_TEMP - NEW_R > 0 THEN
         BEGIN
            NEW_NBR^.DATA := LAST^.DATA;
            X3 := X4;
            Y3 := Y4;
            NEW_VTX^.DATA := VERTEX_TEMP;
            XC := XC_TEMP;
            YC := YC_TEMP;
            R := NEW_R;
```

```
                        XL := XC - R; XR := XC + R;
                        LAST := SORT
                     END   {END IF R_TEMP > NEW_R}

                  (*                                *)
                  (* (X4, Y4) IS OUT OF THE CIRCLE *)
                  (*                                *)
                  ELSE
                     LAST := LAST^.NEXT
               END   {END ELSE IF}

            (*                                                    *)
            (* IF 1) AND 2) ARE SATISFIED,                        *)
            (* WHILE 1) (X4, Y4) IS ON THE LEFT HALF PLANE WITH   *)
            (*          RESPECT TO THE LINE FROM (X1, Y1) TO      *)
            (*          (X3, Y3)                                  *)
            (*       2) NEW_R IS SIGNIGICANTLY GREATER THAN R     *)
            (* THEN KEEP (X3, Y3) AS THE POTENTIAL NEW NEIGHBOUR. *)
            (* GO TO THE NEXT NODE ON THE LINKED LIST 'SORT' AND  *)
            (* KEEP ON TESTING                                    *)
            (*                                                    *)
            ELSE
                LAST := LAST^.NEXT

         (*                                                       *)
         (*IF X4 IS IN THE INTERVAL (XL, XR)                      *)
         (*WHILE (X4, Y4) IS IN THE LEFT HALF PLANE  WITH  RESPECT*)
         (*TO THE LINE FROM (X1, Y1) TO (X2, Y2)                  *)
         (*THEN KEEP (X3, Y3) AS THE POTENTIAL NEW NBR.  GO TO THE*)
         (*NEXT NODE ON THE LINKED LIST 'SORT' AND KEEP ON TESTING*)
         (*                                                       *)
         ELSE
            LAST := LAST^.NEXT

   (*                                                       *)
   (*IF X4 IS OUT OF THE INTERVAL (XL, XR)                  *)
   (*KEEP (X3, Y3) AS THE POTENTIAL NEW NBR.  GO TO THE NEXT*)
   (*NODE ON THE LINKED LIST 'SORT' AND KEEP ON TESTING     *)
   (*                                                       *)
   ELSE
      LAST := LAST^.NEXT

(*                                                               *)
(*(X3, Y3) REMAINS A POTENTIAL NBR AFTER ALL POINTS IN THE 'SORT'*)
(*HAVE BEEN PUT THROUGH THE ABOVE TEST, THEN STOP  THE  TEST  AND*)
(*KEEP (X3, Y3) AS THE NEW NBR, (XC, YC) AS THE NEW VTX          *)
(*                                                               *)
UNTIL
   ( XR < X4 ) OR ( LAST = Z );
(*                                                             *)
(*UPDATE THE NEW NBR FOR THE SUBSEQUENT NEW NBR FINDING PROCESS*)
(*                                                             *)
X2 := X3; Y2 := Y3;
```

```
(*******************************************************************)
(*          ASSIGN 'SECOND' AS THE NEW NBR IF                     *)
(*          THE NEW VTX IS OUT OF THE BOX                         *)
(*******************************************************************)
IF (XC < XMIN - 0.00001) OR (YC > YMAX + 0.00001) OR
   (XC > XMAX + 0.00001) OR (YC < YMIN - 0.00001) THEN
   BEGIN
      NEW_NBR^.DATA := SECOND;
      WITH SECOND DO
         BEGIN
            X2 := X; Y2 := Y
         END;   {END WITH SECOND}
      NEW_VTX^.DATA :=
         VTX_FIND (X1, Y1,
                   NBR_LAST [K]^.DATA.X, NBR_LAST [K]^.DATA.Y,
                   X2, Y2)
   END;

(*                                                 *)
(*DETERMINE IF THE BOOLEAN VARIABLE 'PLUS' IS TRUE*)
(*                                                 *)
PLUS := TRUE;
IF NEW_NBR^.DATA.INDEX <> 0 THEN
   BEGIN
      I := 1;
      REPEAT
         IF NEW_NBR^.DATA.INDEX = NBR [I]^.NEXT^.DATA.INDEX THEN
            PLUS := FALSE;
         I := I + 1
      UNTIL
         ( NOT PLUS ) OR ( I > K + J )
   END
ELSE
   PLUS := FALSE;

(*******************************************************************)
(*  CONNECT THE NEW NBR AND NEW VTX TO NBR [K]'S AND VTX [K]'S    *)
(*  WHICH CONTAIN THEM                                            *)
(*  THE NBR'S AND VTX'S IN EACH NBR [K]'S AND VTX [K]'S ARE       *)
(*  SEQUENCED IN CLOCKWISE ORDER                                  *)
(*******************************************************************)

(*                                       *)
(*IF THE NEW NBR IS NOT A DUMMY POINT...*)
(*                                       *)
IF ( NEW_NBR^.DATA.INDEX <> 0 ) THEN

   (*                                                          *)
   (*IF THE NEW NBR IS NEITHER A DUMMY POINT NOR THE FIRST NBR...*)
   (*                                                          *)
   IF ( ( NEW_NBR^.DATA.X <> NBR_FIRST.X ) OR
        ( NEW_NBR^.DATA.Y <> NBR_FIRST.Y ) ) THEN
      BEGIN
```

```
(*                                           *)
(*IF THE NEW NBR IS NEITHER A DUMMY POINT NOR*)
(*THE FIRST NBR, AND THERE IS STILL NO LINKED*)
(*LIST OF NBR'S CORRESPONDING TO IT          *)
(*                                           *)
IF PLUS THEN
   BEGIN
      J := J + 1;
      IF J >= 1 THEN
         BEGIN
            (*                                     *)
            (*CREATE THE NEW LINKED LIST OF NBR'S*)
            (*CORRESPONDING TO THE NEW NBR       *)
            (*                                     *)
            NEW (NBR_TEMP);
            NBR_TEMP^.NEXT := Z;
            NBR_TEMP^.DATA := NEW_NBR^.DATA;

            NBR_LAST [K + J]^.NEXT := NBR_TEMP;
            NBR_LAST [K + J] := NBR_LAST [K + J]^.NEXT;

            NEW (NBR_TEMP);
            NBR_TEMP^.NEXT := Z;
            NBR_TEMP^.DATA := NBR [K]^.NEXT^.DATA;

            NBR_LAST [K + J]^.NEXT := NBR_TEMP;
            NBR_LAST [K + J] := NBR_LAST [K + J]^.NEXT;

            IF ADD THEN
               BEGIN
                  NEW (NBR_TEMP);
                  NBR_TEMP^.NEXT := Z;
                  NBR_TEMP^.DATA := NBR_LAST [K]^.DATA;

                  NBR_LAST [K + J]^.NEXT := NBR_TEMP;
                  NBR_LAST [K + J] :=
                     NBR_LAST [K + J]^.NEXT
               END;   {END IF ADD}
            (*                                     *)
            (*CREATE THE NEW LINKED LIST OF VTX'S*)
            (*CORRESPONDING TO THE NEW NBR       *)
            (*                                     *)
            NEW (VTX_TEMP);
            VTX_TEMP^.NEXT := Z;
            VTX_TEMP^.DATA := NEW_NBR^.DATA;

            VTX_LAST [K + J]^.NEXT := VTX_TEMP;
            VTX_LAST [K + J] := VTX_LAST [K + J]^.NEXT;

            NEW (VTX_TEMP);
            VTX_TEMP^.NEXT := Z;
            VTX_TEMP^.DATA := NEW_VTX^.DATA;
            VTX_LAST [K + J]^.NEXT := VTX_TEMP;
            VTX_LAST [K + J] := VTX_LAST [K + J]^.NEXT;

