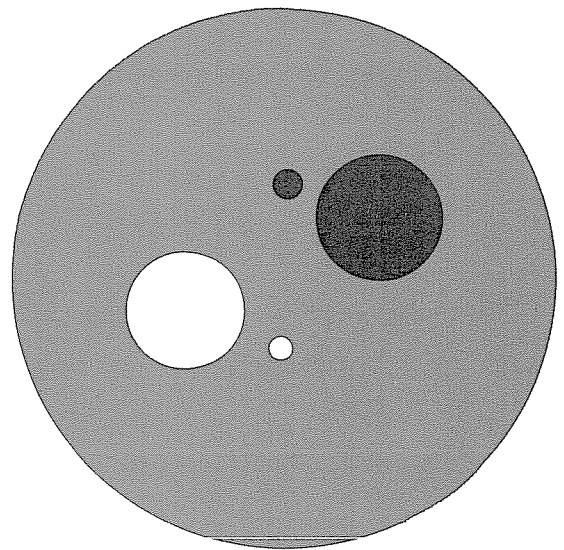


COMPUTER SCIENCES DEPARTMENT

University of Wisconsin-
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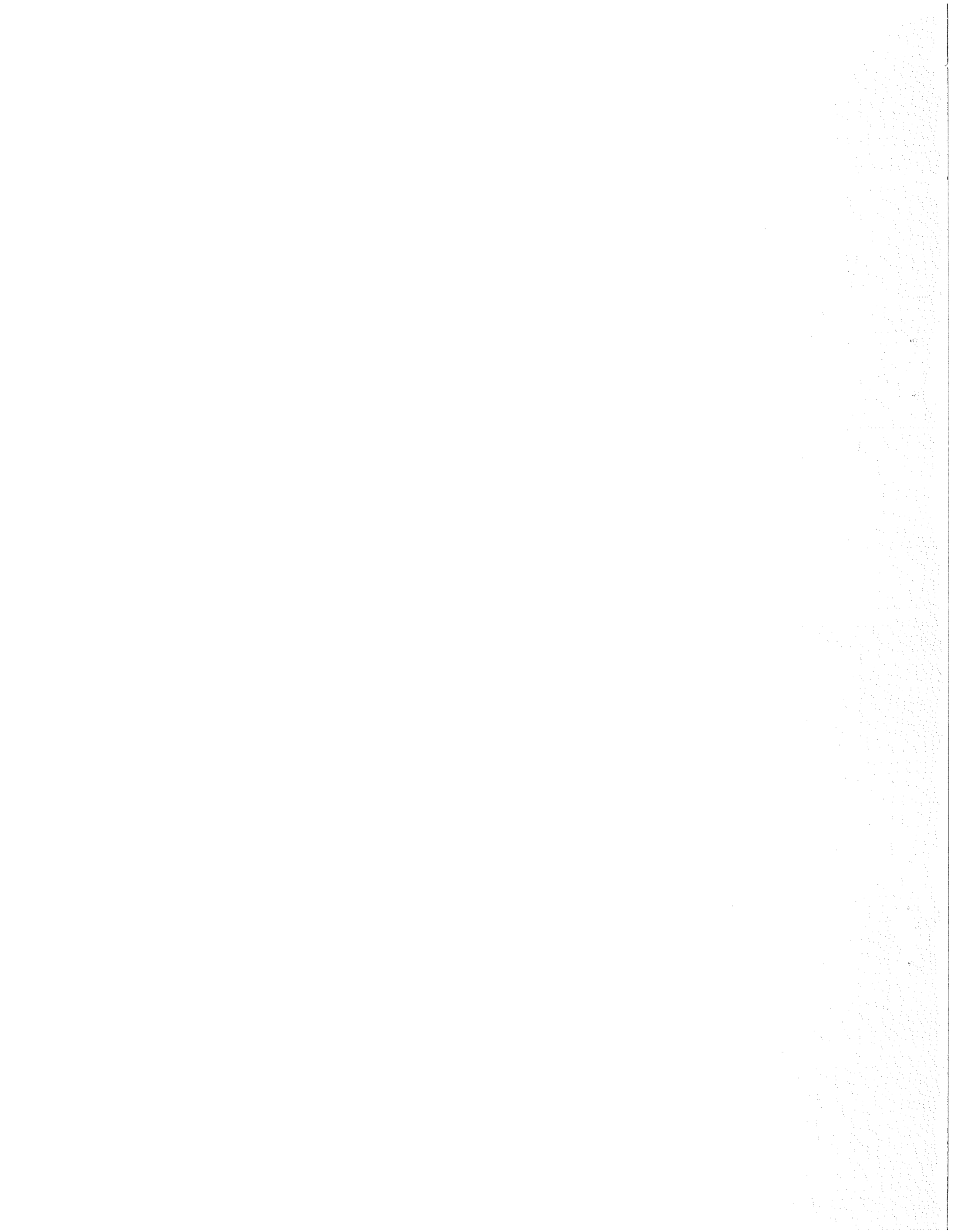
Computer Studies of Interactions of Particles
with Differing Masses

by

Donald Greenspan

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Abstract

In this paper a new type of modeling of physical phenomena is developed for systems of particles of differing masses. Initial value problems must be solved by means of modern, high speed digital computation. Of basic importance is a natural, self-reorganization property of any particle system so modeled. Extensive computer examples are given.



1. Introduction

Recently, new particle-type, computer-oriented models have been developed for the study of natural phenomena related to nonlinear elasticity, heat transfer, shock wave development, and laminar and turbulent fluid flows ([1]-[6]). In each case, the mass of any one particle was the same as the mass of any other particle.

In this paper we will begin the computer study of natural phenomena which result when particles of differing masses interact. We must emphasize, immediately, that this is only a beginning study, since natural phenomena based on such interactions are of exceptional complexity. To indicate the degree of complexity involved, consider, for example, living cell metabolism [7] and geophysical tectonics [8]. In both areas the basic mechanics are, typically, not understood at all. In modeling metabolism, biologists emphasize an electron transfer mechanism, while physical chemists deny any transfer of electrons and emphasize the variation of potentials [9]. In the geophysical area, depending on which experimental results are assumed initially, various accepted models imply, in contradiction, that the core of the earth is solid, or liquid, or iron, or silicate [8].

Now, typically, the modeling of the interaction of particles of differing masses has been implemented by the introduction of a non-homogeneous point continuum whose dynamical behavior is governed by some gross physical law, like a conservation principle. In this way, the sophisticated methods of the calculus and of more advanced forms of mathematical analysis have been found to be useful, especially for

linearized models. However, in replacing the original finite particle set, no matter how large it may have been, by an infinite set of points, one sacrifices the rich physics that exists between atoms and molecules. In this paper, our aim is to maintain the underlying classical particle physics in our modeling and to preserve the highly nonlinear effects. At present, this can only be done by considering a particle to be an aggregate, or clump, of molecules; by restricting ourselves to relatively small sets of particles; and by using modern digital computers to solve dynamical problems. Molecular aggregates are used commonly in modeling, as, for example, in the meteorologists' division of the atmosphere into large parcels of air, each of which is then treated as an atmospheric unit. Analogous ideas were suggested by Schlichting [10] for the study of vortices in viscous fluid flow. In addition, because of the relatively small numbers of particles to be considered, the classical molecular force parameters will have to be rescaled appropriately, in a spirit similar to that recommended by von Neumann [11].

2. Basic Definitions and Formulas

For positive time step Δt , let $t_k = k\Delta t$, $k = 0, 1, 2, \dots$. For $i = 1, 2, \dots, N$, let particle P_i have mass m_i and at time t_k let P_i be located at $\vec{r}_{i,k} = (x_{i,k}, y_{i,k})$, have velocity $\vec{v}_{i,k} = (v_{i,k,x}, v_{i,k,y})$, and have acceleration $\vec{a}_{i,k} = (a_{i,k,x}, a_{i,k,y})$. Let position, velocity and acceleration be related by the "leap-frog" formulas ([1]), p. 107):

$$(2.1) \quad \vec{v}_{i, \frac{1}{2}} = \vec{v}_{i,0} + \frac{\Delta t}{2} \vec{a}_{i,0}$$

$$(2.2) \quad \vec{v}_{i, k+\frac{1}{2}} = \vec{v}_{i, k-\frac{1}{2}} + (\Delta t) \vec{a}_{i,k}, \quad k = 1, 2, \dots$$

$$(2.3) \quad \vec{r}_{i, k+1} = \vec{r}_{i,k} + (\Delta t) \vec{v}_{i, k+\frac{1}{2}}, \quad k = 0, 1, 2, \dots$$

If $\vec{F}_{i,k}$ is the force acting on P_i at time t_k , where $\vec{F}_{i,k} = (F_{i,k,x}, F_{i,k,y})$, then we assume that force and acceleration are related by

$$(2.4) \quad \vec{F}_{i,k} = m_i \vec{a}_{i,k}$$

Once an exact structure is given to $\vec{F}_{i,k}$, the motion of each particle will be determined recursively and explicitly by (2.1)-(2.4) from prescribed initial data. The special structure to be used is described as follows.

