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NUMERICAL SOLUTION OF DISCRETE NONDEGENERATE N-BODY PROBLEMS WITH AN APPLICATION TO FREE SURFACE FLUID FLOW

by

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1. INTRODUCTION

The resulting dynamical behavior of n bodies under the influence of a given set of interactive forces has been of interest in pure and applied science for many years (see, e.g., references [1-3,5,7,8,10,13,15] and the additional references contained therein). Typical important n-body problems occur in the study of Brownian motion under the usual assumptions that n is relatively large and that collisions occur in accordance with an assumed probabilistic distribution, and in the study of the solar system under the usual assumptions that n is relatively small and that capture, but not collision, is admissable.

In this paper we will explore and apply a new numerical method for general, plane, nondegenerate n-body problems. The formulation will be based on a discrete approach to mechanics [4,5] in which the dynamical equations are difference equations and the solutions of the equations are discrete functions, that is, functions defined only on finite point sets. The effects of viscosity and collision will be included in the formulation and the extension of the method to three dimensions will offer no mathematical difficulty, but will require greater storage capacity for the actual computations.

*Supported by the National Science Foundation under Grant No. GJ-578

2. DISCRETE DYNAMICAL EQUATIONS

For $\Delta t > 0$, let $t_k = k\Delta t$, $k = 0,1,\ldots$. Assume that a particle P is in motion on an x-axis and is located at x_k at time t_k. Then, for a given initial velocity v_0, it has been found convenient [4] to define the particle's velocity $v_k = v(t_k)$, $k = 1,2,\ldots$, implicitly by

(2.1) $$\frac{v_k + v_{k-1}}{2} = \frac{x_k - x_{k-1}}{\Delta t}, \quad k = 1,2,\ldots,$$

and the particle's acceleration $a_k = a(t_k)$, $k = 1,2,\ldots$ explicitly by

(2.2) $$a_k = \frac{v_k - v_{k-1}}{\Delta t}, \quad k = 1,2,\ldots$$

It follows readily [4] from (2.1) and (2.2) that

(2.3) $$v_1 = \frac{2}{\Delta t}(x_1 - x_0) - v_0$$

(2.4) $$v_k = \frac{2}{\Delta t}\left\{x_k + (-1)^k x_0 + 2\sum_{j=1}^{k-1}\left[(-1)^j(x_{k-j})\right]\right\} + (-1)^k v_0; \; k \geq 2$$

(2.5) $$a_1 = \frac{2}{(\Delta t)^2}[x_1 - x_0 - v_0\Delta t]$$

(2.6) $$a_2 = \frac{2}{(\Delta t)^2}[x_2 - 3x_1 + 2x_0 + v_0\Delta t]$$

(2.7) $$a_k = \frac{2}{(\Delta t)^2}\left\{x_k - 3x_{k-1} + 2(-1)^k x_0 + 4\sum_{j=2}^{k-1}[(-1)^j x_{k-j}] + (-1)^k \mathbf{v}_0\Delta t\right\}, \; k \geq 3.$$

It has been show [4] that (2.3)-(2.7) and the discrete Newton's equation

(2.8) $$m \cdot a_{k+1} = F(x_k, t_k, v_k)$$

imply the validity of the conservation of energy and momentum and that discrete solutions of initial value problems for (2.8) exist, are unique, and can be generated recursively on a digital computer whether F is linear or nonlinear in its variables.

In order to study n-body problems, we will first extend (2.1) - (2.8) to systems of particles in planar motion as follows. Consider n particles P_i, $i = 1, 2, ., n$. At time $t_k = k\Delta t$, $k = 0, 1, \ldots,$ let P_i be at $(x_{i,k}, y_{i,k})$, have velocity $(v_{i,k,x}, v_{i,k,y})$, and have acceleration $(a_{i,k,x}, a_{i,k,y})$. Then, for each $i = 1, 2, \ldots, n$,

(2.9) $$v_{i,1,x} = \frac{2}{\Delta t}[x_{i,1} - x_{i,0}] - v_{i,0,x}$$

(2.10) $$v_{i,1,y} = \frac{2}{\Delta t}[y_{i,1} - y_{i,0}] - v_{i,0,y}$$

(2.11) $$v_{i,k,x} = \frac{2}{\Delta t}[x_{i,k} + (-1)^k x_{i,0} + 2\sum_{j=1}^{k-1} (-1)^j x_{i,k-j}] + (-1)^k v_{i,0,x};\ k \geq 2$$

(2.12) $$v_{i,k,y} = \frac{2}{\Delta t}[y_{i,k} + (-1)^k y_{i,0} + 2\sum_{j=1}^{k-1} (-1)^j y_{i,k-j}] + (-1)^k v_{i,0,y};\ k \geq 2$$

(2.13) $$a_{i,1,x} = \frac{2}{(\Delta t)^2}[x_{i,1} - x_{i,0} - v_{i,0,x}\Delta t]$$

(2.14) $$a_{i,1,y} = \frac{2}{(\Delta t)^2}[y_{i,1} - y_{i,0} - v_{i,0,y}\Delta t]$$

(2.15) $$a_{i,2,x} = \frac{2}{(\Delta t)^2}[x_{i,2} - 3x_{i,1} + 2x_{i,0} + v_{i,0,x}\Delta t]$$

(2.16) $$a_{i,2,y} = \frac{2}{(\Delta t)^2}[y_{i,2} - 3y_{i,1} + 2y_{i,0} + v_{i,0,y}\Delta t]$$

$$a_{i,k,x} = \frac{2}{(\Delta t)^2}\left\{x_{i,k} - 3x_{i,k-1} + 2\,(-1)^k x_{i,0} + 4\sum_{j=2}^{k-1}[(-1)^j x_{i,k-j}] + (-1)^k v_{i,0,x}\Delta t\right\};\ k \geq 3 \tag{2.17}$$

$$a_{i,k,y} = \frac{2}{(\Delta t)^2}\left\{y_{i,k} - 3y_{i,k-1} + 2\,(-1)^k y_{i,0} + 4\sum_{j=2}^{k-1}[(-1)^j y_{i,k-j}] + (-1)^k v_{i,0,y}\Delta t\right\};\ k \geq 3\,. \tag{2.18}$$

In the usual manner of vector generalization, (2.8) is extended as

$$m\vec{a}_{k+1} = \vec{F}_k\,. \tag{2.19}$$

3. N-BODY PROBLEMS

For Newtonian n-body problems, the components of $\vec{F}$ in (2.19) have factors of the form $-\frac{G}{r^2}$. For our purposes, however, it will be of great advantage to replace such terms by more comprehensive expressions of the form

$$-\frac{G}{(r+\xi)^2} + \frac{H}{(r+\xi)^p} - \alpha\sqrt{v_x^2 + v_y^2}\,, \tag{3.1}$$

where r is the distance between a given pair of interacting particles, G is the universal gravitational constant, H is a nonnegative constant of repulsion, α is a nonnegative damping factor, ξ is a nonnegative parameter which can be used to avoid mathematical singularity when r can equal zero, and p is a constant.

Note, for example, that if $H > 0$, $p > 2$ and $\xi = 0$, then $-\frac{G}{r^2}$ dominates $\frac{H}{r^p}$ for large values of r, while $\frac{H}{r^p}$ dominates $-\frac{G}{r^2}$ for small values of r. Thus, the resulting repulsive effect for small values of r can be used to simulate particle collision without the necessity of actual collision and, of course, also allows us to consider repulsion, itself, as a component of force when it does exist and does have a significant effect.

The resulting dynamical equations, which reduce to a classical n-body Newtonian formulation if $H = \alpha = \xi = 0$ are derived simply by replacing terms of the form $-\frac{G}{r^2}$ in the usual formulas by terms of the form (3.1), are, for $k \geq 0$, therefore

$$(3.2) \qquad a_{i,k+1,x} = \sum_{\substack{j=1 \\ j \neq i}}^{n} \frac{m_j(x_{i,k} - x_{j,k})}{(r_{ij,k} + \xi)} \left\{ -\frac{G}{(r_{ij,k} + \xi)^2} + \frac{H}{(r_{ij,k} + \xi)^p} - \alpha[(v_{i,k,x})^2 + (v_{i,k,y})^2]^{\frac{1}{2}} \right\}$$

$$(3.3) \qquad a_{i,k+1,y} = \sum_{\substack{j=1 \\ j \neq i}}^{n} \frac{m_j(y_{i,k} - y_{j,k})}{(r_{ij,k} + \xi)} \left\{ -\frac{G}{(r_{ij,k} + \xi)^2} + \frac{H}{(r_{ij,k} + \xi)^p} - \alpha[(v_{i,k,x})^2 + (v_{i,k,y})^2]^{\frac{1}{2}} \right\},$$

where $i = 1, 2, \ldots, n$ and where $r_{ij,k}$ is the distance between particles P_i and P_j at time t_k.