            IF ( J > 1 ) AND ( ADD ) THEN
               BEGIN
                  (*                               *)
                  (*INSERT THE NEW NBR AS THE FIRST*)
                  (*NBR TO THE PREVIOUS NBR        *)
                  (*                               *)
                  NEW (NBR_TEMP);
                  NBR_TEMP^.DATA := NEW_NBR^.DATA;

                  NBR_TEMP^.NEXT :=
                      NBR [K + J - 1]^.NEXT^.NEXT;
                  NBR [K + J - 1]^.NEXT^.NEXT := NBR_TEMP;

                  (*                               *)
                  (*INSERT THE NEW VTX AS THE FIRST*)
                  (*VTX TO THE PREVIOUS NBR        *)
                  (*                               *)
                  NEW (VTX_TEMP);
                  VTX_TEMP^.DATA := NEW_VTX^.DATA;

                  VTX_TEMP^.NEXT :=
                      VTX [K + J - 1]^.NEXT^.NEXT;
                  VTX [K + J - 1]^.NEXT^.NEXT := VTX_TEMP
               END   {END IF (J > 1) AND (ADD)}
         END;   {END IF J >= 1}
      (*                                         *)
      (*ASSIGN 'ADD' TO BE TRUE AS  IN  THE  CASE*)
      (*THAT THE NEW NBR IS NEITHER A DUMMY POINT*)
      (*NOR THE FIRST NBR, AND THERE IS STILL  NO*)
      (*LINKED LIST OF NBR  CORRESPONDING  TO  IT*)
      (*                                         *)
      ADD := TRUE
   END   {END IF PLUS}
(*                                                *)
(*ELSE IF THE NEW NBR IS NEITHER A DUMMY POINT NOR*)
(*THE FIRST NBR, BUT THERE IS ALREADY  ONE  LINKED*)
(*LIST OF NBR'S CORRESPONDING TO IT               *)
(*                                                *)
ELSE
   BEGIN
      IF ( ADD = TRUE ) AND ( J >= 1 ) THEN
         BEGIN
            NEW (VTX_TEMP);
            VTX_TEMP^.NEXT := Z;
            VTX_TEMP^.DATA := NEW_VTX^.DATA;
            VTX_TEMP^.NEXT := VTX [K + J]^.NEXT^.NEXT;
            VTX [K + J]^.NEXT^.NEXT := VTX_TEMP
         END;
      ADD := FALSE
   END;   {END ELSE - NOT PLUS}
```

```
      (*                                  *)
      (*ASSIGN THE NEW NBR AS THE LAST NBR*)
      (*TO THE CENTROID BEEN PROCESSED    *)
      (*                                  *)
      NEW (NBR_TEMP);
      NBR_TEMP^.NEXT := Z;
      NBR_TEMP^.DATA := NEW_NBR^.DATA;

      NBR_LAST [K]^.NEXT := NBR_TEMP;
      NBR_LAST [K] := NBR_LAST [K]^.NEXT;
      (*                                  *)
      (*ASSIGN THE NEW VTX AS THE LAST VTX*)
      (*TO THE CENTROID BEEN PROCESSED    *)
      (*                                  *)
      NEW (VTX_TEMP);
      VTX_TEMP^.DATA := NEW_VTX^.DATA;
      VTX_TEMP^.NEXT := Z;

      VTX_LAST [K]^.NEXT := VTX_TEMP;
      VTX_LAST [K] := VTX_LAST [K]^.NEXT
   END
(*                                  *)
(*ELSE IF THE NEW NBR IS NOT A DUMMY*)
(*POINT, BUT IT  IS  THE  FIRST  NBR*)
(*                                  *)
ELSE
   BEGIN
      IF ADD THEN
         BEGIN
            (*                               *)
            (*INSERT THE NEW NBR AS THE FIRST*)
            (*NBR TO THE PREVIOUS NBR        *)
            (*                               *)
            NEW (NBR_TEMP);
            NBR_TEMP^.NEXT := Z;
            NBR_TEMP^.DATA := NEW_NBR^.DATA;

            NBR_TEMP^.NEXT := NBR [K + J]^.NEXT^.NEXT;
            NBR [K + J]^.NEXT^.NEXT := NBR_TEMP;

            (*                              *)
            (*ASSIGN THE PREVIOUS NBR AS THE*)
            (*LAST NBR TO THE FIRST NBR     *)
            (*                              *)
            NEW (NBR_TEMP);
            NBR_TEMP^.NEXT := Z;
            NBR_TEMP^.DATA := NBR_LAST [K]^.DATA;

            NBR_LAST [K + 1]^.NEXT := NBR_TEMP;
            NBR_LAST [K + 1] := NBR_LAST [K + 1]^.NEXT;

            IF J >= 1 THEN
               BEGIN
```

```
                     (*                               *)
                     (*INSERT THE NEW VTX AS THE FIRST*)
                     (*VTX TO THE PREVIOUS NBR        *)
                     (*                               *)
                     NEW (VTX_TEMP);
                     VTX_TEMP^.DATA := NEW_VTX^.DATA;

                     VTX_TEMP^.NEXT := VTX [K + J]^.NEXT^.NEXT;
                     VTX [K + J]^.NEXT^.NEXT := VTX_TEMP;

                     IF J > 1 THEN
                        BEGIN

                           (*                         *)
                           (*ASSIGN THE NEW VTX AS THE*)
                           (*LAST VTX TO THE FIRST NBR*)
                           (*                         *)
                           NEW (VTX_TEMP);
                           VTX_TEMP^.NEXT := Z;
                           VTX_TEMP^.DATA := NEW_VTX^.DATA;

                           VTX_LAST [K + 1]^.NEXT := VTX_TEMP;
                           VTX_LAST [K + 1] :=
                               VTX_LAST [K + 1]^.NEXT
                        END   {END IF J > 1}
                  END   {END IF J >= 1}
            END;  {END IF ADD}

         (*                                                  *)
         (*ASSIGN THE NEW VTX AS THE LAST VTX TO THE CENTROID*)
         (*                                                  *)
         NEW (VTX_TEMP);
         VTX_TEMP^.NEXT := Z;
         VTX_TEMP^.DATA := NEW_VTX^.DATA;

         VTX_LAST [K]^.NEXT := VTX_TEMP;
         VTX_LAST [K] := VTX_LAST [K]^.NEXT

         (*                                             *)
         (*LEAVE THE BOOLEAN VARIABLE 'ADD' UNCHANGED AS*)
         (*IN THE CASE THAT THE NEW NBR IS THE FIRST NBR*)
         (*                                             *)
      END

(*                                       *)
(*ELSE IF THE NEW NBR IS A DUMMY POINT...*)
(*                                       *)
ELSE
   BEGIN
      IF ADD THEN
         BEGIN
            IF J >= 1 THEN
               BEGIN
```

```
                        (*                                *)
                        (*INSERT THE NEW VTX AS THE FIRST*)
                        (*VTX TO THE PREVIOUS NBR         *)
                        (*                                *)
                        NEW (VTX_TEMP);
                        VTX_TEMP^.DATA := NEW_VTX^.DATA;

                        VTX_TEMP^.NEXT := VTX [K + J]^.NEXT^.NEXT;
                        VTX [K + J]^.NEXT^.NEXT := VTX_TEMP
                     END;   {END IF J >= 1}
                  (*                                                  *)
                  (*ASSIGN THE NEW VTX AS THE LAST VTX TO THE CENTROID*)
                  (*                                                  *)
                  NEW(VTX_TEMP);
                  VTX_TEMP^.NEXT := Z;
                  VTX_TEMP^.DATA := NEW_VTX^.DATA;