At time t_k , let $r_{ij,k}$ be the distance between P_i and P_j . Let G (coefficient of attraction), H (coefficient of repulsion),

β (exponent of attraction) and α (exponent of repulsion) be determined by P_i and P_j subject to the constraints $G \geq 0, H \geq 0, \alpha \geq \beta \geq 2$ (see [9]). Then the force $(F_{i,k,x}, F_{i,k,y})$ exerted on P_i by P_j is given by

$$(2.5) \quad F_{i,k,x} = \left[\frac{-G m_i m_j}{r_{ij,k}^\beta} + \frac{H m_i m_j}{r_{ij,k}^\alpha} \right] \frac{x_{i,k} - x_{j,k}}{r_{ij,k}}$$

$$(2.6) \quad F_{i,k,y} = \left[\frac{-G m_i m_j}{r_{ij,k}^\beta} + \frac{H m_i m_j}{r_{ij,k}^\alpha} \right] \frac{y_{i,k} - y_{j,k}}{r_{ij,k}}$$

The total force $(F_{i,k,x}, F_{i,k,y})$ on P_i due to all the other $N-1$ particles is given by

$$(2.7) \quad F_{i,k,x} = \sum_{\substack{j=1 \\ j \neq i}}^N \bar{F}_{i,k,x}; \quad F_{i,k,y} = \sum_{\substack{j=1 \\ j \neq i}}^N \bar{F}_{i,k,y}$$

The formulation (2.1)-(2.7) is explicit and economical, though nonconservative. Conservation of energy and momenta can be achieved [1], but only through an implicit, less economical approach.

Throughout, the time step will be $\Delta t = 10^{-4}$ and the FORTRAN program is that of Greenspan [3].

There is one final parameter which will be of interest in the calculations. In very large bodies, one would not expect two particles which are far apart to interact at all, that is, the force components (2.5) and (2.6) would be negligible in all but local interactions. This will be incorporated into the computations, with extensive economic savings, in the following way. For a preassigned, positive parameter D , set $\bar{F}_{i,k,x} = \bar{F}_{i,k,y} = 0$ whenever $r_{ij,k} > D$. First, let $\delta=10$, $\alpha=6$, $\beta=4$, $G=H=5$. All particles were allowed to interact with all other particles by setting $D=100$. The masses $m_i=10000$ were assigned at random to seven particles, only, while all other particles were assigned masses $m_i=1000$. The seven heavy particles were $P_{10}, P_{22}, P_{23}, P_{43}, P_{48}, P_{58}$, and P_{69} . Figure 2 shows the motion of the system at t_{1000} . In this exceptionally short period of time, the heavier particles, represented by the larger circles, have relocated centrally, which is shown in detail at every hundred time steps in Figure 3, while the lighter particles have moved outward. During the rearrangement, several of the lighter particles have attained escape velocities and have left the system. Such particles will be called exploding particles and, after having left the system, they have been plotted on the outer border of the graph in Figure 2 in order to indicate their distant presence and the direction of their escape.

Changing only the pair α, β in the above example to $\alpha=5, \beta=3$ and $\alpha=4, \beta=2$, and then repeating the calculations showed that a decrease in α and β , simultaneously, resulted in a slower central accumulation of the heavier particles and an increase in the number of exploding

3. Examples.

Computer examples have been run on the UNIVAC 1110 for the parameter choices $N=7, 11, 18, 19, 38, 62$, and 85 , but since interest in relatively large sets is usual, the discussion will be restricted only to the case $N=85$. In all examples, the initial particle positions will be those shown in Figure 1, and listed precisely in Table 1. These positions have been selected so that the force between any pair of particles is zero when the distance between the pair is unity. The entire configuration will then be set into counterclockwise rotation as follows. In terms of the angular velocity parameter δ , let

$$(3.1) \quad v_{i,0,x} = \pm |y_{i,0\delta}|, \quad v_{i,0,y} = \pm |x_{i,0\delta}|,$$

where the choice of signs in (3.1) is determined by the following rule:

- $(x_{i,0}, y_{i,0}) \in \text{Quadrant I} \Rightarrow v_{i,0,x} \leq 0, v_{i,0,y} \geq 0$
- $(x_{i,0}, y_{i,0}) \in \text{Quadrant II} \Rightarrow v_{i,0,x} \leq 0, v_{i,0,y} \leq 0$
- $(x_{i,0}, y_{i,0}) \in \text{Quadrant III} \Rightarrow v_{i,0,x} \geq 0, v_{i,0,y} \leq 0$
- $(x_{i,0}, y_{i,0}) \in \text{Quadrant IV} \Rightarrow v_{i,0,x} \geq 0, v_{i,0,y} \geq 0$.

As will be seen later, the artificial symmetries inherent in the position and velocity choices made above will be offset by assigning mass values in a random fashion.