4. SOLUTION OF N-BODY PROBLEMS

The following simple recursion formulas for the trajectory points $(x_{i,k}, y_{i,k})$, $i = 1,2,\ldots,n$ then follow easily from substitution of (2.13)-(2.18) into (3.2)-(3.3):

$$(4.1)\qquad x_{i,1} = x_{i,0} + v_{i,0,x}\Delta t + \frac{(\Delta t)^2}{2}\left[\sum_{\substack{j=1\\ j\neq i}}^{n} \frac{m_j(x_{i,0} - x_{j,0})}{(r_{ij,0} + \xi)}\left\{-\frac{G}{(r_{ij,0} + \xi)^2} + \frac{H}{(r_{ij,0} + \xi)^p} - \alpha[(v_{i,0,x})^2 + (v_{i,0,y})^2]^{\frac{1}{2}}\right\}\right]$$

$$(4.2)\qquad y_{i,1} = y_{i,0} + v_{i,0,y}\Delta t + \frac{(\Delta t)^2}{2}\left[\sum_{\substack{j=1\\ j\neq i}}^{n} \frac{m_j(y_{i,0} - y_{j,0})}{(r_{ij,0} + \xi)}\left\{-\frac{G}{(r_{ij,0} + \xi)^2} + \frac{H}{(r_{ij,0} + \xi)^p} - \alpha[(v_{i,0,x})^2 + (v_{i,0,y})^2]^{\frac{1}{2}}\right\}\right]$$

$$(4.3)\qquad x_{i,2} = 3x_{i,1} - 2x_{i,0} - v_{i,0,x}\Delta t + \frac{(\Delta t)^2}{2}\left[\sum_{\substack{j=1\\ j\neq i}}^{n} \frac{m_j(x_{i,1} - x_{j,1})}{(r_{ij,1} + \xi)}\left\{-\frac{G}{(r_{ij,1} + \xi)^2} + \frac{H}{(r_{ij,1} + \xi)^p} - \alpha\left([\frac{2}{\Delta t}[x_{i,1} - x_{i,0}] - v_{i,0,x}]^2 + [\frac{2}{\Delta t}[y_{i,1} - y_{i,0}] - v_{i,0,y}]^2\right)^{\frac{1}{2}}\right\}\right]$$

$$(4.4)\qquad y_{i,2} = 3y_{i,1} - 2y_{i,0} - v_{i,0,y}\Delta t + \frac{(\Delta t)^2}{2}\left[\sum_{\substack{j=1\\ j\neq i}}^{n} \frac{m_j(y_{i,1} - y_{j,1})}{(r_{ij,1} + \xi)}\left\{-\frac{G}{(r_{ij,1} + \xi)^2}\right.\right.$$

$$+ \frac{H}{(r_{ij,1} + \xi)^p} - \alpha\left([\frac{2}{\Delta t}[x_{i,1} - x_{i,0}] - v_{i,0,x}]^2\right.$$

$$\left.\left.\left. + [\frac{2}{\Delta t}[y_{i,1} - y_{i,0}] - v_{i,0,y}]^2\right)^{\frac{1}{2}}\right\}\right]$$

and, for $k \geq 2$,

$$(4.5)\qquad x_{i,k+1} = 3x_{i,k} + 2(-1)^k x_{i,0} - 4\sum_{j=2}^{k} [(-1)^j x_{i,k-j+1}] + (-1)^k v_{i,0,x}\Delta t$$

$$+ \frac{(\Delta t)^2}{2}\left[\sum_{\substack{j=1\\ j\neq i}}^{n} \frac{m_j(x_{i,k} - x_{j,k})}{(r_{ij,k} + \xi)}\left\{-\frac{G}{(r_{ij,k} + \xi)^2} + \frac{H}{(r_{ij,k} + \xi)^p}\right.\right.$$

$$- \alpha\left([\frac{2}{\Delta t}[x_{i,k} + (-1)^k x_{i,0} + 2\sum_{j=1}^{k-1} (-1)^j x_{i,k-j}] + (-1)^k v_{i,0,x}]^2\right.$$

$$\left.\left.\left. + [\frac{2}{\Delta t}[y_{i,k} + (-1)^k y_{i,0} + 2\sum_{j=1}^{k-1} (-1)^j y_{i,k-j}] + (-1)^k v_{i,0,y}]^2\right)^{\frac{1}{2}}\right\}\right]$$

$$(4.6)\qquad y_{i,k+1} = 3y_{i,k} + 2(-1)^k y_{i,0} - 4\sum_{j=2}^{k} [(-1)^j y_{i,k-j+1}] + (-1)^k v_{i,0,y}\Delta t$$

$$+ \frac{(\Delta t)^2}{2}\left[\sum_{\substack{j=1\\ j\neq i}}^{n} \frac{m_j(y_{i,k} - y_{j,k})}{(r_{ij,k} + \xi)} \left\{ - \frac{G}{(r_{ij,k} + \xi)^2} + \frac{H}{(r_{ij,k} + \xi)^p}\right.\right.$$

$$- \alpha\left([\frac{2}{\Delta t} [x_{i,k} + (-1)^k x_{i,0} + 2\sum_{j=1}^{k-1} (-1)^j x_{i,k-j}] + (-1)^k v_{i,0,x}]^2\right.$$

$$\left.\left.\left. + [\frac{2}{\Delta t} [y_{i,k} + (-1)^k y_{i,0} + 2\sum_{j=1}^{k-1} (-1)^j y_{i,k-j}] + (-1)^k v_{i,0,y}]^2 \right)^{\frac{1}{2}} \right\}\right].$$

That n-body initial value problems have unique solutions is now a consequence of the following theorem.

Theorem 4.1 For given $\xi > 0$, $\alpha \geq 0$ and arbitrary $x_{i,0}$, $y_{i,0}$, $v_{i,0,x}$ and $v_{i,0,y}$, $i = 1,2,\ldots,n$, the n-body problem defined by (3.2)-(3.3) has a unique discrete solution which is given constructively by (4.1)-(4.6).

Proof: The proof is a direct consequence of the observation that the right-hand sides of (4.1)-(4.6) are always real, defined, and single valued.

It is important to note also that the recursive structure of (4.1)-(4.6) is what makes the solution particularly amenable to evaluation on a high speed digital computer.

5. FREE SURFACE FLUID FLOW

Free surface fluid problems have long been of wide interest in both pure and applied science (see, e.g., references [6,9,11-14,16-18] and the additional references contained therein), and liquids, in particular, have been modeled traditionally as being continuous and as consisting of an infinite number of point particles. The resulting nonlinear differential equations, even when linearized, can rarely be solved analytically.

In order to illustrate the methods and theory of Sections 1-4, we will model a particular free surface liquid flow problem as a discrete n-body problem. By Theorem 4.1, the dynamical equations of motion will be solved easily on a digital computer. Unfortunately, the present state of computer design does not as yet allow us to choose relatively large values of n. Nevertheless, it will still be of interest to note that, even though the example to be described consists of only 100 particles, still the flow does crudely approximate the actual flow constructed in our hydraulics laboratory and, indeed, a mechanism for the development of rotation is observed easily from the resulting numerical computations.

The problem to be considered, called the open gate problem, can be formulated physically as follows. The wall CD of square container ABCD, shown in Figure 5.1, is hinged at D and can be opened at will. The container is filled with liquid and then DC is opened quickly in such a fashion that C rotates on a circle with center D to the new position C', as shown in Figure 5.1. Thus, the gate has been opened. The problem is to describe the motion of the liquid as it flows out of the container.

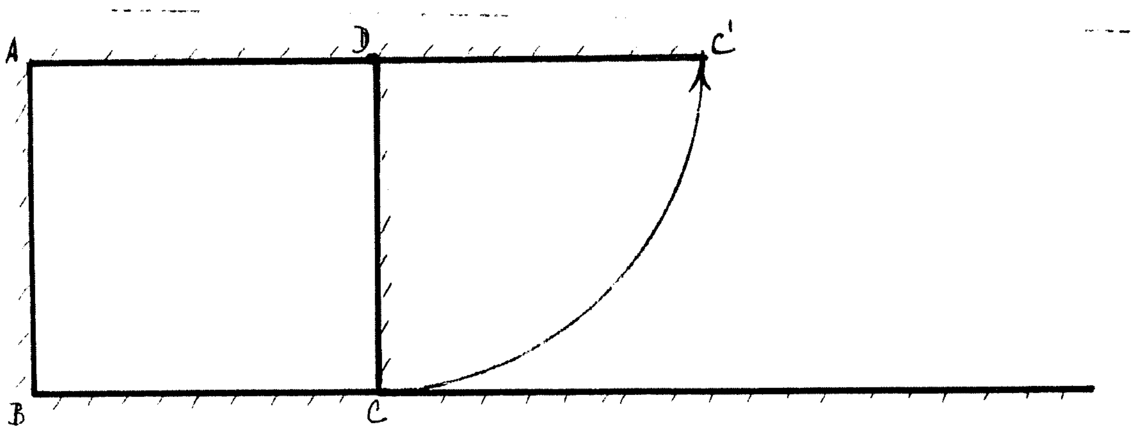

FIGURE 5.1

In cgs units, consider then a liquid which is represented by 100 circular, homogeneous particles, $P_1, P_2, \ldots, P_{100}$, each of mass 8, which are arranged as shown in Figure 5.2. For simplicity, let the diameter d of each particle be unity and let the x-axis contain the centers of the bottom row of particles while the y-axis contains the centers of the left column of particles. In this manner the mass centers $(x_{i,0}, y_{i,0})$ of P_i, $i = 1,2,\ldots,100$, are at nodal points of the form $(m_1 h, m_2 h)$, where $h = d = 1$; $m_1 = 0,1,\cdot,9$; and $m_2 = 0,1,\cdot,9$.