                  VTX_LAST [K]^.NEXT := VTX_TEMP;
                  VTX_LAST [K] := VTX_LAST [K]^.NEXT
               END   {END IF ADD}
            (*                                                        *)
            (*ELSE IF THE NEW NBR IS A DUMMY POINT;  'ADD'  IS  FALSE;*)
            (*i.e., THE PREVIOUS NEW NBR IS A DUMMY POINT OR THE FIRST*)
            (*NBR EITHER TO THE VERY CENTROID PROCESSED PREVIOUSLY  OR*)
            (*TO THE CENTROID PRESENTLY BEEN PROCESSED,  AND  THE  NEW*)
            (*VTX IS ONE OF THE VERTICES OF THE BOX...                *)
            (*                                                        *)
            ELSE
               IF ( NEW_VTX^.DATA.X <> VTX_LAST [K]^.DATA.X ) OR
                  ( NEW_VTX^.DATA.Y <> VTX_LAST [K]^.DATA.Y ) THEN
                  BEGIN
                     NEW (VTX_TEMP);
                     VTX_TEMP^.NEXT := Z;
                     VTX_TEMP^.DATA := NEW_VTX^.DATA;

                     VTX_LAST [K]^.NEXT := VTX_TEMP;
                     VTX_LAST [K] := VTX_LAST [K]^.NEXT
                  END;
            (*                                       *)
            (*ASSIGN 'ADD' TO BE FALSE AS IN THE CASE*)
            (*THAT THE NEW NBR IS A DUMMY POINT      *)
            (*                                       *)
            ADD := FALSE
         END   {END ELSE - NEW_NBR^.DATA.INDEX = 0}

(*                                            *)
(*STOP PROCESSING THE CENTROID PRESENTLY BEING*)
(*PROCESSED AS ALL IT'S NBR'S HAD BEEN FOUND  *)
(*                                            *)
UNTIL
   ( NEW_NBR^.DATA.X = NBR_FIRST.X ) AND
   ( NEW_NBR^.DATA.Y = NBR_FIRST.Y );
   K := K + 1; J := J - 1;
   IF K <= NUM_LOOP THEN
      BEGIN
         NBR_FIRST := NBR [K]^.NEXT^.NEXT^.DATA;
         NEW_NBR^.DATA := NBR_LAST [K]^.DATA
      END   {END IF K <= NUM_LOOP}

(*                                                                      *)
(*STOP THE LOOP AS ALL LINKED LISTS OF NBR'S AND VTX'S HAD BEEN CREATED*)
(*                                                                      *)
UNTIL
   K > NUM_LOOP;

FOR K := 1 TO NUM_LOOP DO
   BEGIN
      WRITELN (NBRFILE);
      WRITELN (NBRFILE, '  THE # ', K:3, ' LINKED LIST OF NBR IS:');
      NBR_LAST [K] := NBR [K]^.NEXT;
      WITH NBR_LAST [K]^.DATA DO
         BEGIN
            WRITELN (NBRFILE, INDEX, ' ', X, ' ', Y, ' ', DIA);
            X1 := X;
            Y1 := Y
         END;   {END WITH NBR_LAST [K]^.DATA}
      NBR_LAST [K] := NBR_LAST [K]^.NEXT;

      WHILE NBR_LAST [K] <> Z DO
         BEGIN
            WITH NBR_LAST [K]^.DATA DO
               BEGIN
                  WRITELN (NBRFILE, INDEX, ' ', X, ' ', Y, ' ', DIA);
                  WRITELN (DELAUNAY, X1, Y1, X, Y)
               END;   {END WITH NBR_LAST [K]^.DATA}
            NBR_LAST [K] := NBR_LAST [K]^.NEXT
         END   {END WHILE NBR_LAST [K] <> Z}
   END;   {END FOR K := 1 TO NUM_LOOP}

FOR K := 1 TO NUM_LOOP DO
   BEGIN
      WRITELN (VTXFILE);
      VTX_LAST [K] := VTX [K]^.NEXT^.NEXT;

      WHILE VTX_LAST [K] <> Z DO
         BEGIN
            WITH VTX_LAST [K]^.DATA DO
               WRITELN (VTXFILE, X, ' ', Y);
            VTX_LAST [K] := VTX_LAST [K]^.NEXT
         END   {END WHILE VTX_LAST [K] <> Z}
   END;   {END FOR K := 1 TO K DO}

(***************************************************************************)
(*                   THE VORONOI DIAGRAM IS COMPLETED HERE                *)
(***************************************************************************)
```

```
(***************************************************************************)
(*   FIND 1) THE 'TOP', 'BOTTOM', 'LEFT', AND 'RIGHT', SUCH THAT           *)
(*   THE FOUR LINES Y = TOP, Y = BOTTOM, X = LEFT, X = RIGHT TOGETHER      *)
(*   FORMS THE INNER BOX.                                                  *)
(***************************************************************************)
(*                                                                         *)
(*SORT THE ARRAY OF LINKED LIST OF NBR'S USING THE INDICES OF CENTER DISKS *)
(*AS THE KEY.  NAME THE SORTED ARRAY 'GNBR'.                               *)
(*                                                                         *)
FOR K := 1 TO NUM_LOOP DO
   BEGIN
      J := NBR [K]^.NEXT^.DATA.INDEX;
      GNBR [J] := NBR [K]^.NEXT;
      NBR_LAST [J] := GNBR [J];
      WITH NBR_LAST [J]^.DATA DO
         BEGIN
            X1 := X; Y1 := Y
         END;   {END WITH NBR_LAST [J]^.DATA}
      NBR_LAST [J] := NBR_LAST [J]^.NEXT;
      REPEAT
         WITH NBR_LAST [J]^.DATA DO
            BEGIN
               X2 := X; Y2 := Y
            END;   {END WITH NBR_LAST [J]^.DATA}
         NBR_LAST [J]^.DATA.ANGLE := THETA  (X1, Y1, X2, Y2);
         NBR_LAST [J] := NBR_LAST [J]^.NEXT
      UNTIL
         NBR_LAST [J] = Z
   END;
(*                                                 *)
(*FIND THE MINIMUM Y-COORDINATE ON THE TOP BOUNDARY*)
(*NAME IT 'TOP' TEMPERARILY                        *)
(*                                                 *)
K := CORNER2.INDEX;
NBR_LAST [K] := GNBR [K];
TOP := NBR_LAST [K]^.DATA.Y;
NBR_LAST [K] := NBR_LAST [K]^.NEXT;
REPEAT
   MIN := 180;
   REPEAT
      ALFA := 90 - NBR_LAST [K]^.DATA.ANGLE;
      IF ALFA > 0 THEN
         BEGIN
            IF ALFA < MIN THEN
               BEGIN
                  MIN :=  ALFA;
                  J := NBR_LAST [K]^.DATA.INDEX
               END
         END   {END IF ALFA > 0}
      ELSE IF ( ALFA < -180 ) AND ( MIN - ALFA > 360 ) THEN
         BEGIN
            MIN := 360 + ALFA;
            J := NBR_LAST [K]^.DATA.INDEX
         END;
      NBR_LAST [K] := NBR_LAST [K]^.NEXT
   UNTIL
      NBR_LAST [K] = Z;
   K := J;
   NBR_LAST [K] := GNBR [K];
   IF NBR_LAST [K]^.DATA.Y < TOP THEN
      TOP := NBR_LAST [K]^.DATA.Y;
   NBR_LAST [K] := NBR_LAST [K]^.NEXT
UNTIL
   K = CORNER3.INDEX;
(*                                                    *)
(*FIND THE MAXIMUM Y-COORDINATE ON THE BOTTOM BOUNDARY*)
(*NAME IT 'BOTTOM' TEMPERARILY                        *)
(*                                                    *)
K := CORNER4.INDEX;
NBR_LAST [K] := GNBR [K];
BOTTOM := NBR_LAST [K]^.DATA.Y;
NBR_LAST [K] := NBR_LAST [K]^.NEXT;
REPEAT
   MIN := 180;
   REPEAT
      ALFA := 270 - NBR_LAST [K]^.DATA.ANGLE;
      IF ( 0 < ALFA ) AND ( ALFA < MIN ) THEN
         BEGIN
            MIN := ALFA;
            J := NBR_LAST [K]^.DATA.INDEX
         END;
      NBR_LAST [K] := NBR_LAST [K]^.NEXT
   UNTIL
      NBR_LAST [K] = Z;
   K := J;
   NBR_LAST [K] := GNBR [K];
   IF NBR_LAST [K]^.DATA.Y > BOTTOM THEN
      BOTTOM := NBR_LAST [K]^.DATA.Y;
   NBR_LAST [K] := NBR_LAST [K]^.NEXT
UNTIL
   K = CORNER1.INDEX;
(*                                                  *)
(*FIND THE MAXIMUM X-COORDINATE ON THE LEFT BOUNDARY*)
(*NAME IT 'LEFT' TEMPERARILY                        *)
(*                                                  *)
K := CORNER1.INDEX;
NBR_LAST [K] := GNBR [K];
LEFT := NBR_LAST [K]^.DATA.X;
NBR_LAST [K] := NBR_LAST [K]^.NEXT;
REPEAT
   MIN := 180;
   REPEAT
      ALFA := 180 - NBR_LAST [K]^.DATA.ANGLE;
      IF ( 0 < ALFA ) AND ( ALFA < MIN ) THEN
         BEGIN
            MIN := ALFA;
            J := NBR_LAST [K]^.DATA.INDEX
         END;
      NBR_LAST [K] := NBR_LAST [K]^.NEXT
   UNTIL
      NBR_LAST [K] = Z;
   K := J;
   NBR_LAST [K] := GNBR [K];
   IF NBR_LAST [K]^.DATA.X > LEFT THEN
      LEFT := NBR_LAST [K]^.DATA.X;
   NBR_LAST [K] := NBR_LAST [K]^.NEXT
UNTIL
   K = CORNER2.INDEX;
(*                                                   *)
(*FIND THE MINIMUM X-COORDINATE ON THE RIGHT BOUNDARY*)
(*NAME IT 'RIGHT' TEMPERARILY                        *)
(*                                                   *)
K := CORNER3.INDEX;
NBR_LAST [K] := GNBR [K];
RIGHT:= NBR_LAST [K]^.DATA.X;
NBR_LAST [K] := NBR_LAST [K]^.NEXT;
REPEAT
   MIN := 180;
   REPEAT
      ALFA := - NBR_LAST [K]^.DATA.ANGLE;
      IF ( ALFA < -180 ) AND ( MIN - ALFA > 360 ) THEN
         BEGIN
            MIN := 360 + ALFA;
            J := NBR_LAST [K]^.DATA.INDEX
         END;
      NBR_LAST [K] := NBR_LAST [K]^.NEXT
   UNTIL
      NBR_LAST [K] = Z;
   K := J;
   NBR_LAST [K] := GNBR [K];
   IF NBR_LAST [K]^.DATA.X < RIGHT THEN
      RIGHT := NBR_LAST [K]^.DATA.X;
   NBR_LAST [K] := NBR_LAST [K]^.NEXT
UNTIL
   K = CORNER4.INDEX;