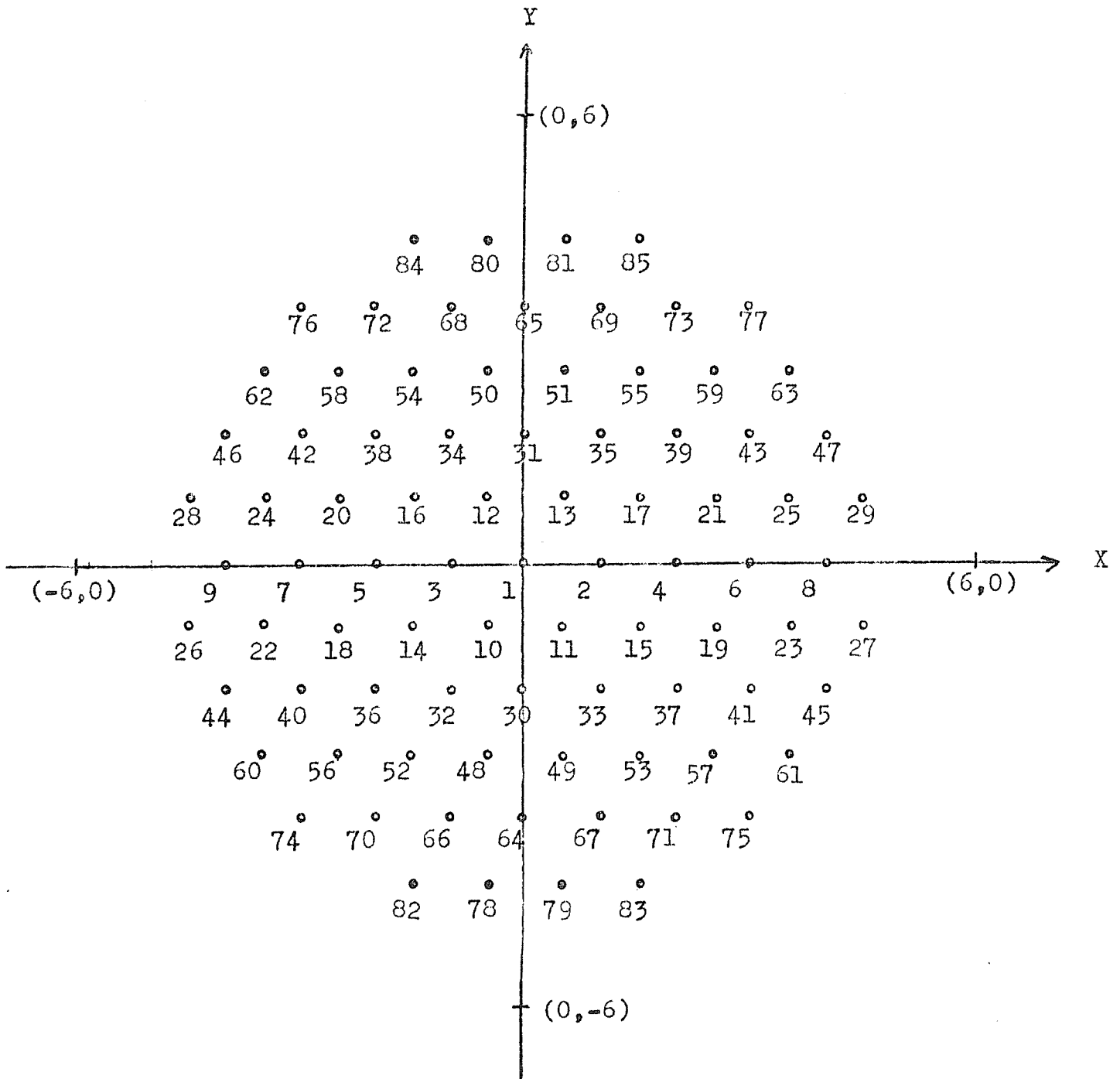


FIGURE 1

TABLE 1

P_i	$x_{i,0}$	$y_{i,0}$
P ₁	0	0
P ₂	1	0
P ₃	-1	0
P ₄	2	0
P ₅	-2	0
P ₆	3	0
P ₇	-3	0
P ₈	4	0
P ₉	-4	0
P ₁₀	-0.5	-0.87
P ₁₁	0.5	-0.87
P ₁₂	-0.5	0.87
P ₁₃	0.5	0.87
P ₁₄	-1.5	-0.87
P ₁₅	1.5	-0.87
P ₁₆	-1.5	0.87
P ₁₇	1.5	0.87
P ₁₈	-2.5	-0.87
P ₁₉	2.5	-0.87
P ₂₀	-2.5	0.87
P ₂₁	2.5	0.87
P ₂₂	-3.5	-0.87
P ₂₃	3.5	-0.87
P ₂₄	-3.5	0.87
P ₂₅	3.5	0.87
P ₂₆	-4.5	-0.87
P ₂₇	4.5	-0.87
P ₂₈	-4.5	0.87

P_i	$x_{i,0}$	$y_{i,0}$
P ₂₉	4.5	0.87
P ₃₀	0	-1.73
P ₃₁	0	1.73
P ₃₂	-1	-1.73
P ₃₃	1	-1.73
P ₃₄	-1	1.73
P ₃₅	1	1.73
P ₃₆	-2	-1.73
P ₃₇	2	-1.73
P ₃₈	-2	1.73
P ₃₉	2	1.73
P ₄₀	-3	-1.73
P ₄₁	3	-1.73
P ₄₂	-3	1.73
P ₄₃	3	1.73
P ₄₄	-4	-1.73
P ₄₅	4	-1.73
P ₄₆	-4	1.73
P ₄₇	4	1.73
P ₄₈	-0.5	-2.6
P ₄₉	0.5	-2.6
P ₅₀	-0.5	2.6
P ₅₁	0.5	2.6
P ₅₂	-1.5	-2.6
P ₅₃	1.5	-2.6
P ₅₄	-1.5	2.6
P ₅₅	1.5	2.6
P ₅₆	-2.5	-2.6
P ₅₇	2.5	-2.6

P_i	$x_{i,0}$	$y_{i,0}$
P ₅₈	-2.5	2.6
P ₅₉	2.5	2.6
P ₆₀	-3.5	-2.6
P ₆₁	3.5	-2.6
P ₆₂	-3.5	2.6
P ₆₃	3.5	2.6
P ₆₄	0	-3.46
P ₆₅	0	3.46
P ₆₆	-1	-3.46
P ₆₇	1	-3.46
P ₆₈	-1	3.46
P ₆₉	1	3.46
P ₇₀	-2	-3.46
P ₇₁	2	-3.46
P ₇₂	-2	3.46
P ₇₃	2	3.46
P ₇₄	-3	-3.46
P ₇₅	3	-3.46
P ₇₆	-3	3.46
P ₇₇	3	3.46
P ₇₈	-0.5	-4.33
P ₇₉	0.5	-4.33
P ₈₀	-0.5	4.33
P ₈₁	0.5	4.33
P ₈₂	-1.5	-4.33
P ₈₃	1.5	-4.33
P ₈₄	-1.5	4.33
P ₈₅	1.5	4.33

particles.

In all three of the above cases, the collapse effect of the heavy particles could be slowed to an arbitrary rate, and even avoided, by decreasing D , and, to a lesser extent, by decreasing H and G . Consider, for example, the case $\delta=10$, $\alpha=6$, $\beta=4$, $G=H=5$, and $D=\sqrt{5}$. The particles P_{10} , P_{22} , P_{23} , P_{43} , P_{48} , P_{58} and P_{69} were assigned mass $m_i=10000$ and all other particles were assigned mass $m_i=1000$. Figure 4 shows the resulting configuration after 12000 time steps.

The heavy particles, represented by triangles, are shown to have organized into three separate, bonded units, in the second, third, and fourth quadrants, near the points $(-17,5)$, $(-4,-30)$ and $(17,-7)$. Each such unit has a heavy core surrounded by a ring of lighter particles. Lighter particles are also scattered thinly throughout XY space and, again, exploding particles have been plotted on the boundary of the graph.

Interestingly enough, some of the exploding particles are escaping as coupled subunits. The dynamical behavior in this example is suggestive of the evolution of gas and liquid subunits from a parent, hot fluid, and similar results were obtained for the parameter choice $D=3$ in place of $D=5$, and also for $H=G=1$ in place of $H=G=5$ with $D=5$.

In the next examples, we will try to limit the number of particles which explode and try to have the particles stratify themselves according to mass. Let us fix $\alpha=6$, $\beta=4$ and $G=H=5$. Preliminary investigations, using the mass system considered thus far, and for the fifteen cases resulting from all combinations of $\delta=7.5, 5, 2.5$ and $D=\sqrt{3}, \sqrt{5}, 3, 4, 5$, yielded a modicum of exploding particles only in the case $\delta=2.5, D=5$,