At time t_k let the mass center of P_i be $(x_{i,k}, y_{i,k})$. Then introducing the effect of gravity results in the following particular choices for (3.2) and (3.3):

$$(5.1) \qquad a_{i,k+1,x} = 8\sum_{\substack{j=1 \\ j\neq i}}^{100} \left\{ \frac{(x_{i,k} - x_{j,k})}{(r_{ij,k} + .75)} \left[\frac{H_{ij,k}}{(r_{ij,k} + .75)} - \alpha \left(v_{i,k,x}^{2} + v_{i,k,y}^{2}\right)^{\frac{1}{2}} \right] \right\}$$

$$(5.2) \qquad a_{i,k+1,y} = 8\sum_{\substack{j=1 \\ j\neq i}}^{100} \left\{ \frac{(y_{i,k} - y_{j,k})}{(r_{ij,k} + .75)} \left[\frac{H_{ij,k}}{(r_{ij,k} + .75)} - \alpha \left(v_{i,k,x}^{2} + v_{i,k,y}^{2}\right)^{\frac{1}{2}} \right] \right\} - \frac{980\beta_j}{m}$$

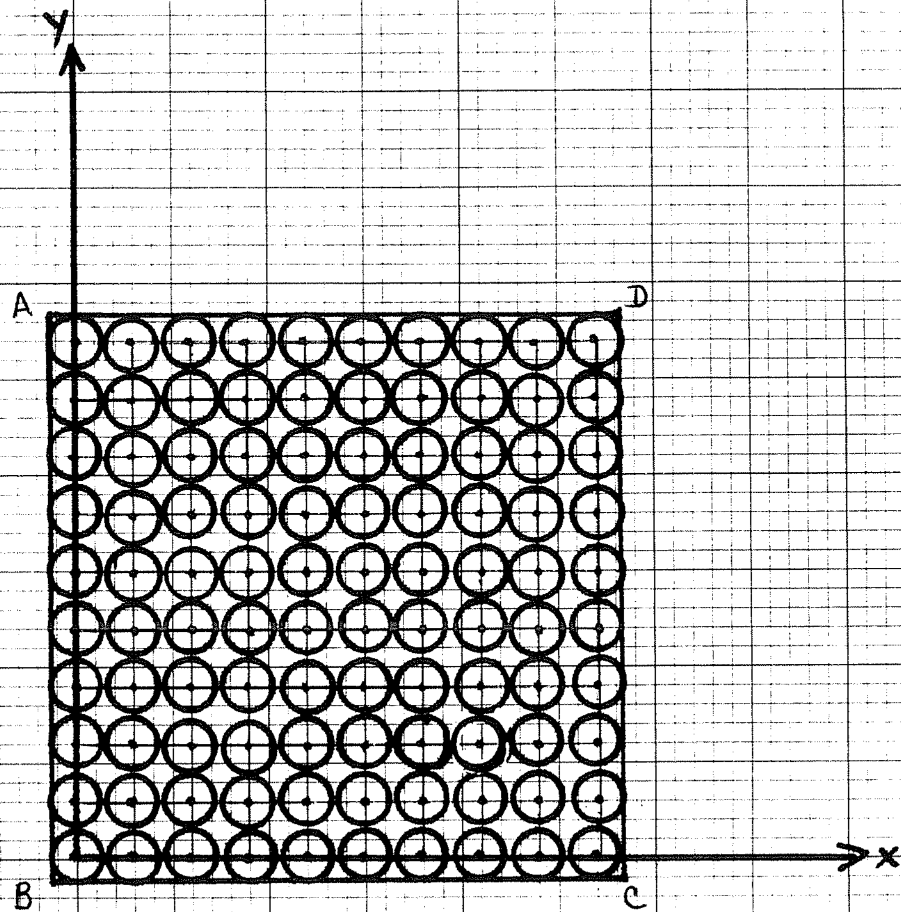

FIGURE 5.2

where the repulsion coefficient $H_{ij,k}$ is defined by

(5.3) $$H_{ij,k} = \begin{cases} 0, \text{ if } r_{ij,k} > 1 \\ 1, \text{ if } r_{ij,k} \leq 1 , \end{cases}$$

and where the viscosity coefficient α is defined by

(5.4) $$\alpha = \begin{cases} 10^{-4}, \text{ if } y_{i,k} > 0 \\ 10^{-3}, \text{ if } y_{i,k} = 0 . \end{cases}$$

The constant G has been set equal to zero because of the overwhelming effect of the attraction of each particle to the earth. The definition of β_i will require the following additional remarks.

At time t_k, let the shadow of particle P_i be the rectangle whose vertices are $(x_{i,k} + \frac{1}{2}, 0)$, $(x_{i,k} + \frac{1}{2}, y_{i,k})$, $(x_{i,k} - \frac{1}{2}, y_{i,k})$, $(x_{i,k} - \frac{1}{2}, 0)$, as shown in Figure 5.3. If there are no particles in the shadow of P_i, we would wish to choose $\beta_i = 1$ and thus have the full force of gravity acting upon P_i. On the other hand, if the shadow area of P_i contains portions of other particles, we would wish to choose β_i different from unity to reflect the amount of support which P_i has below it. The measure β_i is then defined as follows. One lists all particles P_j different from P_i whose mass centers satisfy both

(5.5) $$x_{i,k} - 1 < x_{j,k} < x_{i,k} + 1$$

(5.6) $$y_{j,k} < y_{i,k} ,$$

and defines

$$\sigma = \sum_j [1 - |x_{i,k} - x_{j,k}|] .$$

Note that if no particle P_j exists whose center satisfies (5.5) and (5.6), then $\sigma = 0$. Finally, β_i is defined by

$$\beta_i = \begin{cases} 0, \text{ if } y_{i,k} = 0 \\ \left(1 - \dfrac{\sigma}{y_{i,k}}\right)^2, \text{ if } 0 < \dfrac{\sigma}{y_{i,k}} < 1 \\ (.00005)\left(1 - \dfrac{1+\sigma}{1+y_{i,k}}\right), \text{ if } \dfrac{\sigma}{y_{i,k}} \geq 1. \end{cases} \tag{5.7}$$

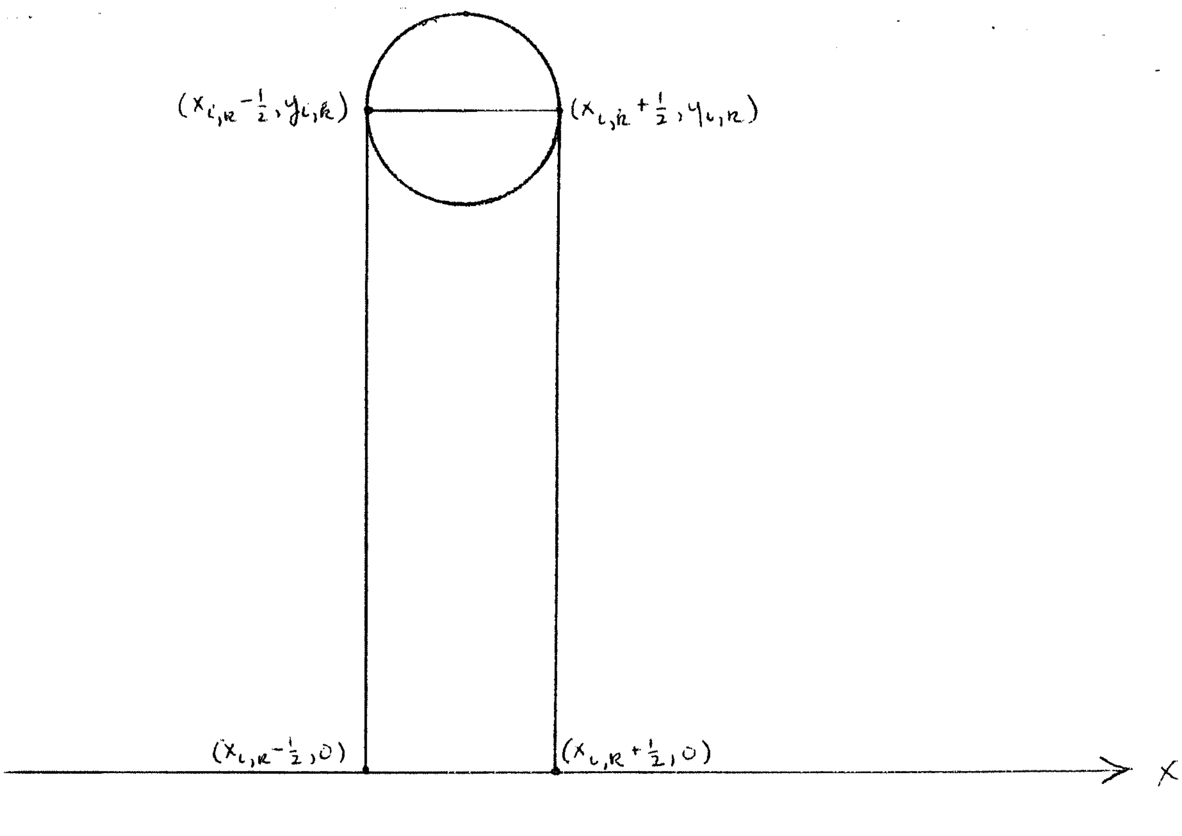

FIGURE 5.3

The calculations which result after replacing (5.1) and (5.2) by recursion formulas of the types (4.1)-(4.6) are then carried out as follows. Initial velocities $v_{i,0,x}$ and $v_{i,0,y}$ which result from the opening of the gates are given by

$$(5.5)\qquad v_{i,0,y} = 0$$

$$(5.6)\qquad v_{i,0,x} = (2.7)\,(9 - y_{i,0})\left(\frac{27}{40} + \frac{x_{i,0}}{40}\right)^{14-x} .$$

Formula (5.6) is only one of several which reflect the assumption that $v_{i,0,x}$ increases with depth and with horizontal distance from the left wall when the gate is opened. If at any time $x_{i,k}$ satisfies $x_{i,k} \le \frac{1}{2}$, then the associated particle is reset immediately to $(\frac{1}{2}, y_{i,k})$ and its velocity is reset as $(0, v_{i,k,y})$. If at any time any $y_{i,k}$ satisfies $y_{i,k} < 0$, then the associated particle is reset immediately to $(x_{i,k}, 0)$ and its velocity is reset at $(0, -.0025v_{i,k,y})$, which imparts some bounce to the particle.