WRITELN (BOX);
WRITELN (BOX, '  MINIMUM DISTANCE BETWEEN THE TOP AND BOTTOM BOUNDARIES: ',
               TOP - BOTTOM);
WRITELN (BOX, '  MINIMUM DISTANCE BETWEEN THE LEFT AND RIGHT BOUNDARIES: ',
               RIGHT - LEFT);
IF TOP - BOTTOM < 4 * DMAX THEN
   BEGIN
      WRITELN (BOX);
      WRITELN (BOX, '  NOT EXECUTABLE ENSEMBLE!');
      WRITELN (BOX, '  NO INNER BOX CAN BE FIXED FOR THE GIVEN ENSEMBLE ');
      WRITELN (BOX, '  BECAUSE THE MINIMUM DISTANCE BETWEEN THE TOP AND');
      WRITELN (BOX, '  BOTTOM BOUNDARIES IS TOO SMALL.');
      WRITELN (BOX, '  BYE!');
      WRITELN (BOX);
      GOTO 100
   END;   {END IF TO - BOTTOM < 4 * DMAX}
IF RIGHT - LEFT < 4 * DMAX THEN
   BEGIN
      WRITELN (BOX);
      WRITELN (BOX, '  NOT EXECUTABLE ENSEMBLE!');
      WRITELN (BOX, '  NO INNER BOX CAN BE FIXED FOR THE GIVEN ENSEMBLE.');
      WRITELN (BOX, '  BECAUSE THE MINIMUM DISTANCE BETWEEN THE RIGHT AND');
      WRITELN (BOX, '  LEFT BOUNDARIES IS TOO SMALL.');
      WRITELN (BOX, '  BYE!');
      WRITELN (BOX);
      GOTO 100
   END;   {END IF RIGHT - LEFT < 4 * DMAX}

(*                                              *)
(*GENERATE A INNER BOX WITH 'HEIGHT' AND 'WIDTH'*)
(*                                              *)
Y1 := BOTTOM;
Y2 := TOP;
X1 := LEFT;
X2 := RIGHT;

YC := (Y1 + Y2) / 2;
XC := WIDE / 2;

IF (XC - X1 < 2 * DMAX) OR (X2 - XC < 2 * DMAX) THEN
   BEGIN
      WRITELN (BOX);
      WRITELN (BOX, '  NOT EXECUTABLE ENSEMBLE!');
      WRITELN (BOX, '  NO INNER BOX CAN BE FIXED FOR THE GIVEN ENSEMBLE.');
      WRITELN (BOX, '  BECAUSE THE MINIMUM DISTANCE BETWEEN THE CENTER AND');
      WRITELN (BOX, '  EITHER THE LEFT OR THE RIGHT BOUNDARY IS TOO SMALL.');
      WRITELN (BOX, '  BYE!');
      WRITELN (BOX);
      GOTO 100
   END;   {END IF}

BOTTOM := YC - HEIGHT / 2;
TOP := YC + HEIGHT / 2;
LEFT := XC - WIDTH / 2;
RIGHT := XC + WIDTH / 2;

STOP := FALSE;
IF (BOTTOM < Y1 + 2 * DMAX) OR (TOP > Y2 - 2 * DMAX) THEN
   BEGIN
      STOP := TRUE;
      WRITELN (BOX);
      WRITELN (BOX, '  THE HEIGHT OF THE INNER BOX SELECTED IS TOO ',
                    'LARGE.');
      WRITELN (BOX, '  CHOOSE A HEIGHT SMALLER THAN ',
                       Y2 - Y1 - 4 * DMAX, ' AND RUN AGAIN.')
   END;   {END IF}
```