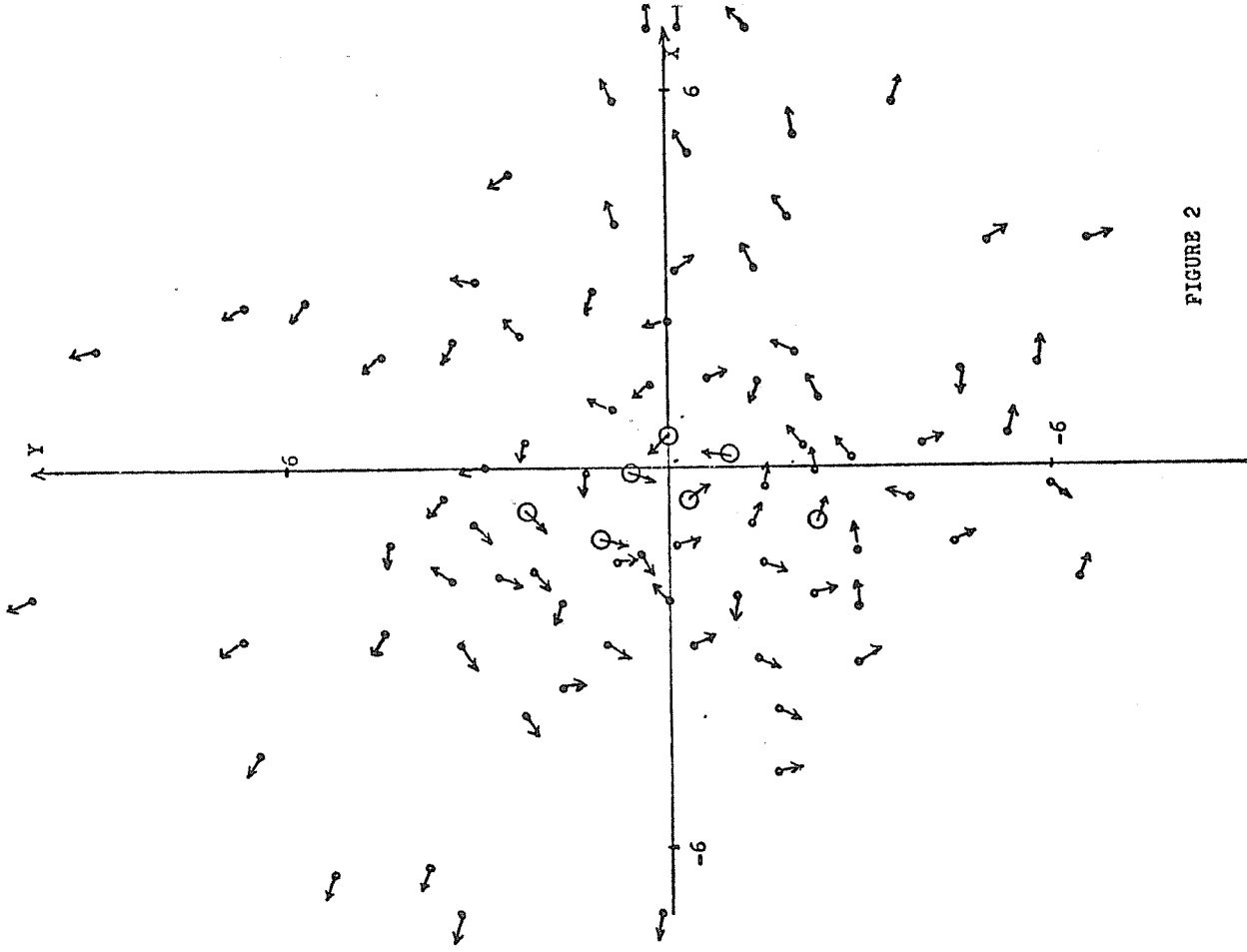


FIGURE 2

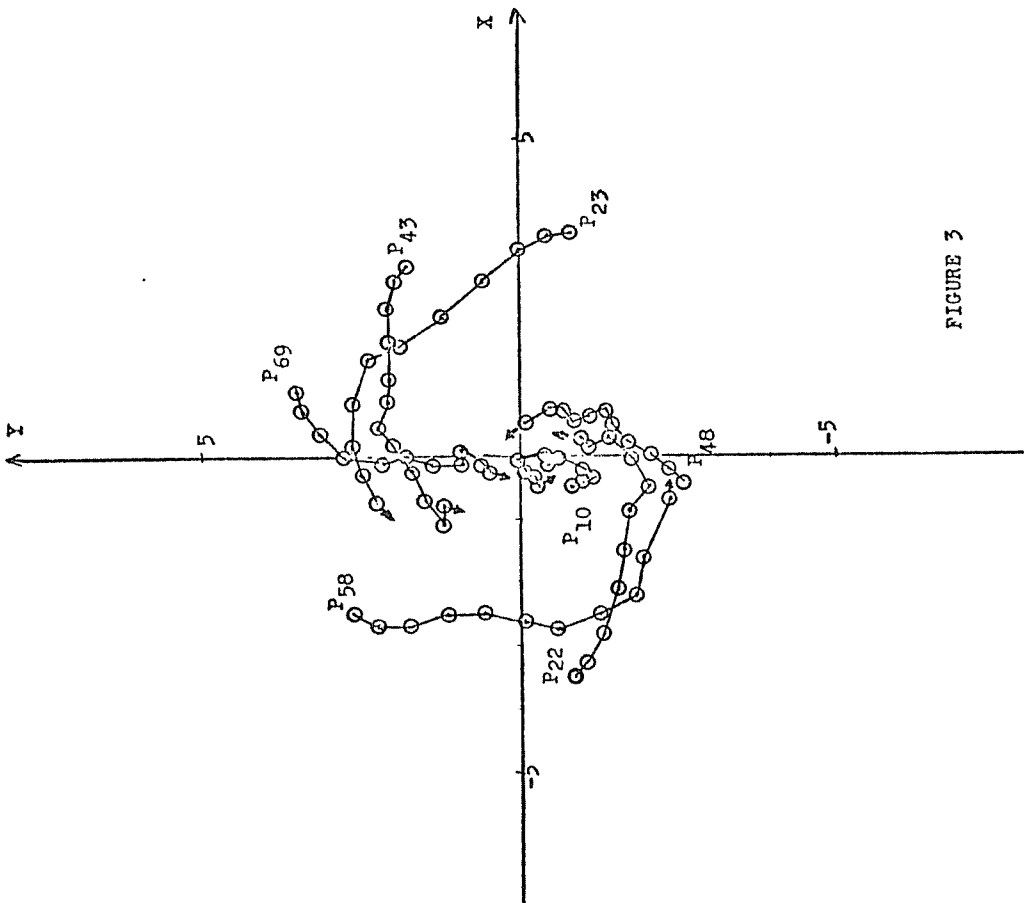


FIGURE 3

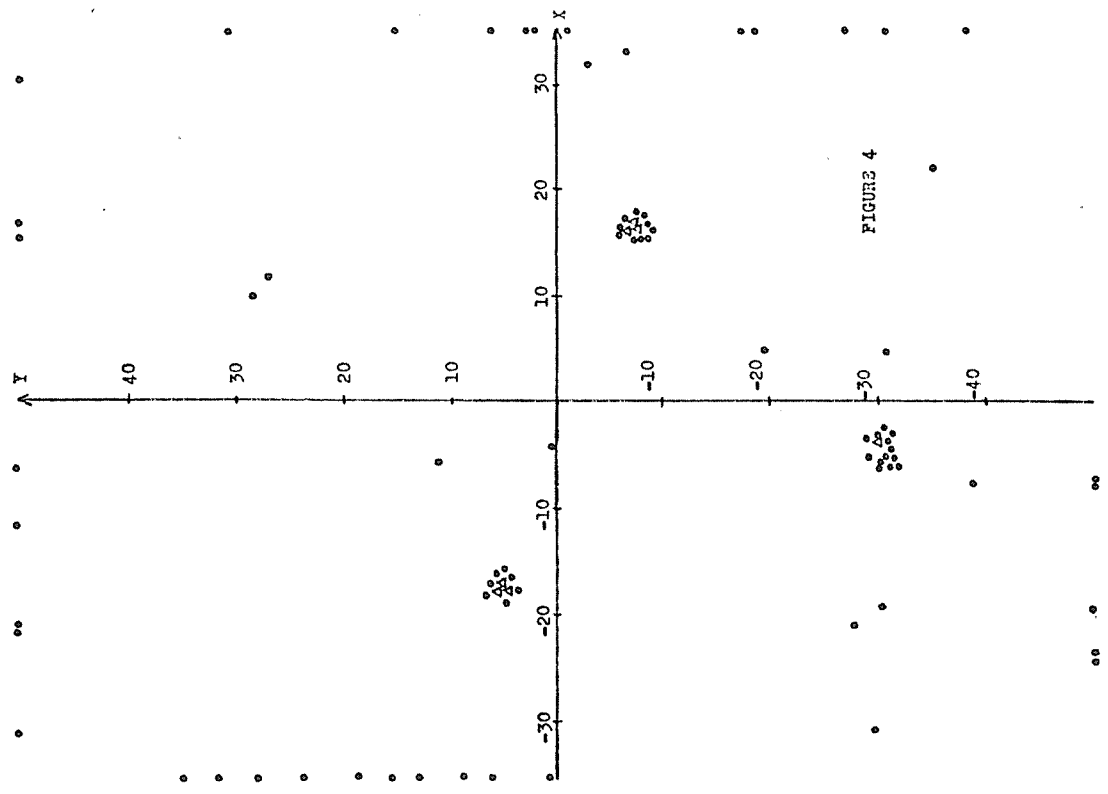


FIGURE 4

so these parameter choices will also be fixed. Next, consider resetting the particle masses. Throughout, we will keep $m_i=10000$ for P_{10} , P_{22} , P_{23} , P_{43} , P_{48} , P_{58} and P_{69} , and reset the masses of the other particles. First assign masses $m_i=8000$ to thirteen of the remaining particles, at random, and let the rest have masses 1000. Within one thousand time steps, then, all but one of the particles with mass 1000 had exploded while the rest were relatively stably organized. This happened also when the subset of thirteen particles were assigned masses of 6000 and then of 4000, so that the minimum mass had to be chosen greater than 1000. Next, in addition to the seven particles of masses 10000, masses $m_i=8000$ were assigned at random to thirteen particles, masses $m_i=6000$ assigned at random to seventeen particles, masses $m_i=4000$ assigned at random to thirty particles, and the remaining particles were assigned masses $m_i=2000$. After ten thousand time steps, most of the particles with mass $m_i=2000$ had exploded while the self-stratification of the remaining particles was proceeding at a very slow rate. In order to accentuate the process, then, the mass distribution was finally reset as follows. In addition to the seven particles of mass 10000, the mass $m_i=7000$ was assigned at random to thirty particles and all remaining particles were assigned the masses $m_i=4000$. This configuration is shown in Figure 5, where the particles of mass 10000 are represented by the largest circles, the particles of mass 7000 are represented by darkened circles, and the particles of mass 4000 are represented by small circles. The interaction was studied over 85000 time steps. Figure 6 shows the state of the system after 5000 time steps. The largest particles are beginning to relocate centrally.

In anticipation of later computations, Figure 7 shows, by triangular enclosures, those particles at time t_{5000} which, eventually, will escape. Figure 8 gives the velocity field at this time and reveals that molecular-type interactions have become prevalent with the inward movement of the largest particles. Nevertheless, the gross motion of the particles is still counterclockwise, as is shown in the velocity field of Figure 9, where the particles gross velocities, defined by

$$\vec{v}_{i,5000}^* = \frac{\vec{r}_{i,7000} - \vec{r}_{i,5000}}{0.2}$$

have been graphed. Particles whose motion is not counterclockwise, as in the upper left hand section of Quadrant II of Figure 9, can be related to the explosion of nearby particles, as can be observed by comparison with the same region in Figure 7. Figure 10 shows, at time t_{10000} , the central relocation of the largest particles and the formation of a band of the smallest particles around the configuration. Two of the smallest particles have escaped. Figures 11 and 12 show the continued development at the respective times t_{30000} and t_{70000} . Throughout, the stratification in terms of density is clear. Of course, it need not be entirely spherical because of the highly fluid nature of the system.