Calculations on the UNIVAC 1108 for $\Delta t = .01$ and in which the left wall is kept wet, that is, no particle with $x_{i,0} = 0$ is allowed to move, are shown typically for time steps t_{25}, t_{60}, t_{100}, t_{175}, t_{250} and t_{350} in Figures 5.4 - 5.9, respectively. Approximations to the actual surfaces at each time step are shown in Figures 5.10-5.15, in which smooth curves have been drawn freely above the particle configurations. In Figure 5.16 is shown an actual three dimensional cavity with a string attachment for opening a left gate. In Figures 5.17 and 5.18 are shown the actual patterns as water flows to the left during and after the opening of the gate.

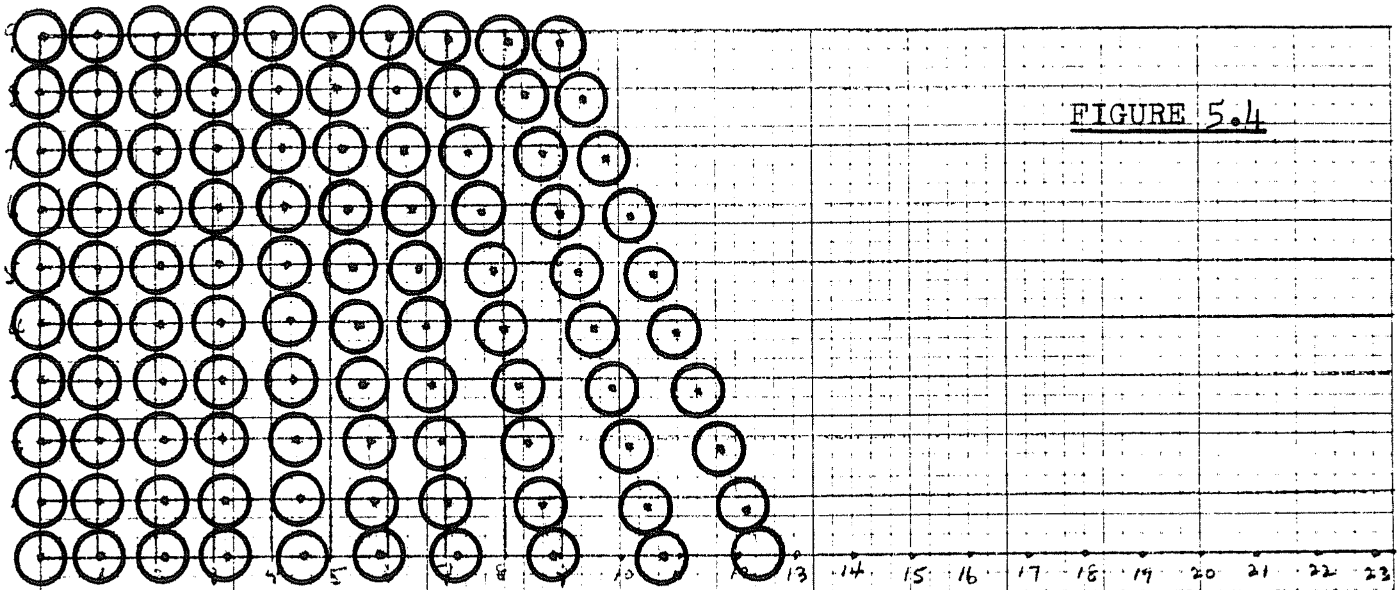

FIGURE 5.4

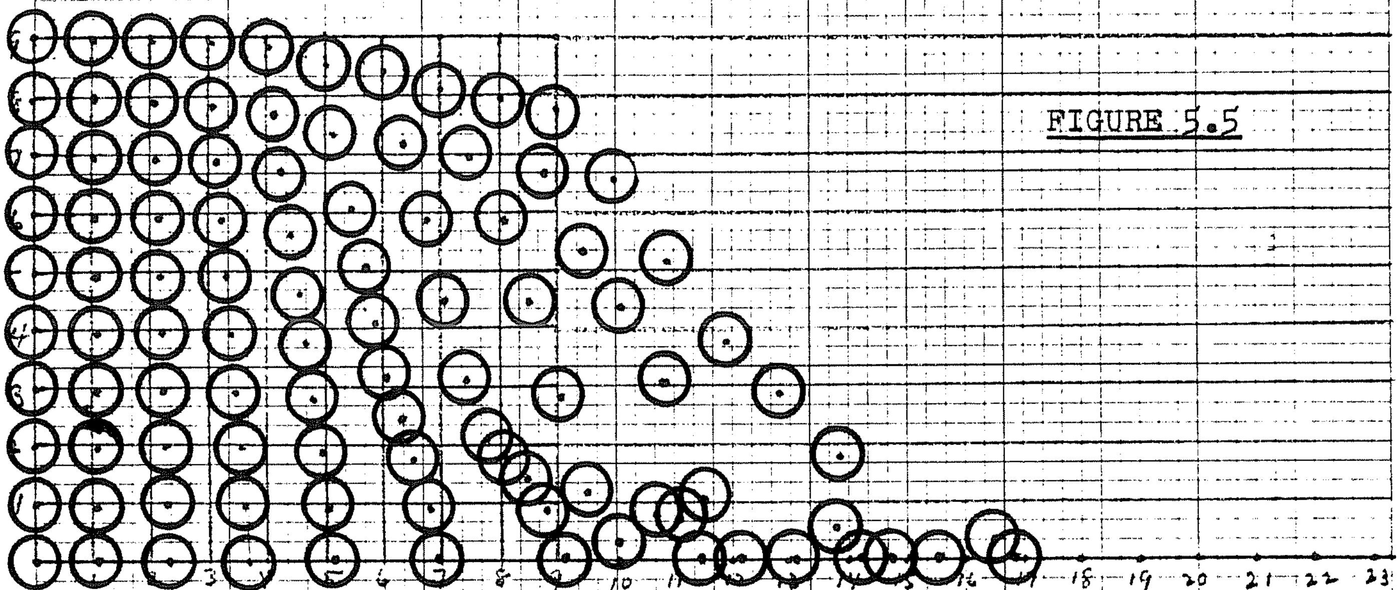