```
IF (LEFT < X1 + 2 * DMAX) OR (RIGHT > X2 - 2 * DMAX) THEN
   BEGIN
      STOP := TRUE;
      WRITELN (BOX);
      WRITELN (BOX, '  THE WIDTH OF THE INNER BOX SELECTED IS TOO ',
              'LARGE.');
      IF (XC - X1 < X2 - XC) THEN
         WRITELN (BOX, '  CHOOSE A WIDTH SMALLER THEN ',
                  2 * (XC - X1 - 2 * DMAX), ' AND RUN AGAIN.')
      ELSE
         WRITELN (BOX, '  CHOOSE A WIDTH SMALLER THEN ',
                  2 * (X2 - XC - 2 * DMAX), ' AND RUN AGAIN.')
   END;   {END IF}
IF DEFINE_PF_BOX THEN
   BEGIN
      IF PF_L < 0 THEN
         BEGIN
            STOP := TRUE;
            WRITELN (BOX);
            WRITELN (BOX, 'PF_L IS TOO SMALL.');
            WRITELN (BOX, 'CHOOSE A PF_L NO LESS THAN 0 AND RUN AGAIN.')
         END;   {END IF}
      IF PF_R > WIDE THEN
         BEGIN
            STOP := TRUE;
            WRITELN (BOX);
            WRITELN (BOX, 'PF_R IS TOO LARGE.');
            WRITELN (BOX, 'CHOOSE A PF_R NO GREATER THAN ', WIDE,
                          ' AND RUN AGAIN.')
         END;   {END IF}
      IF PF_B < 0 THEN
         BEGIN
            STOP := TRUE;
            WRITELN (BOX);
            WRITELN (BOX, 'PF_B IS TOO SMALL.');
            WRITELN (BOX, 'CHOOSE A PF_B NO LESS THAN 0 AND RUN AGAIN.')
         END;   {END IF}
      IF PF_T > Y2 - 2 * DMAX THEN
         BEGIN
            STOP := TRUE;
            WRITELN (BOX);
            WRITELN (BOX, 'PF_T IS TOO LARGE.');
            WRITELN (BOX, 'CHOOSE A PF_T NO GREATER THAN ', Y2 - 2 * DMAX,
                          ' AND RUN AGAIN.')
         END   {END IF}
   END;   {END IF DEFINE_PF_BOX}
IF STOP THEN
   GOTO 100
ELSE
   BEGIN
      WRITELN (BOX);
      WRITELN (BOX, '  $THE EXTREMA OF THE INNER BOX IS:');
      WRITELN (BOX);
      WRITELN (BOX, '  XMIN = ', LEFT, ' XMAX = ', RIGHT);
      WRITELN (BOX, '  YMIN = ', BOTTOM, ' YMAX = ', TOP);
      IF DEFINE_PF_BOX THEN
         BEGIN
            WRITELN (BOX);
            WRITELN(BOX,'  $THE EXTREMA OF THE BOX FOR CALCULATIN P.F. IS:');
            WRITELN (BOX);
            WRITELN (BOX, '  PF_L = ', PF_L, ' PF_R = ', PF_R);
            WRITELN (BOX, '  PF_B = ', PF_B, ' PF_T = ', PF_T)
         END   {END IF DEFINE_PF_BOX}
   END;   {END ELSE - NOT STOP}

(****************************************************************************)
(*         FIND THE INNER DISKS CONSTRAINED BY THE INNER BOX                *)
(****************************************************************************)

MAKE_COPY (SORT, SORT_COPY);
FIND_INNER (SORT_COPY, LEFT, RIGHT, BOTTOM, TOP, INNER);

(****************************************************************************)
(*  1) FIND ARRAY OF LINKED LIST OF GEOMETRIC NEIGHBOURS FOR INNER DISKS,   *)
(*     NAME THE ARRAY 'INNERG'                                              *)
(*  2) FIND THE NUMBER DISTRIBUTION AND EXPECTED  NUMBER  OF  GEOMETRIC     *)
(*     NEIGHBOUR FOR INNER DISKS                                            *)
(****************************************************************************)
LAST := INNER;
K := 1;

REPEAT
   J := LAST^.DATA.INDEX;
   INNERG [K] := GNBR [J];
   NBR_LAST [K] := INNERG [K]^.NEXT;
   NUM_GN [K] := 0;

   REPEAT
      NBR_LAST [K] := NBR_LAST [K]^.NEXT;
      NUM_GN [K] := NUM_GN [K] + 1
   UNTIL
      NBR_LAST [K] = Z;
   LAST := LAST^.NEXT;
   K := K + 1
UNTIL
   LAST = Z;
NUM_IN := K - 1;

WRITELN (BOX);
WRITELN (BOX, '  $NUMBER OF INNER DISKS FOUND EXISTING WITHIN OR ON THE ',
              'INNER BOX: ', NUM_IN);
NUM_DST (NUM_GN, NUM_IN, NMIN, NMAX, DST);
NUM_DST_GN := DST;
SUM := 0;
FOR K := NMIN TO NMAX DO SUM := SUM + NUM_DST_GN [K] * K;
AVG_GN := SUM / NUM_IN;
```

```
(***************************************************************************)
(*1) PICK OUT STRUCTRUAL NEIGHBOURS FROM GEOMETRICAL NEIGHBOURS, FORM ARRAY*)
(*   'INNERS' OF LINKED LISTS OF STRUCTRUAL NEIGHBOURS FOR EACH INNER DISK *)
(*2) FIND THE NUMBER  DISTRIBUTION  AND  EXPECTED  NUMBER  OF  STRUCTUUAL  *)
(*   NEIGHBOUR FOR INNER DISKS                                             *)
(*3) FIND THE ANGULAR  DISTRIBUTION  AND  EXPECTED  ANGLE  OF  STRUCTURAL  *)
(*   NEIGHBOUR FOR INNER DISKS                                             *)
(***************************************************************************)
FOR K := 1 TO NUM_IN DO
   BEGIN
      NBR_LAST [K] := INNERG [K];
      WITH NBR_LAST [K]^.DATA DO
         BEGIN
            X1 := X;
            Y1 := Y;
            DIA1 := DIA
         END;   {END WITH NBR_LAST [K]^.DATA}

      NEW (INNERS [K]);
      INNERS [K]^.NEXT := Z;
      INNERS [K]^.DATA := NBR_LAST [K]^.DATA;
      SNBR_LAST [K] := INNERS [K];

      NBR_LAST [K] := NBR_LAST [K]^.NEXT;
      NUM_SN [K] := 0;
      REPEAT
         WITH NBR_LAST [K]^.DATA DO
            BEGIN
               X2 := X;
               Y2 := Y;
               DIA2 := DIA
            END;   {END WITH NBR_LAST [K]^.DATA}

         IF SQRT ( SQR ( X2 - X1 ) + SQR ( Y2 - Y1 ) ) <
                 ( 1 + TOLERANCE ) * ( DIA1 / 2 + DIA2 / 2 ) THEN
            BEGIN
               NEW ( NBR_TEMP);
               NBR_TEMP^.NEXT := Z;
               NBR_TEMP^.DATA := NBR_LAST [K]^.DATA;

               SNBR_LAST [K]^.NEXT := NBR_TEMP;
               SNBR_LAST [K] := SNBR_LAST [K]^.NEXT;
               NUM_SN [K] := NUM_SN [K] + 1
            END;
         NBR_LAST [K] := NBR_LAST [K]^.NEXT
      UNTIL
         NBR_LAST [K] = Z
   END;   {END FOR K := 1 TO NUM_IN}
FOR K := 1 TO NUM_IN DO
   BEGIN
      WRITELN (SNBRFILE);
      WRITELN (SNBRFILE, '  THE # ', K:5, ' LINKED LIST OF STRUCTURAL',
                         ' NEIGHBOUR FOR INNER DISKS IS:');
      SNBR_LAST [K] := INNERS [K];
      WITH SNBR_LAST [K]^.DATA DO
         WRITELN (SNBRFILE, INDEX, ' ', X, ' ', Y, ' ', DIA);
      SNBR_LAST [K] := SNBR_LAST [K]^.NEXT;
      WHILE SNBR_LAST [K] <> Z DO
         BEGIN
            WITH SNBR_LAST [K]^.DATA DO
            WRITELN (SNBRFILE, INDEX, ' ', X, ' ', Y, ' ', DIA, ' ', ANGLE);
            SNBR_LAST [K] := SNBR_LAST [K]^.NEXT
         END   {END WHILE SNBR_LAST [K] <> Z}
   END;   {END FOR K := 1 TO NUM_IN}
SUM := 0;
NUM_DST (NUM_SN, NUM_IN, SMIN, SMAX, DST);
NUM_DST_SN := DST;
FOR K := SMIN TO SMAX DO
   SUM := SUM + NUM_DST_SN [K] * K;
AVG_SN := SUM / NUM_IN;
(***************************************************************************)
(*    1.  COMPUTE THE MEAN NEAREST NEIGHBOUR RADIUS                        *)
(*        AND THE MEDIAN NEAREST NEIGHBOUR RADIUS                          *)
(*        IN CASE WHETHER THE GIVEN ENSEMBLE IS A RANDOM CLOSE PACKING     *)
(*        OR NOT IS UNKNOWN.                                               *)
(*                                                                         *)
(*    2.  FIND THE CUMULATIVE PROBABILITY OF THE DISTRIBUTION OF           *)
(*        NEAREST NEIGHBOUR RADIUS IF THE GIVEN ENSEMBLE ARE IN SAME SIZE. *)
(***************************************************************************)
IF NOT KNOWN_TO_BE_RCP THEN
   BEGIN
      FIND_NNR (INNERS, GNBR, NUM_IN, NNR);
      SUM := 0;
      FOR K := 1 TO NUM_IN DO
         SUM := SUM + NNR [K];
      MEAN_NNR := SUM / NUM_IN;
      WRITELN (BOX);
      WRITELN (BOX, '  $MEAN NEAREST NEIGHBOUR RADIUS IS: ', MEAN_NNR);
      ARRAY_SORT (NNR, NUM_IN);
      IF NUM_IN - NUM_IN DIV 2 * 2 = 0 THEN
         MEDIAN_NNR := NNR[NUM_IN DIV 2]
      ELSE
         MEDIAN_NNR := NNR[NUM_IN DIV 2 + 1];
      WRITELN (BOX);
      WRITELN (BOX, '  $MEDIAN NEAREST NEIGHBOUR RADIUS IS: ', MEDIAN_NNR);