Finally, let us try to introduce a solidification process. For this purpose, we eliminate the fifteen escaped particles at t_{70000} and consider only the remaining seventy particles, whose masses, positions, and velocities are given, for convenience, in Table 2.

For simplicity, we will model loss of heat by radiation as follows. At each time t_k , let the center of mass be (x_k, y_k) . Any particle P_i whose distance to (x_k, y_k) at t_k is greater than two units will be called an outer particle. We will allow only outer particles to radiate heat, which will be implemented by resetting the velocity of each outer particle to

$$\vec{v}_{i,k} = (\delta v_{i,k,x}, \delta v_{i,k,y}), \quad 0 \leq \delta < 1,$$

where δ is a damping parameter.

In order to analyze change of physical state after the onset of radiation, it will be convenient to have the concept of temperature. The molecular temperature $T_{i,k}^*$ of P_i at t_k is defined by

$$T_{i,k}^* = \frac{1}{2} m v_k^2.$$

The normalized molecular temperature $T'_{i,k}$ of P_i at t_k is defined by

$$T'_{i,k} = T_{i,k}^* / 1000.$$

The temperature $T_{i,k}$ of P_i at t_k , which is a measured quantity, thus requiring a positive time period, is defined after t_{70000} by [1,p 78]:

$$T_{i,70000+k} = \frac{1}{k} \sum_{r=1}^k T'_{i,70000+r}, \quad k = 1, 2, \dots$$

In order to determine from its temperature whether a particle is solid or fluid, the following simplistic rule of thumb was used. Throughout the calculations, it was observed that, in general, particles of masses 10000, 7000, and 4000 would not bond with particles of the same mass when their speeds were greater than about 25, 21 and 16,