FIGURE 5.5

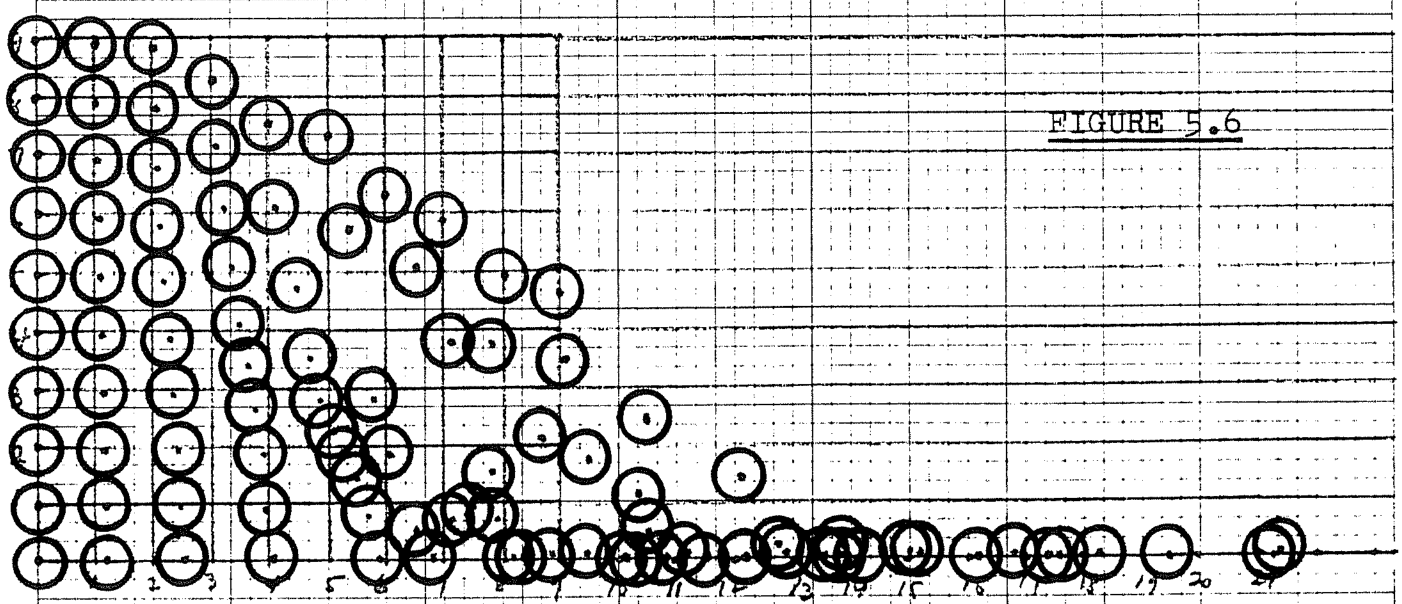

FIGURE 5.6

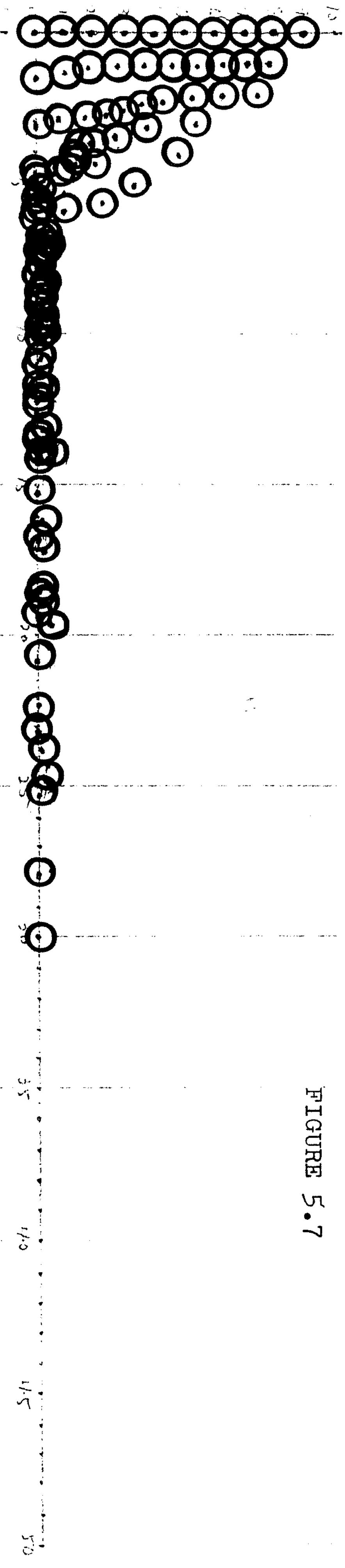

FIGURE 5.7

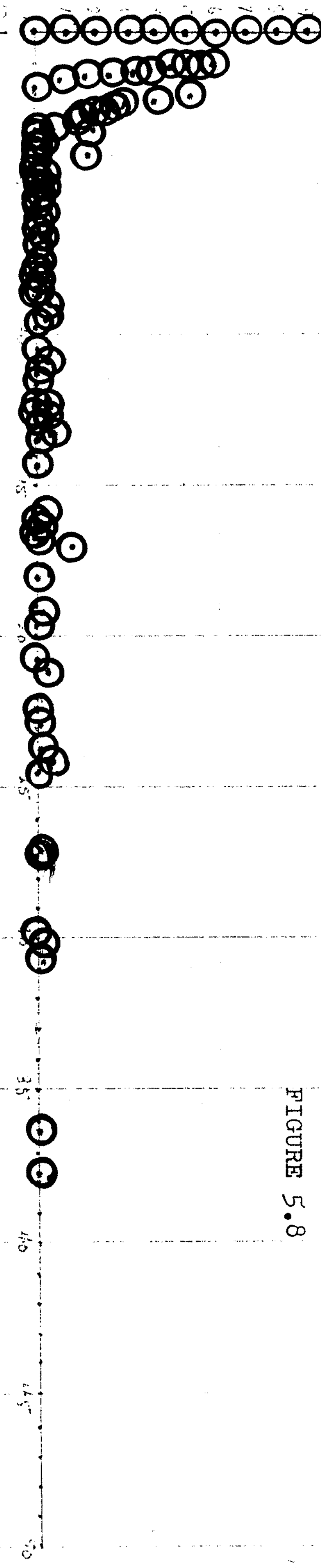

FIGURE 5.8

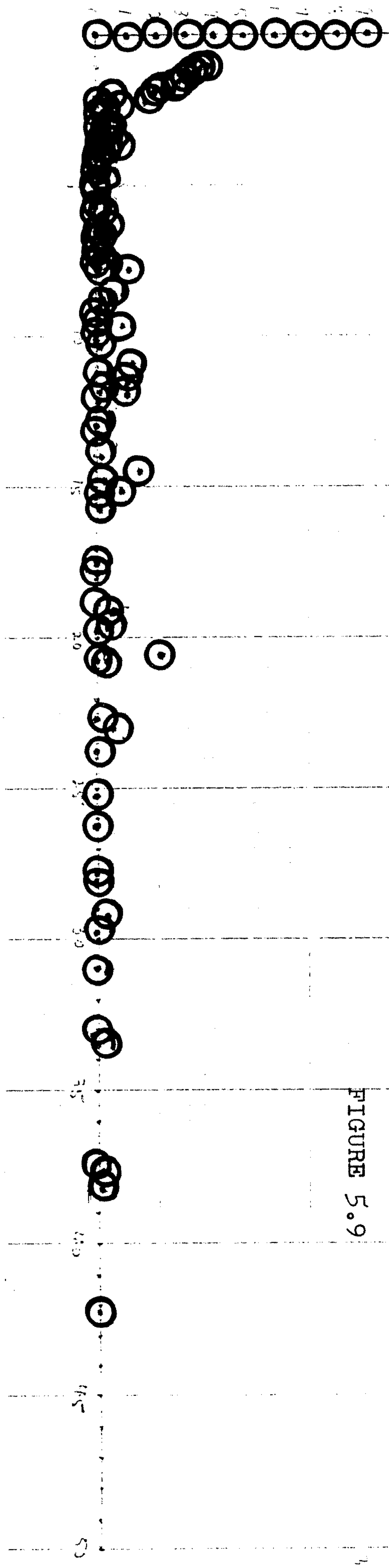

FIGURE 5.9

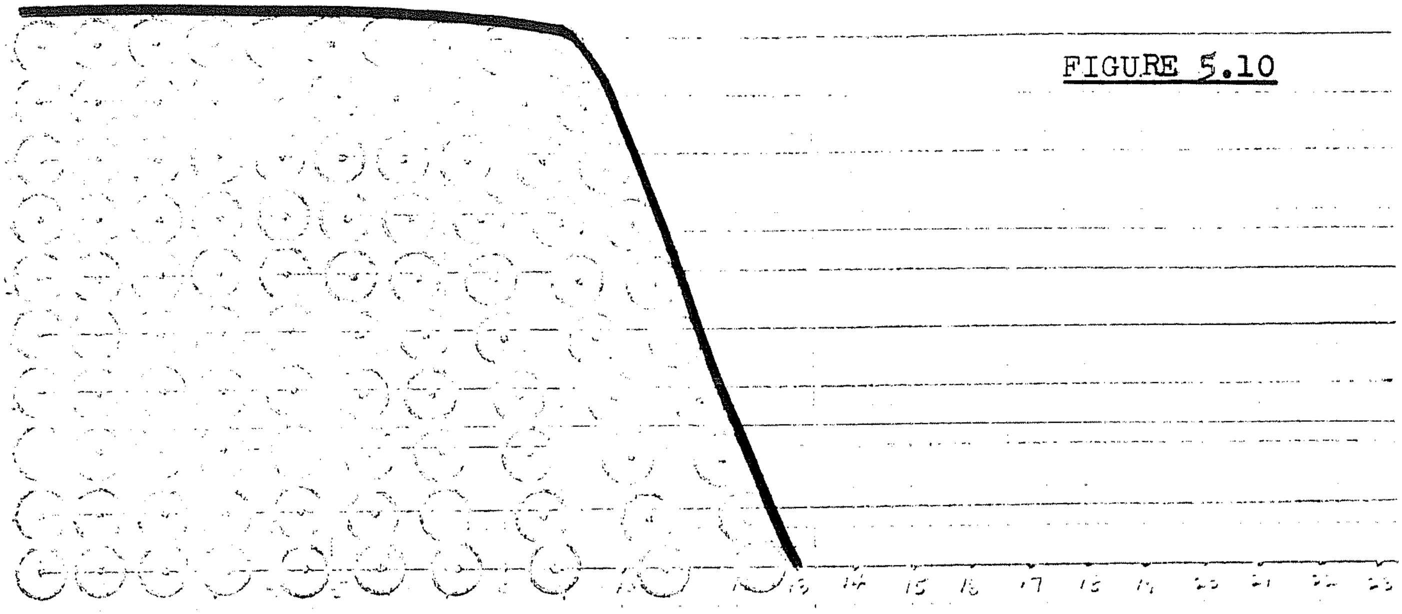

FIGURE 5.10

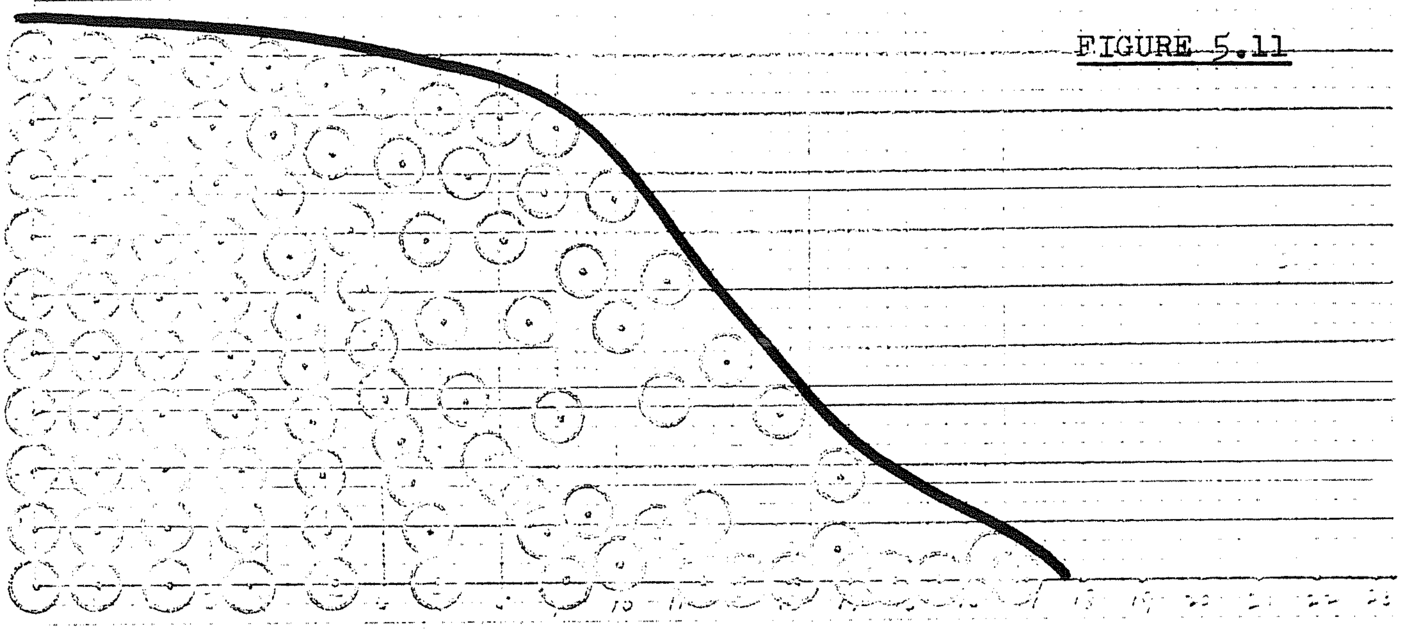

FIGURE 5.11

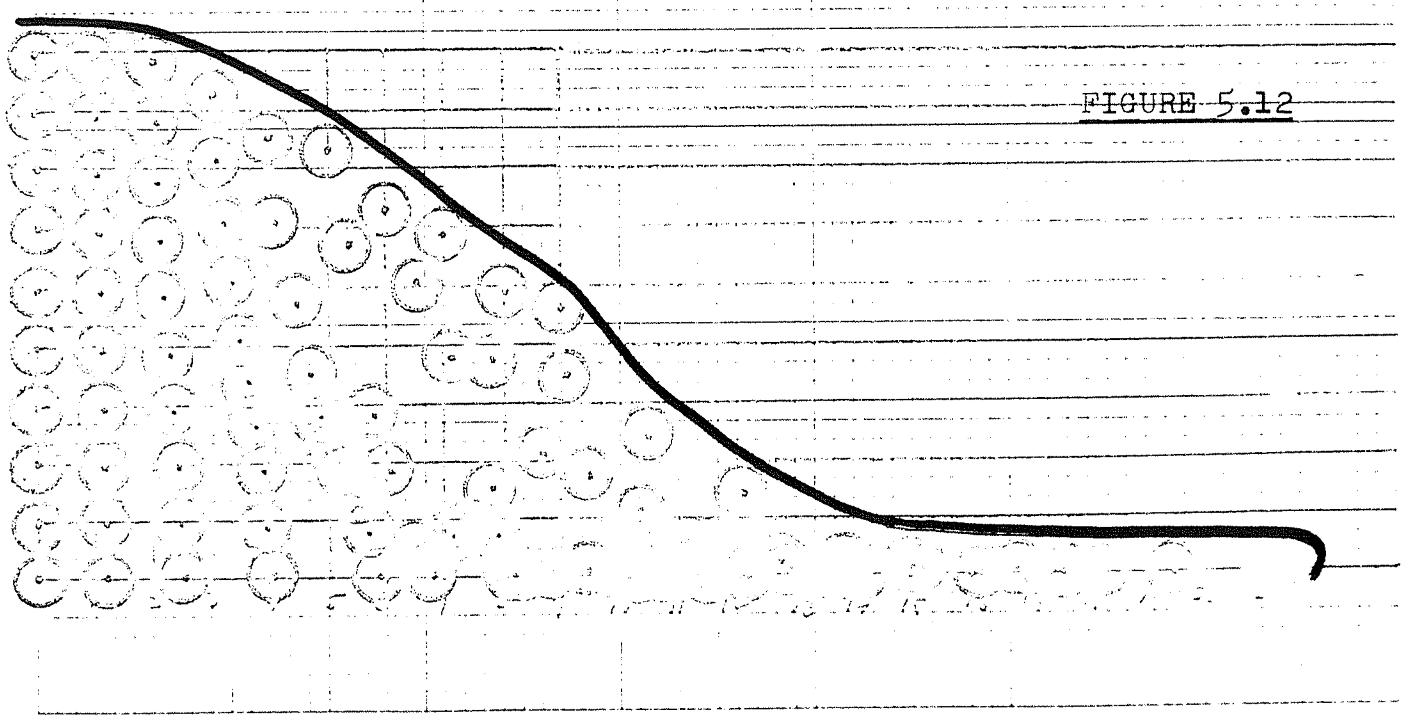

FIGURE 5.12

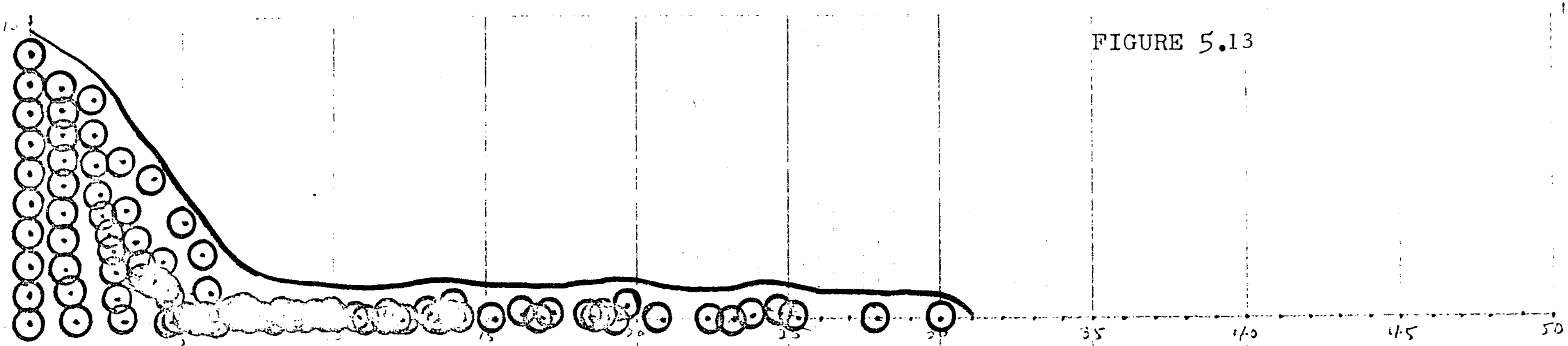

FIGURE 5.13

FIGURE 5.14

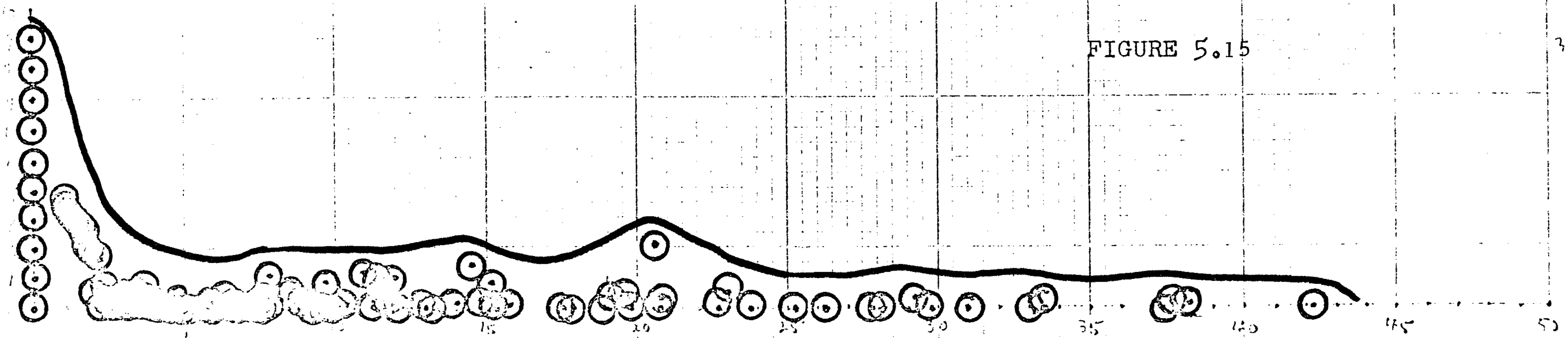

FIGURE 5.15

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pages ~~18, 19, 20~~ 19-20-21

Note that Figures 5.12 and 5.17 compare favorably while Figures 5.15 and 5.18 both exhibit the development of a downstream bore. Also, from the very large number of other examples run, it should be noted that the computations were very sensitive to the choices of (5.4), (5.6) and magnitude of bounce allowed.

In Figures 5.19 and 5.20 are shown the positions of the particles of the 5^{th} row at the respective time steps t_{50} and t_{250}. In Figure 5.21 are shown the positions of the particles of the 4^{th} column at time step t_{125}. Note here that certain particles originally above other particles have fallen below them due to less dense shadow regions and a greater resultant force of gravity. The effect shown in Figure 5.21 is, interestingly enough, one of rotation.

Finally, because of the experimental nature of our work, we find it necessary to include our Fortran program in an Appendix, so that others can reproduce our work in its entirety.