      IF EQ_DISKS THEN
         IF MEDIAN_NNR > (1 + TOLERANCE) * DMAX THEN
            BEGIN
               WRITELN (BOX, '  WHICH IS GREATER THEN (1 + TOLERENCE) * ',
                             'DMAX.');
               WRITELN (BOX, '  IT IS THUS SHOWN THAT THE GIVEN ENSEMBLE IS',
                       ' NOT A RANDOM CLOSE PACKING!');
               WRITELN (BOX, '  BYE!');
               GOTO 100
            END   {END IF MEDIAN_NNR > (1 + TOLERANCE) * DMAX}
         ELSE
            BEGIN
               CP_NNR[0] := 0;
               DIVISION := (MEDIAN_NNR - DMAX) / 5;
               MIN := DMAX + DIVISION;
               K := 1;
               J := 0;
               I := 0;
               REPEAT
                  I := I + 1;
                  WHILE (NNR[K] <= MIN) AND (K <= NUM_IN) DO
                     K := K + 1;
                  CP_NNR[I] := CP_NNR[I - 1] + (K - 1 - J) / NUM_IN;
                  J := K - 1;
                  MIN := MIN + DIVISION
               UNTIL
                  (CP_NNR[I] > 0.99999) OR (I = 100);
               NUM_RAD_DIV := I
            END   {END ELSE}
   END;   {END IF NOT KNOWN_TO_BE_RCP}
(*                                                            *)
(*SORT EACH ELEMENT IN THE ARRAY OF LINKED LIST 'INNERS', SUCH*)
(*THAT THE STRUCTURAL NEIGHBOURS IN EACH ELEMENT ARE LINKED TO*)
(*THE CENTER DISK IN INCREASING ANGLE SEQUENCE                *)
(*                                                            *)
FOR K := 1 TO NUM_IN DO
   BEGIN
      NBR_LAST [K] := INNERS [K]^.NEXT;
      ALFA := NBR_LAST [K]^.DATA.ANGLE;
      STOP := FALSE;
      WHILE ( NBR_LAST [K]^.NEXT <> Z ) AND ( NOT STOP ) DO
         IF ALFA < NBR_LAST [K]^.NEXT^.DATA.ANGLE THEN
            BEGIN
               STOP := TRUE;
               NBR_TEMP := NBR_LAST [K]^.NEXT;
               NBR_LAST [K]^.NEXT := Z;
               NBR_LAST [K] := NBR_TEMP;
               WHILE NBR_LAST [K]^.NEXT <> Z DO
                  NBR_LAST [K] := NBR_LAST [K]^.NEXT;
               NBR_LAST [K]^.NEXT := INNERS [K]^.NEXT;
               INNERS [K]^.NEXT := NBR_TEMP
            END   {END IF ALFA < NBR_LAST [K]^.NEXT^.DATA.ANGLE}
         ELSE
            NBR_LAST [K] := NBR_LAST [K]^.NEXT
   END;   {END FOR K := 1 TO NUM_IN}
(*                                                                          *)
(*1) FORM ARRAY 'GROUP_SN [K]' WHICH GROUP INNER DISKS WITH THE SAME NUMBER*)
(*   'K', OF STRUCTURAL NEIGHBOUR TOGETHER.                                 *)
(*   NOTE: DISKS WITH 0 STRUCTURAL NEIGHBOURS ARE EXCLUDED.                 *)
(*2) GET 'GROUP_SUM [K]', THE NUMBER OF DISK WITH  K  STRUCTURAL  NEIGHBOUR*)
(*   THAT ARE GROUPED IN GROUP_SN [K].                                      *)
FOR K := 1 TO 6 DO
   GROUP_SUM [K] := 0;
```

```
FOR K := 1 TO NUM_IN DO
   CASE NUM_SN [K] OF
      1: BEGIN
            GROUP_SUM [1] := GROUP_SUM [1] + 1;
            GROUP_SN [1, GROUP_SUM [1]] := INNERS [K]
         END;   {END CASE NUM_SN [K] OF 1}
      2: BEGIN
            GROUP_SUM [2] := GROUP_SUM [2] + 1;
            GROUP_SN [2, GROUP_SUM [2]] := INNERS [K]
         END;   {END CASE NUM_SN [K] OF 2}
      3: BEGIN
            GROUP_SUM [3] := GROUP_SUM [3] + 1;
            GROUP_SN [3, GROUP_SUM [3]] := INNERS [K]
         END;   {END CASE NUM_SN [K] OF 3}
      4: BEGIN
            GROUP_SUM [4] := GROUP_SUM [4] + 1;
            GROUP_SN [4, GROUP_SUM [4]] := INNERS [K]
         END;   {END CASE NUM_SN [K] OF 4}
      5: BEGIN
            GROUP_SUM [5] := GROUP_SUM [5] + 1;
            GROUP_SN [5, GROUP_SUM [5]] := INNERS [K]
         END;   {END CASE NUM_SN [K] OF 5}
      6: BEGIN
            GROUP_SUM [6] := GROUP_SUM [6] + 1;
            GROUP_SN [6, GROUP_SUM [6]] := INNERS [K]
         END   {END CASE NUM_SN [K] OF 6}
   END;   {END CASE}
(*                                                                       *)
(*FOR EACH GROUP OF DISKS WITH K STRUCTURAL NEIGHBOURS, FIND THE EXPECTED*)
(*ANGLE FOR THE Jth STRUCTURAL NEIGHBOUR.  WHERE J IS FROM 1 TO K.       *)
(*                                                                       *)
ANG_DST (GROUP_SN, GROUP_SUM, SMIN, SMAX, NUM_ANG_DIV, DST_SN);
ANG_DST_SN := DST_SN;
FOR K := SMIN TO SMAX DO
   BEGIN
      FOR J := 1 TO GROUP_SUM [K] DO
         NBR_LAST [J] := GROUP_SN [K, J]^.NEXT;
      FOR J := 1 TO K DO
         BEGIN
            SUM := 0;
            FOR I := 1 TO GROUP_SUM [K] DO
               BEGIN
                  SUM := SUM + NBR_LAST [I]^.DATA.ANGLE;
                  NBR_LAST [I] := NBR_LAST [I]^.NEXT
               END;   {END FOR I := 1 TO GROUP_SUM [K]}
            EXPECT_ANGLE [K, J] := SUM / GROUP_SUM [K]
         END   {END FOR J := 1 TO K}
   END;   {END FOR K := SMIN TO SMAX}