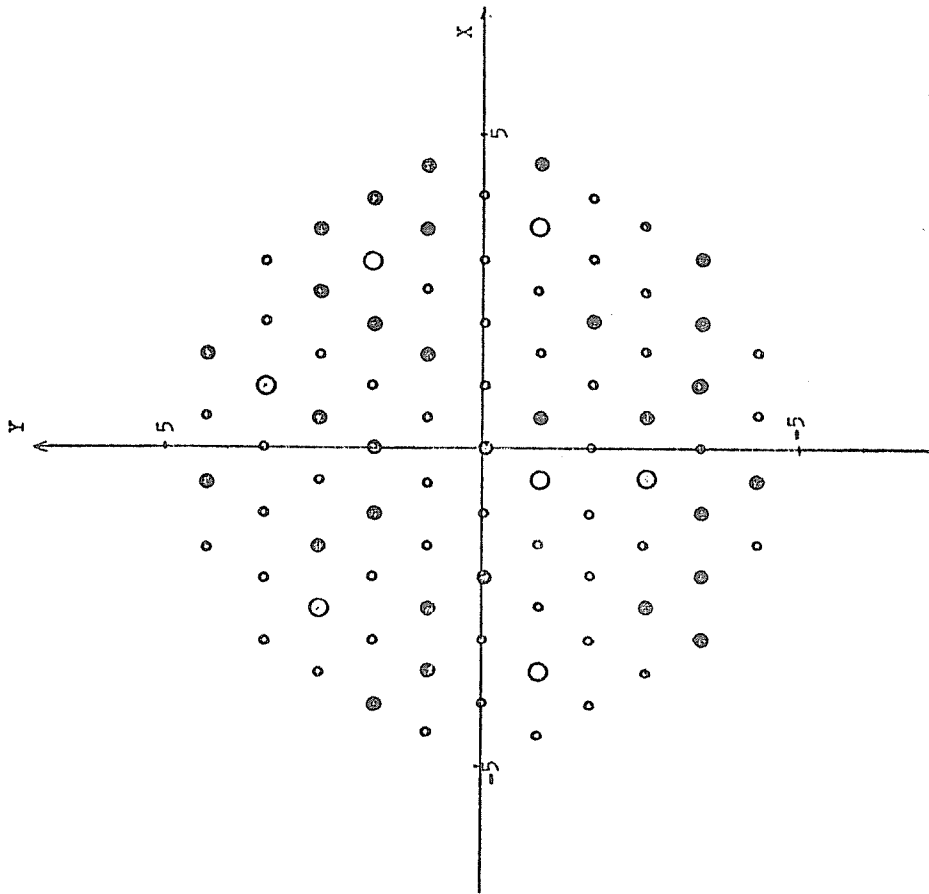


FIGURE 5

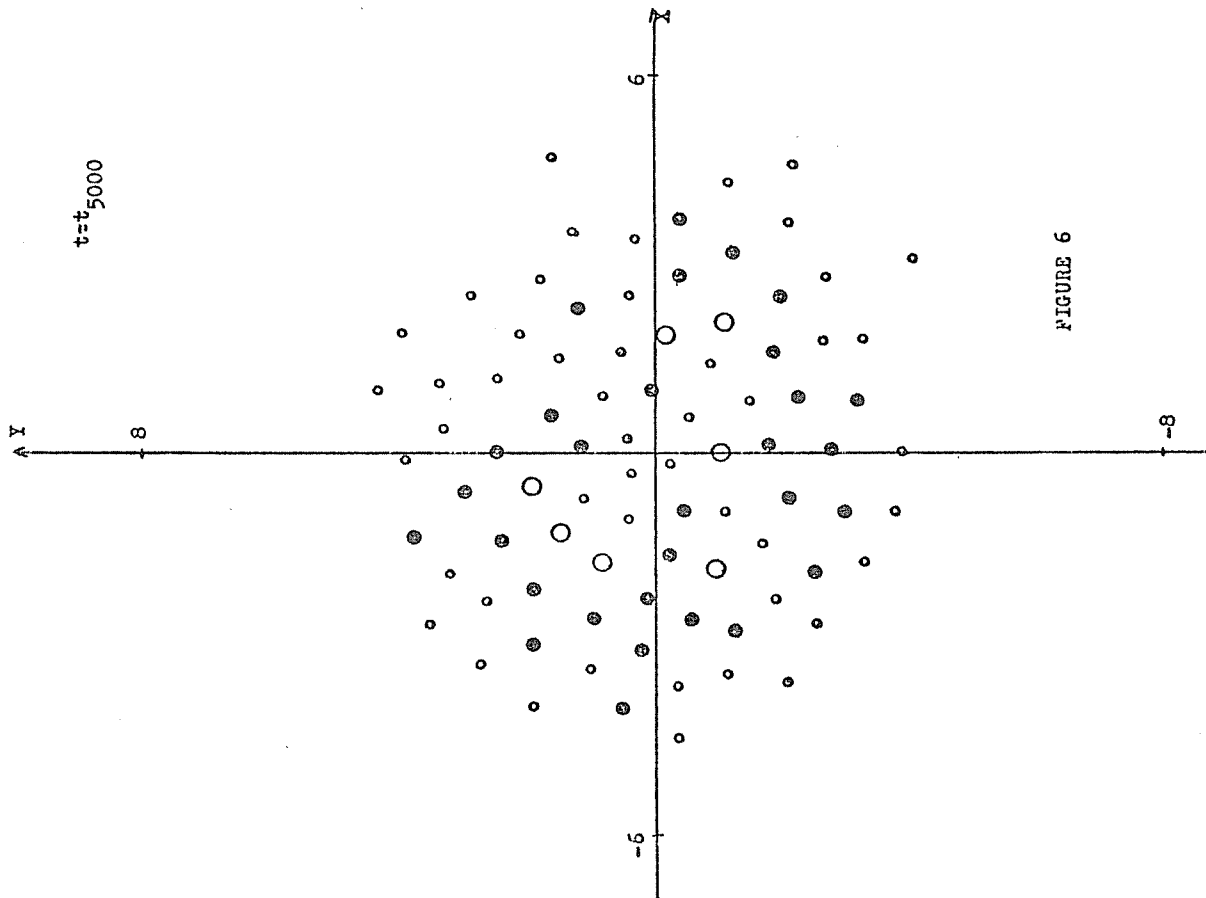


FIGURE 6

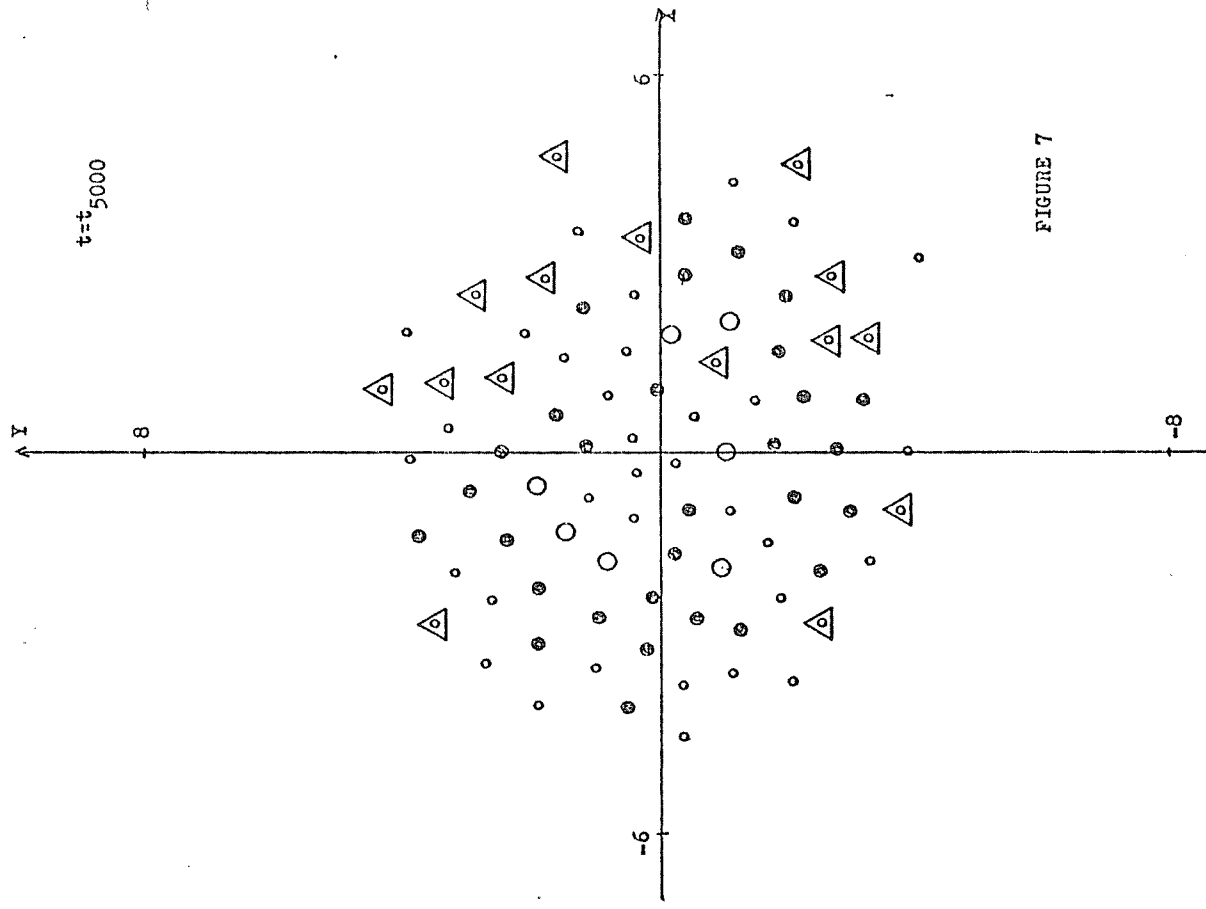


FIGURE 7

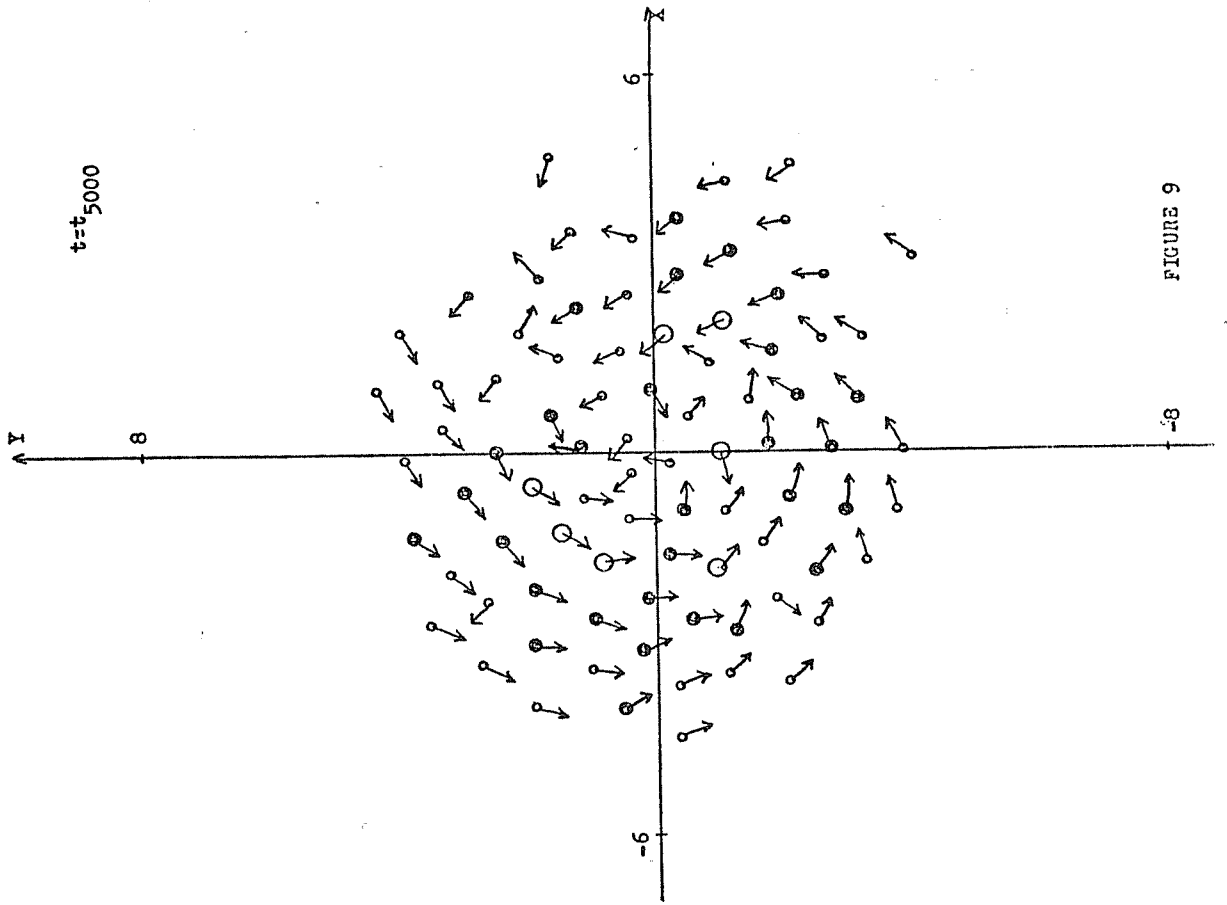


FIGURE 9

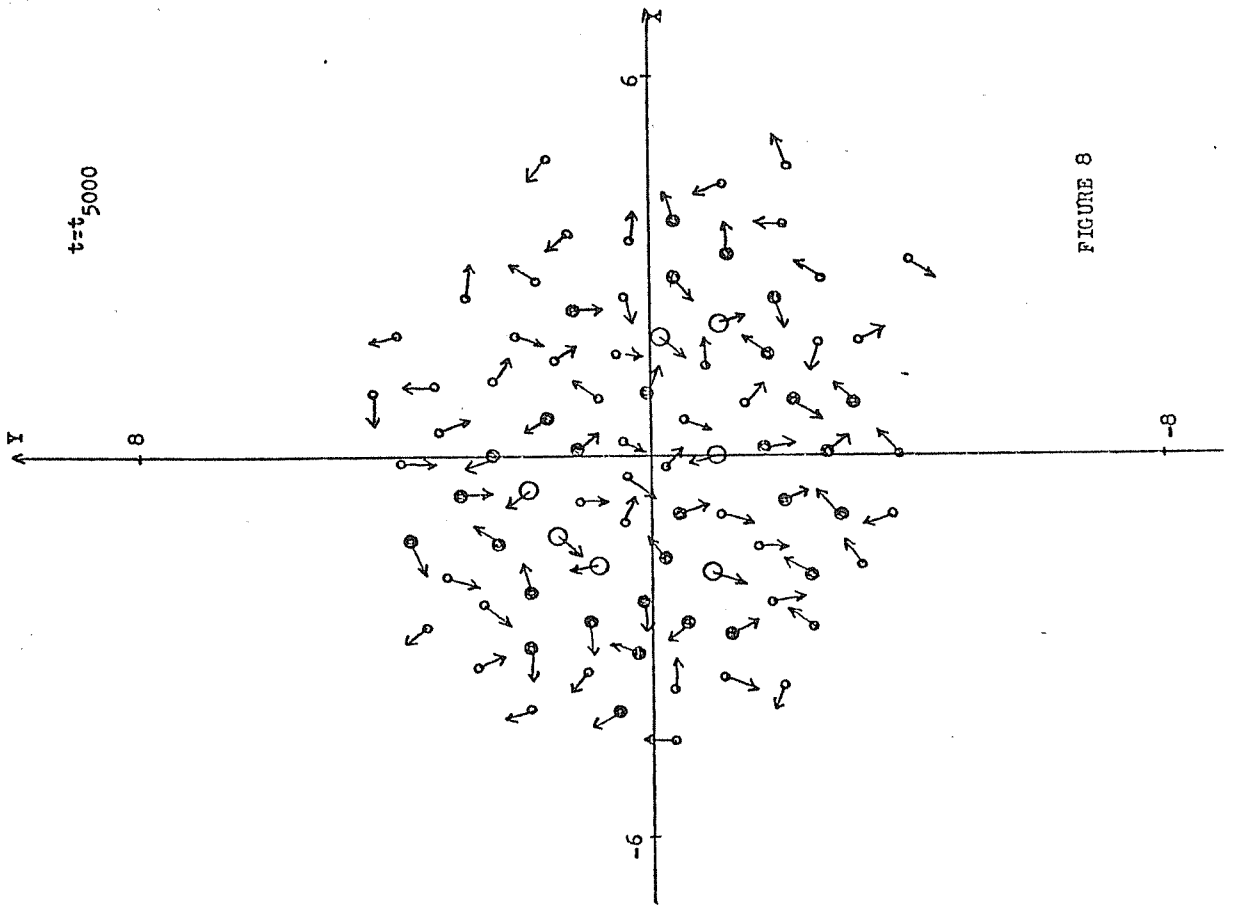


FIGURE 8

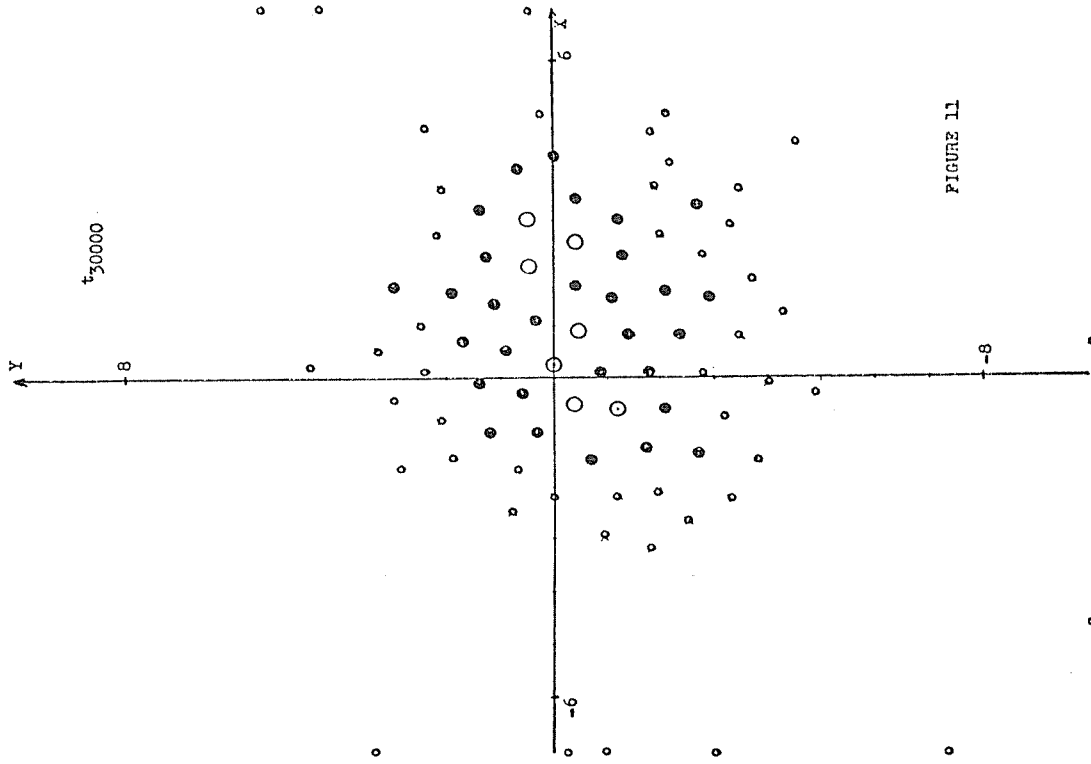


FIGURE 11

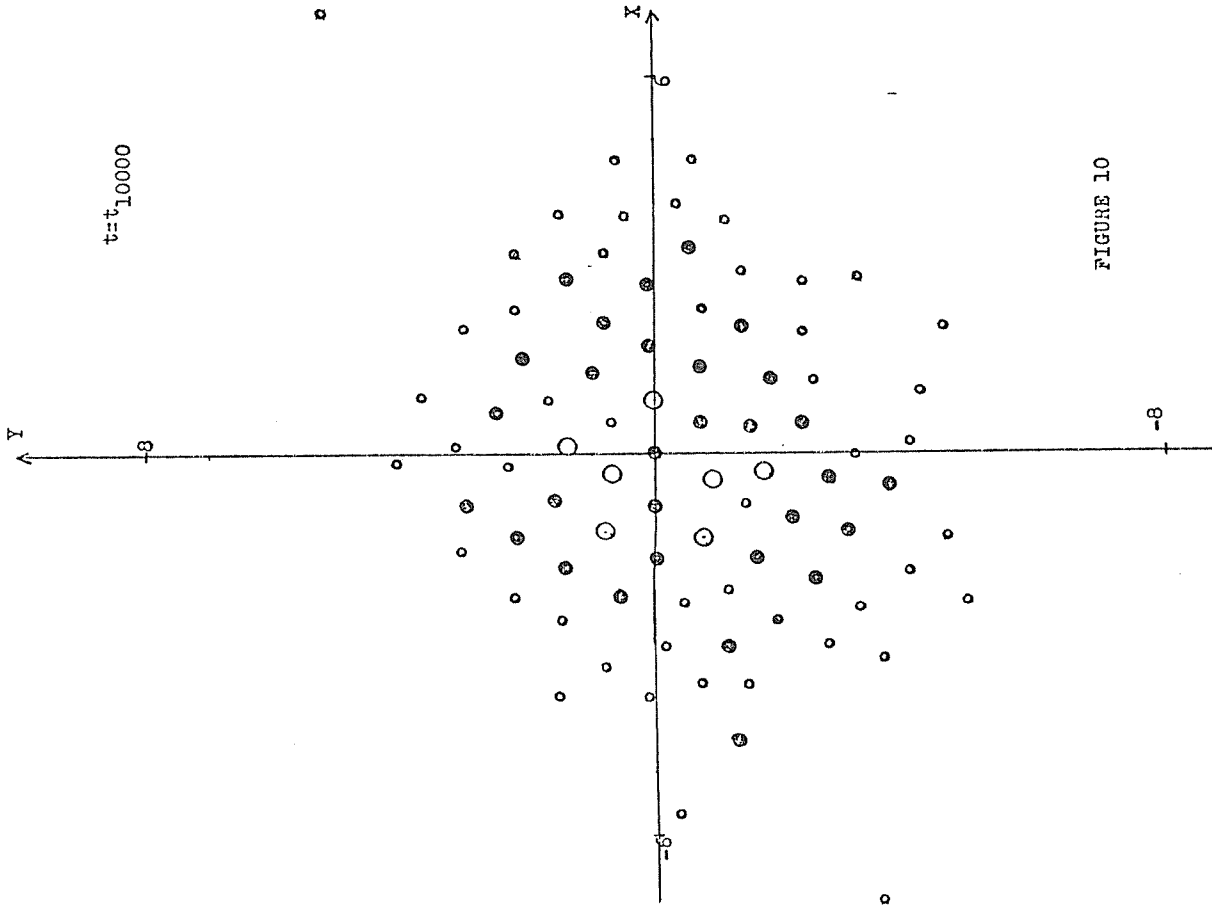


FIGURE 10

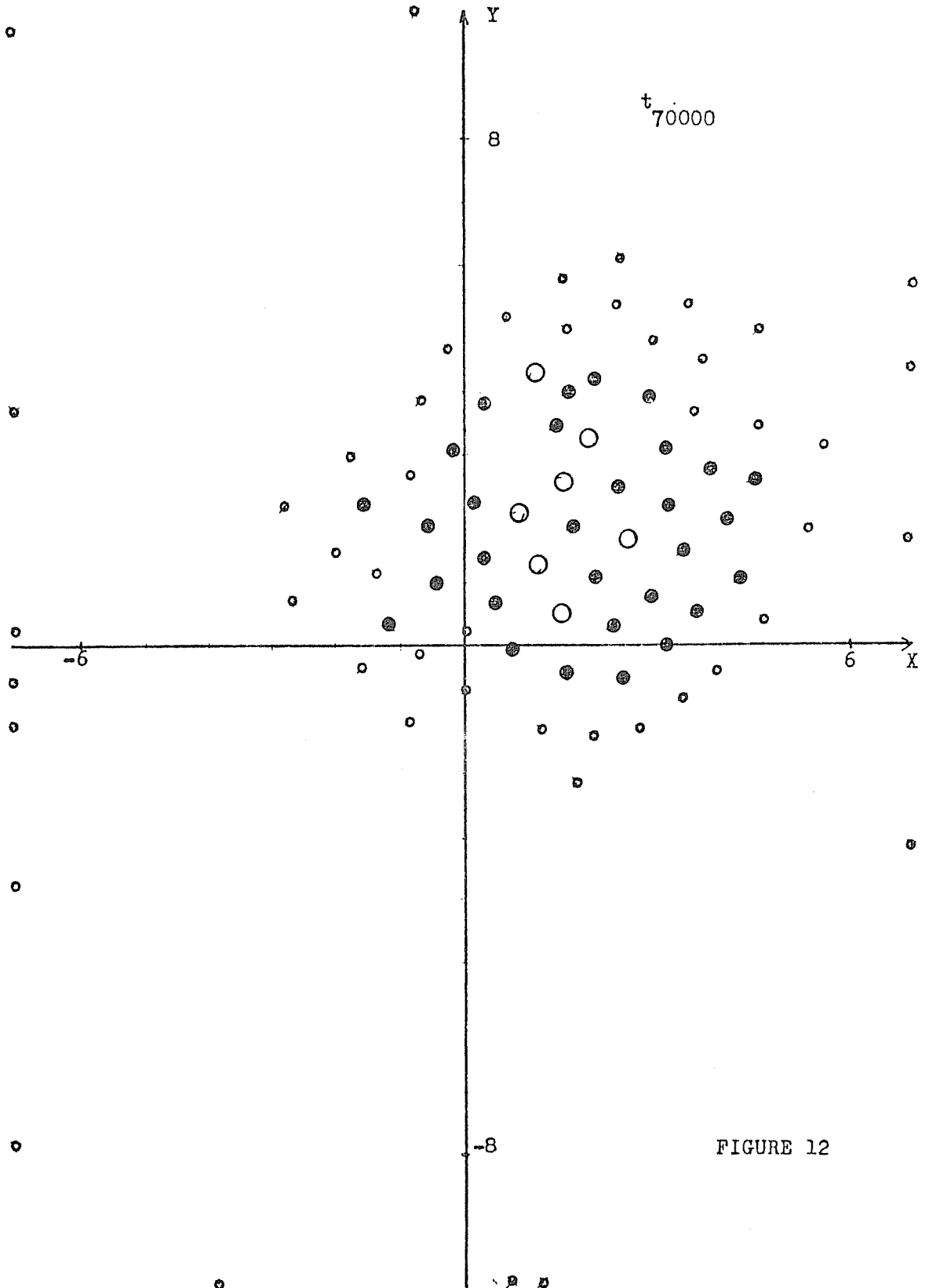


FIGURE 12

TABLE 2

m	x	y	v _x	v _y
10000.00000	1.56030	2.79100	-48.54180	-11.74170
10000.00000	2.53430	1.67580	-39.33610	47.14220
10000.00000	1.13120	1.27290	-29.74250	2.54730
10000.00000	.93500	2.13320	9.55340	6.56470
10000.00000	1.46150	.42230	87.60250	-24.21680
10000.00000	2.18460	3.37400	20.70670	9.13660
10000.00000	1.10030	4.52040	-21.75620	16.74070
7000.00000	.59720	3.73040	23.20220	31.14740
7000.00000	2.32530	-.72770	-8.43120	-4.27770
7000.00000	2.83890	.84570	15.11520	9.87560
7000.00000	3.10220	2.26650	-20.37360	-1.79940
7000.00000	-.12470	3.20130	28.85020	-1.86350
7000.00000	.83480	3.03380	48.01350	-59.98630
7000.00000	2.36410	.24880	-6.58200	-32.59970
7000.00000	4.29840	1.38940	-12.16270	-51.65620
7000.00000	3.91840	3.00010	4.98840	22.26540
7000.00000	.15480	2.43340	-49.29330	-22.18740
7000.00000	3.93700	2.11820	14.11930	37.02920
7000.00000	3.18760	.00510	68.57520	-29.86810
7000.00000	2.98830	3.13420	-43.62630	-16.04270
7000.00000	.50600	.58650	-11.71100	71.38840
7000.00000	2.76630	4.03640	1.03910	13.46670
7000.00000	2.00980	4.47150	33.57680	7.74930
7000.00000	2.37970	2.54050	-42.66930	22.00120