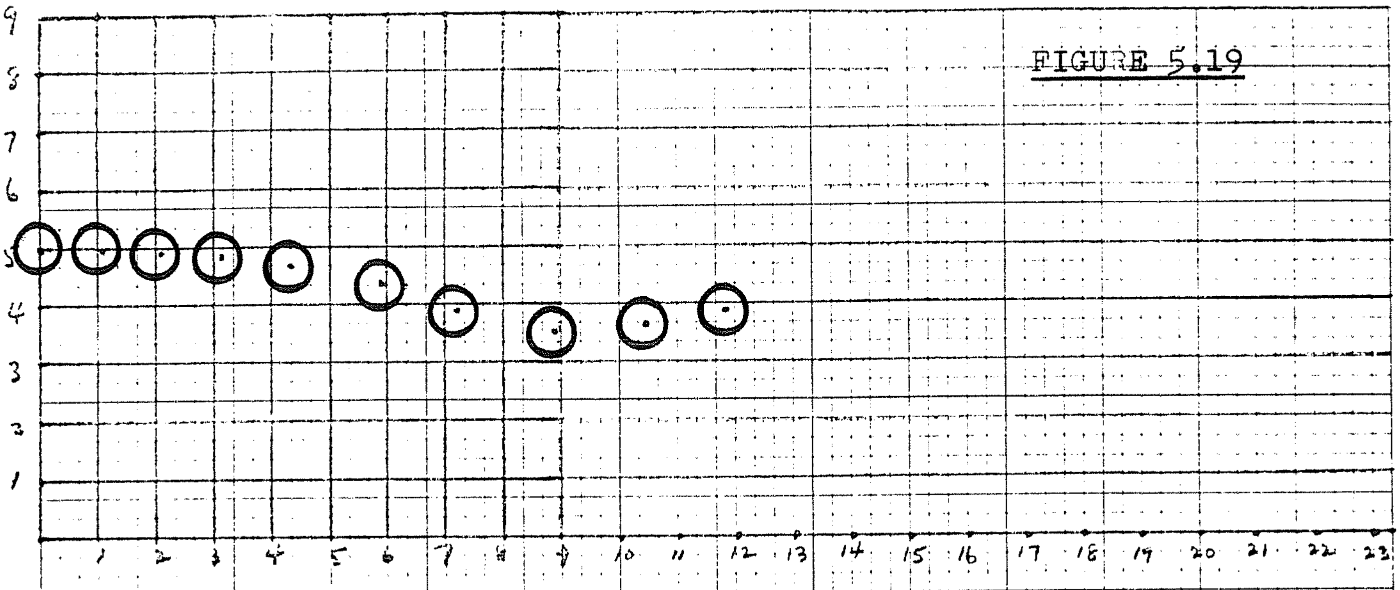

FIGURE 5.19

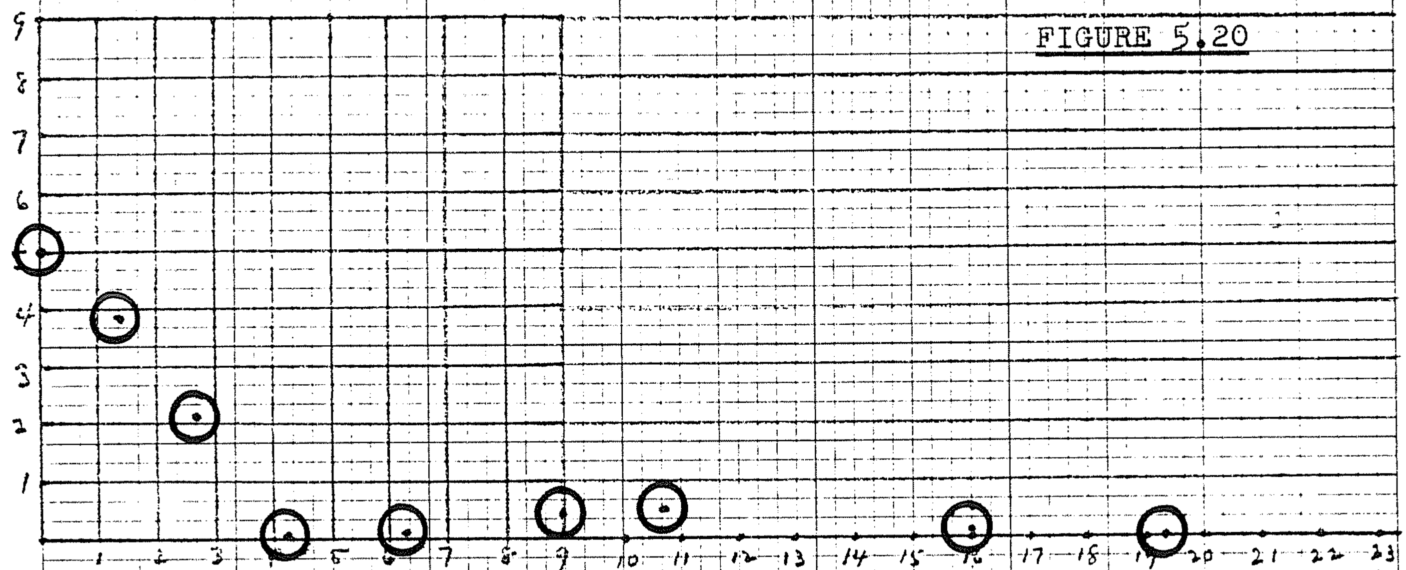

FIGURE 5.20

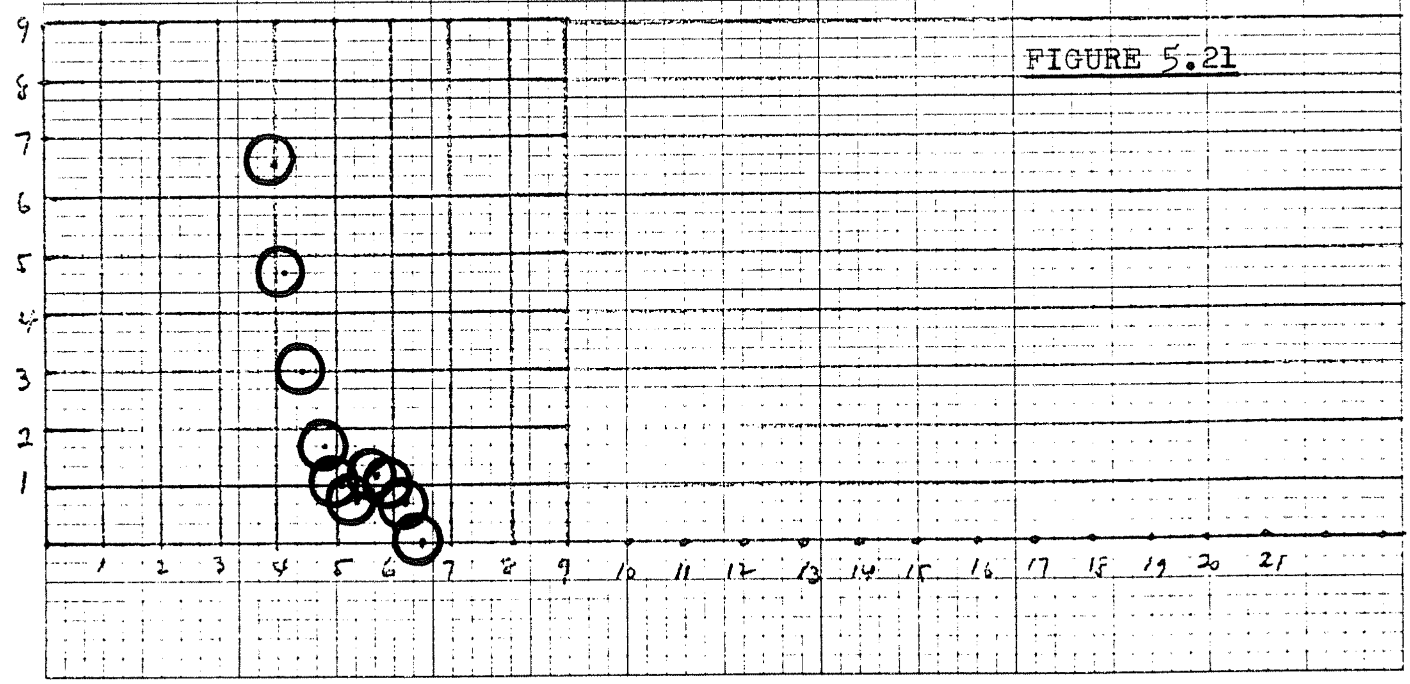

FIGURE 5.21

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```
      DIMENSION X1(100),Y1(100),VOX(100),VOY(100),D(100),Q(100),F(100),
     1E(100),VX(100),VY(100),AX(100),AY(100),A(100),
     2X(100,50),Y(100,50),R(100,100),KTIM(100,2),ZX(100),ZY(100)
C     SET UP PARAMETERS
      NP=100
      RR=.75
      NPP=90
      CC=2.7
      AM=8.0
      H=1.
      A1=.0001
      A2=.001
      A3=.0025
      A4=.00005
      KL=0
      LQ=0
      DT=.01
      NN=50
      NZP=3
      LW=0
      KS=1
      NZ=0
      Z=1
      NS=1
      II=0
C    CALCULATE INITIAL VELOCITY
      DO 33 I=1,10
      DO 33 J=1,9
      II=II+1
      Y1(II)=I-1
      VOY(II)=0
      X1(II)=J
      P1=14-J
      R1=((27./40.)+(J/40.))**P1
33    VOX(II)=((10.-I)*R1)*CC
      DO 334 I=1,10
      II=II+1
      Y1(II)=I-1
334   X1(II)=0.
30    FORMAT(9E8.1,/,9E8.1,/,9E8.1)
      DO 443 K=1,NN
      DO 443 I=91,100
      X(I,K)=X1(I)
443   Y(I,K)=Y1(I)
      DO 71 I=1,NP
      D(I)=0
      ZX(I)=1
      ZY(I)=1.
      Q(I)=0
      F(I)=0
71    E(I)=0
C     PRINT OUT LIST OF PARAMETERS
      PRINT 80,AM,H,DT,A4
      PRINT 81,CC,RR,A1,A2
      PRINT 976,A3
976   FORMAT(1X,' A3=',E10.4)
81    FORMAT(' CC=',E10.4,' R+=',E10.4,' A1=',E10.4,' A2=',E10.4)
80    FORMAT(1H1,'AM=',E10.4,' H=',E10.4,' DT=',E10.4,' A4=',E10.4)
72    FORMAT (100(E10.4,15X,E10.4,/))
      PRINT 73
73    FORMAT(5X,10('   X      Y    '))
```