FOR K := SMIN TO SMAX DO
   BEGIN
      FOR J := 1 TO GROUP_SUM [K] DO
         NBR_LAST [J] := GROUP_SN [K, J]^.NEXT;
      FOR J := 1 TO K DO
         BEGIN
            SUM := 0;
            SUMS := 0;
            FOR I := 1 TO GROUP_SUM [K] DO
               BEGIN
                  SUM := SUM + NBR_LAST [I]^.DATA.ANGLE;
                  SUMS := SUMS + SQR ( NBR_LAST [I]^.DATA.ANGLE );
                  NBR_LAST [I] := NBR_LAST [I]^.NEXT
               END;   {END FOR I := 1 TO GROUP_SUM [K]}
            IF GROUP_SUM [K] > 1 THEN
               STD_DVA [K, J] := SQRT (ABS
               ( (SUMS - SQR (SUM) / GROUP_SUM [K]) / (GROUP_SUM [K] - 1) ) )
         END   {END FOR J := 1 TO K}
   END;   {END FOR K := SMIN TO SMAX}

IF SMIN < NMIN THEN NMIN := SMIN;
IF SMAX > NMAX THEN NMAX := SMAX;

(****************************************************************************)
(*                  MAKE OUTPUT FILE TABLE.DAT                              *)
(****************************************************************************)
WRITELN (TABLE);
WRITELN (TABLE, '**********************************************************',
                '***********************');
WRITELN (TABLE, '*                                  PARAMETERS              ',
                '                     *');
WRITELN (TABLE, '**********************************************************',
                '***********************');
WRITELN (TABLE);
WRITELN (TABLE, '  NUMBER OF DISK         : ', NUM_DISK);
WRITELN (TABLE, '  TOLERANCE              : ', TOLERANCE);
WRITELN (TABLE, '  HEIGHT OF THE INNER BOX: ', HEIGHT);
WRITELN (TABLE, '  WIDTH OF THE INNER BOX : ', WIDTH );
WRITELN (TABLE, '  AREA OF THE INNER BOX  : ', HEIGHT * WIDTH );
WRITELN (TABLE);
WRITELN (TABLE, '**********************************************************',
                '**********************');
WRITELN (TABLE, '*                      INFORMATIONS ON INNER DISKS:        ',
                '                    *');
WRITELN (TABLE, '**********************************************************',
                '**********************');
WRITELN (TABLE);
WRITELN (TABLE, '  INDEX  # OF G.N.  GEOMETRIC NBRS  # OF S.N.',
                '  STRUCTRUAL NBRS     THETA ');
WRITELN (TABLE);
LAST := INNER;
FOR K := 1 TO NUM_IN DO
   BEGIN
      WRITELN (TABLE, '----------------------------------------------------',
                      '----------------------------');
      NBR_LAST [K] := INNERG [K]^.NEXT;
      SNBR_LAST [K] := INNERS [K]^.NEXT;
      WRITELN (TABLE, ' ', LAST^.DATA.INDEX:5,
                      '       ', NUM_GN [K]:1,
                      '           ', NBR_LAST [K]^.DATA.INDEX:5,
                      '          ', NUM_SN [K]:1,
                      '            ', SNBR_LAST [K]^.DATA.INDEX:5,
                      '     ', SNBR_LAST [K]^.DATA.ANGLE);
      NBR_LAST [K] := NBR_LAST [K]^.NEXT;
      SNBR_LAST [K] := SNBR_LAST [K]^.NEXT;
      WHILE SNBR_LAST [K] <> Z DO
         BEGIN
            WRITELN (TABLE, ' ':25,
                    NBR_LAST [K]^.DATA.INDEX:5, ' ':23,
                    SNBR_LAST [K]^.DATA.INDEX:5, ' ':5,
                    SNBR_LAST [K]^.DATA.ANGLE);
            NBR_LAST [K] := NBR_LAST [K]^.NEXT;
            SNBR_LAST [K] := SNBR_LAST [K]^.NEXT
         END;   {END WHILE SNBR_LAST [K] <> Z}
      WHILE NBR_LAST [K] <> Z DO
         BEGIN
            WRITELN (TABLE, ' ':20,
                     NBR_LAST [K]^.DATA.INDEX);
            NBR_LAST [K] := NBR_LAST [K]^.NEXT
         END;   {END WHILE NBR_LAST [K] <> Z}
      LAST := LAST^.NEXT
   END;   {FOR K := 1 TO NUM_IN}
WRITELN (TABLE);
WRITELN (TABLE, '----------------------------------------------------------',
                '----------------------');
WRITELN (TABLE);
WRITELN (TABLE, '   MEAN  ', AVG_GN, '               ', AVG_SN);

WRITELN (TABLE);
WRITELN (TABLE, '**********************************************************',
                '**********************');
WRITELN (TABLE, '*          CUMULATIVE PROBALITY OF THE RADIAL DISTRIBUTION',
                '                     *');
WRITELN (TABLE, '*          OF THE NEAREST NEIGHBOUR RADIUS                ',
                '                     *');
WRITELN (TABLE, '**********************************************************',
                '**********************');
WRITELN (TABLE);
WRITELN (TABLE, '      RADIAL RANGE                CUMULATIVE PROBABILITY');
WRITELN (TABLE);
WRITELN (TABLE, '----------------------------------------------------------',
                '----------------------');
MIN := DMAX;
FOR K := 1 TO NUM_RAD_DIV DO
   BEGIN
      WRITELN (TABLE, '  ', MIN, ' - ', MIN + DIVISION,
                      '          ', CP_NNR[K]);
      MIN := MIN + DIVISION
   END;
WRITELN (TABLE);
WRITELN (TABLE, '**********************************************************',
                '**********************');
WRITELN (TABLE, '*               DISTRIBUTION OF THE NUMBER OF GEOMETRIC   ',
                '                     *');
WRITELN (TABLE, '*               AND STRUCTURAL NEIGHBOUR FOR INNER DISKS. ',
                '                     *');
WRITELN (TABLE, '**********************************************************',
                '**********************');
WRITELN (TABLE);
WRITELN (TABLE, '  NUMBER', '     ', ' GEOMETRIC NEIGHBOUR', '     ',
                ' STRUCTURAL NEIGHBOUR');
WRITELN (TABLE);
WRITELN (TABLE, '----------------------------------------------------------',
                '----------------------');
FOR K := NMIN TO NMAX DO
   WRITELN (TABLE, K:6, '        ', NUM_DST_GN [K],
                        '                ', NUM_DST_SN [K]);
WRITELN (TABLE, '----------------------------------------------------------',
                '----------------------');
WRITELN (TABLE, '   TATAL', '      ', NUM_IN:10,
                '                ', NUM_IN:10);
WRITELN (TABLE);
WRITELN (TABLE, '**********************************************************',
                '**********************');
WRITELN (TABLE, '* THE MEAN VALUE OF ANGLE ASSOCIATED WITH EACH SEQUENCIAL ',
                'STRUCTURAL NEIGHBOUR *');
WRITELN (TABLE, '**********************************************************',
                '**********************');
WRITELN (TABLE);
WRITELN (TABLE, ' NUMBER OF                     STRUCTURAL NEIGHBOUR IN',
                ' SEQUENCE');
WRITELN (TABLE, ' STURCTURAL  ----------------------------------------------',
                '----------------------');
WRITELN (TABLE, ' NEIGHBOUR          1          2          3     ',
                '      4          5          6');
WRITELN (TABLE, '----------------------------------------------------------',
                '----------------------');
FOR K := SMIN TO SMAX DO
   BEGIN
      IF K = 1 THEN
         BEGIN
            WRITE (TABLE, '     ', K:1);
            WRITELN (TABLE, '         ', EXPECT_ANGLE [K, 1]:10)
         END    {END IF K = 1}
      ELSE IF K > 1 THEN
         BEGIN
            WRITE (TABLE, '     ', K:1);
            WRITE (TABLE, '        ', EXPECT_ANGLE [K, 1]:10);
            FOR J := 2 TO K - 1 DO
               WRITE (TABLE, ' ', EXPECT_ANGLE [K, J]:10);
            WRITELN (TABLE, ' ', EXPECT_ANGLE [K, K]:10)
         END    {ELSE IF K > 1}
   END;    {END FOR K := SMIN TO SMAX}
```