7000.00000	1.54570	-.34850	-33.98820	-4.89870
7000.00000	2.02210	1.08230	15.64410	4.10260
7000.00000	.71220	-.25190	6.22250	-26.23950
7000.00000	.35380	1.56540	-5.60650	27.93330
7000.00000	-1.59330	.40150	-7.26170	21.22850
7000.00000	3.84170	.68650	-42.75540	-6.33050
7000.00000	-1.52570	1.64030	-3.79490	11.92660
7000.00000	-.22500	.90510	-14.00210	6.25230
7000.00000	4.70530	2.55750	30.36750	-16.55160
7000.00000	1.42630	3.74770	8.45250	10.00980
7000.00000	3.36040	1.49100	-3.03360	-10.47180
7000.00000	-.43930	1.90390	70.49240	-76.71200
7000.00000	1.71870	1.88640	-9.53290	24.02670
4000.00000	-.10890	-1.29360	-36.25870	-13.39550
4000.00000	3.39890	-2.03840	.31140	-5.47610
4000.00000	4.28940	5.19970	-25.62660	-19.45880
4000.00000	4.30430	.00690	2.41410	44.76230
4000.00000	2.90470	4.92660	-97.66210	-18.10270
4000.00000	-.09500	-.20310	38.50530	-3.53890
4000.00000	5.32580	1.73330	-14.76920	-2.62810
4000.00000	3.49700	3.74720	-47.22760	18.79350
4000.00000	.31110	4.39270	5.39290	23.53150
4000.00000	3.62040	4.52810	-34.14450	2.13490
4000.00000	2.50260	-1.84140	71.40450	83.67520
4000.00000	-1.87570	-.52700	36.07200	-7.73050
4000.00000	-2.68480	.26490	-25.93690	70.97110
4000.00000	-1.37490	-1.05370	76.48730	5.13310
4000.00000	-1.03270	.99730	-6.29860	-43.78980
4000.00000	3.13570	5.73240	-67.94810	16.79080
4000.00000	4.98690	.86870	2.62650	41.41030
4000.00000	-1.70500	3.35870	-17.85540	28.65940
4000.00000	2.58120	6.78580	-4.10720	-38.79370
4000.00000	-1.89830	2.42390	92.37920	42.61370
4000.00000	1.44540	5.35220	24.02640	-25.49170