```
C       PRINT OUT INITIAL POSITIONS
        IZ=101
        DO 120 L1=1,10
        IZ=IZ-1
        IT=1+9*(L1-1)
        IN=91-IT
        IB=IN-8
120     PRINT 74,LQ,X1(IZ),Y1(IZ),(X1(I),Y1(I),I=IB,IN)
        PRINT 32
32      FORMAT(1X,/)
74      FORMAT(I5,10(F5.2,F5.2,1X))
C       RUN EACH CASE FOR NN*NZP TIME STEPS
        DO 1 IZP=1,NZP
        DO 91 KK=KS,NN
        K=KK
        IF(KK .EQ. 1) GO TO 829
        GO TO 831
829     DO 830 KQ=1,NP
        X(KQ,K)=X1(KQ)
830     Y(KQ,K)=Y1(KQ)
        DO 50 I=1,NP
        DO 50 J=1,NP
C        FIND DISTANCE BETWEEN PARTICLES
C       FOR FIRST TIME STEP
50      R(I,J)=SQRT(((X1(I)-X1(J))**2)+((Y1(I)-Y1(J))**2)) +RR
831     DO 91 I=1,NPP
        DO 811 KP=1,2
811     KTIM(I,KP)=KTIM(I,KP)+1
        ZX(I)=-ZX(I)
        ZY(I)=-ZY(I)
        K=KTIM(I,1)
        IF(K-2)6,7,7
C       SET X VELOCITY TO INITIAL VELOCITY
6       VX(I)=VOX(I)
7       K=KTIM(I,2)
        IF(K-2)806,807,807
C       SET Y VELOCITY TO INITIAL VELOCITY
806     VY(I)=VOY(I)
807     IF(KK .EQ. 1) GO TO 10
        K=KK
        K=K-1
C        FIND DISTANCE BETWEEN PARTICLES
C       FOR TIME STEPS GREATER THAN ONE
        DO 54 J=1,NP
54      R(I,J)=SQRT(((X(I,K)-X(J,K))**2)+((Y(I,K)-Y(J,K))**2)) +RR
        K=KTIM(I,1)
        IF(K-2)412,17,412
17      CONTINUE
        K=KK-1
C        CALCULATE X VELOCITY FOR SECOND TIME STEP
410     VX(I)=(2./DT)*(X(I,K)-X1(I))-VOX(I)
412     K=KTIM(I,2)
        IF(K-2)53,814,53
814     K=KK-1
C        CALCULATE Y VELOCITY FOR SECOND TIME STEP
510     VY(I)=(2./DT)*(Y(I,K)-Y1(I))-VOY(I)
53      CONTINUE
        K=KTIM(I,1)
        IF(K-2)816,816,815
815     K=KK-1
C        CALCULATE X VELOCITY FOR TIME STEPS GREATER THAN 2
```

```
110     D(I)=-D(I)-X(I,K-1)
        Z=ZX(I)
        VX(I)=(2./DT)*(X(I,K)-Z*X1(I)+2.*D(I))-Z*VOX(I)
816     K=KTIM(I,2)
        IF(K-2)2,2,817
817     K=KK-1
C        CALCULATE Y VELOCITY FOR TIME STEPS GREATER THAN 2
112     Q(I)=-Q(I)-Y(I,K-1)
        Z=ZY(I)
        VY(I)=(2./DT)*(Y(I,K)-Z*Y1(I)+2.*Q(I))-Z*VOY(I)
2       CONTINUE
10      CONTINUE
        CVX=ABS(VX(I))
        CVY=ABS(VY(I))
        IF(CVX  -10000.)77,869,869
77      IF(CVY  -10000.)3,869,869
3       A(I)=SQRT(((VX(I))**2)+((VY(I))**2))
C       DETERMINE DAMPING COEFFICIENT
        IF(KK .EQ. 1) GO TO 4019
        K=KK-1
        GO TO 4020
4019    K=KK
4020    CONTINUE
        IF(Y(I,K)-.0)617,618,617
618     AA=A2
        GO TO 619
617     AA=A1
619     CONTINUE
        D1=0
        D2=0
        DO 24 I1=1,NP
        IF(I1 .EQ. I) GO TO 24
C       DETERMINE REPULSION COEFFICIENT
        IF(R(I,I1) .GE. 1.) GO TO 917
        H=1.
        GO TO 918
917     H=.0
918     CONTINUE
C       FIND ACCELERATION OF PARTICLES
        D2=D2+((Y(I,K)-Y(I1,K))/R(I,I1))*(H/((R(I,I1))**1)-AA*A(I))
        D1=D1+((X(I,K)-X(I1,K))/R(I,I1))*(H/((R(I,I1))**1)-AA*A(I))
24      CONTINUE
        QQ=0
C       DETERMINE BETA I
        IF(Y(I,K)-.0)600,211,600
600     CONTINUE
        DO 200 I2=1,NP
        IF(Y(I,K)-Y(I2,K))200,200,202
202     P=ABS(X(I,K)-X(I2,K))
        IF(P .GE. 1.) GO TO 200
        P=1.-P
        QQ=QQ+P
200     CONTINUE
        DP=QQ/Y(I,K)
        IF(DP-1.)212,3012,3012
212     BI=1.-DP
        BI=BI*BI
        GO TO 213
3012    BI=A4*(1.-(QQ+1)/(Y(I,K)+1))
        GO TO 213
211     BI=0.
```

```
C     FIND X POSITION FOR THIRD  TIME STEP
610   E(I)=-E(I)+X(I,K-2)
      Z=ZX(I)
      X(I,K)=3.*X(I,K-1)-2.*Z*X1(I)-4.*E(I)-Z*DT*VOX(I)+(DT*DT/2.)*AX(I
     1)
C     IF X LESS THAN .5 RESET X VALUE
      IF(X(I,K)-.5)66,91,91
66    X(I,K)=.5
      VOX(I)=.0
      X1(I)=.5
      E(I)=0.
      D(I)=0.
      ZX(I)=NS
      KTIM(I,1)=0
      GO TO 91
822   K=KK
      Z=ZY(I)
C     FIND Y POSITION FOR THIRD  TIME STEP
612   F(I)=-F(I)+Y(I,K-2)
      Y(I,K)=3.*Y(I,K-1)-2.*Z*Y1(I)-4.*F(I)-Z*DT*VOY(I)+(DT*DT/2.)*AY(I
     1)
C     IF Y LESS THAN 0 RESET Y VALUE
67    IF(Y(I,K)-.0)68,91,91
68    Y(I,K)=.0
      Y1(I)=.0
      F(I)=0.
      Q(I)=0.
      VOY(I)=-A3*VY(I)
      KTIM(I,2)=0
      ZY(I)=NS
65    CONTINUE
91    CONTINUE
      GO TO 969
869   CONTINUE
      PRINT 870,K
870   FORMAT(20X,'****',I3)
969   CONTINUE
C     PRINT RESULTS
      DO 288 K=KS,NN
      IZ=101
      LK=K+LW
      PRINT 32
      DO 28 L1=1,10
      IZ=IZ-1
      IT=1+9*(L1-1)
      IN=91-IT
      IB=IN-8
28    PRINT 74,LK,X1(IZ),Y1(IZ),(X(I,K),Y(I,K),I=IB,IN)
288   CONTINUE
      IF(NZP .EQ. 1) GO TO 1
      DO 29 LM=1,NPP
      X(LM,2)=X(LM,NN)
      Y(LM,2)=Y(LM,NN)
      X(LM,1)=X(LM,NN-1)
29    Y(LM,1)=Y(LM,NN-1)
      KS=3
      LW=NN-2+LW
1     CONTINUE
      END
```

```
213     CONTINUE
106     AX(I)=AM*D1
        AY(I)=AM*D2-(980.*BI/AM)
20      CONTINUE
        DO 91 KQ=1,2
        K=KTIM(I,KQ)
        IF(K-2)12,13,14
12      IF(KQ .EQ. 2) GO TO 820
        K=KK
C       FIND X POSITION FOR FIRST TIME STEP
        X(I,K)=X1(I)+DT*VOX(I)+((DT*DT)/2.)*AX(I)
C       IF X LESS THAN .5 RESET X VALUE
        IF(X(I,K)-.5)26,91,91
26      X(I,K)=.5
        VOX(I)=.0
        X1(I)=.5
        D(I)=0.
        ZX(I)=NS
        KTIM(I,1)=0
        GO TO 91
820     K=KK
C       FIND Y POSITION FOR FIRST  TIME STEP
        Y(I,K)=Y1(I)+DT*VOY(I)+((DT*DT)/2.)*AY(I)
C       IF Y LESS THAN 0 RESET Y VALUE
27      IF(Y(I,K)-.0)75,91,91
75      Y(I,K)=.0
        Y1(I)=.0
        Q(I)=0.
        VOY(I)=-A3*VY(I)
        ZY(I)=NS
        KTIM(I,2)=0
        GO TO 91
13      IF(KQ .EQ. 2) GO TO 821
        K=KK
        L=K-1
C       FIND X POSITION FOR SECOND TIME STEP
        X(I,K)=3.*X(I,L)-2.*X1(I)-DT*VOX(I)+(DT*DT/2.)*AX(I)
C       IF X LESS THAN .5 RESET X VALUE
        IF(X(I,K)-.5)61,91,91
61      X(I,K)=.5
        X1(I)=.5
        D(I)=0.
        VOX(I)=.0
        ZX(I)=NS
        KTIM(I,1)=0
        GO TO 91
821     K=KK
        L=K-1
C       FIND Y POSITION FOR SECOND TIME STEP
        Y(I,K)=3.*Y(I,L)-2.*Y1(I)-DT*VOY(I)+(DT*DT/2.)*AY(I)
C       IF Y LESS THAN 0 RESET Y VALUE
62      IF(Y(I,K)-.0)63,91,91
63      Y(I,K)=.0
        Y1(I)=.0
        Q(I)=0.
        VOY(I)=-A3*VY(I)
        ZY(I)=NS
        KTIM(I,2)=0
        GO TO 91
14      IF(KQ .EQ. 2) GO TO 822
        K=KK
```