```
WRITELN (TABLE);
WRITELN (TABLE, '**********************************************************',
                '**********************');
WRITELN (TABLE, '*           THE STANDARD DEVIATION OF THE ANGLE ASSOCIATED',
                '                     *');
WRITELN (TABLE, '*           WITH EACH SEQUENCIAL STRUCTURAL NEIGHBOUR      ',
                '                     *');
WRITELN (TABLE, '**********************************************************',
                '**********************');
WRITELN (TABLE);
WRITELN (TABLE, ' NUMBER OF                     STRUCTURAL NEIGHBOUR IN',
                ' SEQUENCE');
WRITELN (TABLE, ' STURCTURAL   --------------------------------------------',
                '----------------------');
WRITELN (TABLE, ' NEIGHBOUR         1          2          3     ',
                '     4          5          6');
WRITELN (TABLE, '----------------------------------------------------------',
                '----------------------');
FOR K := SMIN TO SMAX DO
   IF GROUP_SUM [K] > 1 THEN
      BEGIN
         WRITE (TABLE, '     ', K:1);
         IF K = 1 THEN
            WRITELN (TABLE, '        ', STD_DVA [K, 1]:10)
         ELSE IF K > 1 THEN
            BEGIN
               WRITE (TABLE, '        ', STD_DVA [K, 1]:10);
               FOR J := 2 TO K - 1 DO
                  WRITE (TABLE, ' ', STD_DVA [K, J]:10);
               WRITELN (TABLE, ' ', STD_DVA [K, K]:10)
            END   {END ELSE IF K > 1}
      END;   {END IF GROUP_SUM [K] > 1}

WRITELN (TABLE);
WRITELN (TABLE, '**********************************************************',
                '**********************');
WRITELN (TABLE, '*            ANGULAR DISTRUBUTION OF STRUCTURAL NEIGHBOURS',
                '                     *');
WRITELN (TABLE, '**********************************************************',
                '**********************');
GAMMA := 360 / NUM_ANG_DIV;
FOR K := SMIN TO SMAX DO
   FOR J := 1 TO K DO
      BEGIN
         WRITELN (TABLE);
         WRITELN (TABLE, ' THE ANGULAR DISTRIBUTION OF # ', J:1,
                         ' STRUCTURAL NEIGHBOUR');
         WRITELN (TABLE, ' IN DISKS WITH ', K:1,
                         ' STRUCTURAL NEIGHBOURS');
         WRITELN (TABLE, '----------------------------------------------',
                         '----------------------------------');
         WRITELN (TABLE, '     ANGLE RANGE', '              ',
                         ' # OF STRUCTURAL NEIGHBOUR');
         WRITELN (TABLE, '----------------------------------------------',
                         '----------------------------------');
         ALFA := 0;
         BETA := GAMMA;
         FOR I := 0 TO NUM_ANG_DIV - 1 DO
            BEGIN
               WRITELN (TABLE, ALFA, ' - ', BETA, '          ',
                               ANG_DST_SN [K, J, I]);
               ALFA := BETA;
               BETA := ALFA + GAMMA
            END;   {END FOR I := 0 TO NUM_ANG_DIV - 1}
         WRITELN (TABLE, '----------------------------------------------',
                         '----------------------------------');
         WRITELN (TABLE, '   TOTAL', ' ':29, NUM_DST_SN [K]);
         WRITELN (TABLE)
      END;   {END FOR J := 1 TO K}
(***************************************************************************)
(*               FIND THE PACKING FRACTION                                 *)
(***************************************************************************)
WRITELN (TABLE);
WRITELN (TABLE, '**********************************************************',
                '**********************');
WRITELN (TABLE, '*                                 PACKING FRACTION        ',
                '                     *');
WRITELN (TABLE, '**********************************************************',
                '**********************');
WRITELN (TABLE);
WRITELN (TABLE, '   PF_L        PF_R        PF_B        PF_T     INNER DISK',
                ' AREA PACKING FRACTION');
WRITELN (TABLE);
WRITELN (TABLE, '----------------------------------------------------------',
                '----------------------');
IF DEFINE_PF_BOX THEN
   BEGIN

      (*                                 *)
      (*DISPOSE THE LINKED LIST SORT_COPY*)
      (*                                 *)
      LAST := INNER;
      WHILE LAST <> Z DO
         BEGIN
            NBR_TEMP := LAST;
            LAST := LAST^.NEXT;
            DISPOSE (NBR_TEMP)
         END;   {END WHILE LAST <> Z}

      LEFT := PF_L;
      RIGHT := PF_R;
      BOTTOM := PF_B;
      TOP := PF_T;
      MAKE_COPY (SORT, SORT_COPY);
      FIND_INNER (SORT_COPY, LEFT, RIGHT, BOTTOM, TOP, INNER);
      FIND_PF (INNER, LEFT, RIGHT, BOTTOM, TOP, ETA, SUM);
      WRITELN (TABLE);
      WRITELN (TABLE, '  PACKING FRACTION WITHIN USER DEFINED PF_BOX:');
      WRITELN (TABLE);
      WRITELN (TABLE, LEFT, RIGHT, BOTTOM, TOP, ' ', SUM, '   ', ETA)
   END   {END IF DEFINE_PF_BOX}
ELSE
   BEGIN
      WRITELN (TABLE);
      WRITELN (TABLE, '  PACKING FRACITON WITHIN THE INNER BOX:');
      WRITELN (TABLE);
      FIND_PF (INNER, LEFT, RIGHT, BOTTOM, TOP, ETA, SUM);
      WRITELN (TABLE, LEFT, RIGHT, BOTTOM, TOP, ' ', SUM, '   ', ETA)
   END;   {END ELSE}

IF EQ_DISKS AND FIND_WALL_EFFECT THEN
   BEGIN
      WRITELN (TABLE);
      WRITELN (TABLE, '  PACKING FRACTION VARIATION BY WALL EFFECT:');
      WRITELN (TABLE);
      LEFT := 0;
      RIGHT := DMAX;

      (*                                 *)
      (*DISPOSE THE LINKED LIST SORT_COPY*)
      (*                                 *)
      REPEAT
         LAST := INNER;
         WHILE LAST <> Z DO
            BEGIN
               NBR_TEMP := LAST;
               LAST := LAST^.NEXT;
               DISPOSE (NBR_TEMP)
            END;   {END WHILE LAST <> Z}

         MAKE_COPY (SORT, SORT_COPY);
         FIND_INNER (SORT_COPY, LEFT, RIGHT, BOTTOM, TOP, INNER);
         FIND_PF (INNER, LEFT, RIGHT, BOTTOM, TOP, ETA, SUM);
         WRITELN (TABLE, LEFT, RIGHT, BOTTOM, TOP, ' ', SUM, '   ', ETA);
         RIGHT := RIGHT + 0.001 * WIDE
      UNTIL
         RIGHT > WIDE;

      LAST := INNER;
      WHILE LAST <> Z DO
         BEGIN
            NBR_TEMP := LAST;
            LAST := LAST^.NEXT;
            DISPOSE (NBR_TEMP)
         END;   {END WHILE LAST <> Z}

      RIGHT := WIDE;
      MAKE_COPY (SORT, SORT_COPY);
      FIND_INNER (SORT_COPY, LEFT, RIGHT, BOTTOM, TOP, INNER);
```

```
         FIND_PF (INNER, LEFT, RIGHT, BOTTOM, TOP, ETA, SUM);
         WRITELN (TABLE, LEFT, RIGHT, BOTTOM, TOP, ' ', SUM, '   ', ETA)
      END;   {END IF EQ_DISKS}
   100: CLOSE (DISKIN);
   CLOSE (NBRFILE);
   CLOSE (VTXFILE);
   CLOSE (BOX);
   CLOSE (DELAUNAY);
   CLOSE (SNBRFILE);
   CLOSE (TABLE)
END.
```

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