4000.00000	4.41710	4.03720	5.57530	22.10890
4000.00000	5.27060	3.34710	-16.47850	38.69040
4000.00000	3.59760	-1.25750	18.67890	-58.06110
4000.00000	-.93420	-.12260	56.24810	21.45010
4000.00000	1.56580	6.15380	17.77290	46.86250
4000.00000	1.62690	-1.26500	-37.93260	22.09020
4000.00000	-.67630	3.86170	15.57210	-44.37460
4000.00000	2.30530	5.62660	-17.31100	-13.16010
4000.00000	.86770	-1.03330	22.78250	-39.60600
4000.00000	-.87210	2.66760	47.28810	-102.73510
4000.00000	.60670	5.24550	-3.70840	-21.21010
4000.00000	-2.34060	1.48330	-13.37190	25.21530

respectively. Thus, particles of masses 10000, 7000 and 4000 are defined to be solid particles when their temperatures are less than 3125, 1544, and 512, respectively. Otherwise, they are defined to be fluid particles.

For $\delta=0$, Figure 13 shows the rapid formation of solid particles, shown within squares, by the time t_{70400} . Figure 14 shows this continued development at time t_{71000} , while Figure 15 shows the complete formation of a crust at the time t_{74000} . Two fluid particles lie on the crust at t_{74000} , one of the heaviest particles has solidified, and the interior fluid particles have very high temperatures. Note also that the entire configuration has contracted, as was to be expected. Completely analogous results were obtained with $\delta=.95$, but the reaction was much slower, with the first solid particle appearing at t_{77400} .

Further, more refined studies of solidification could not be undertaken at the present time due to a depletion of funds.

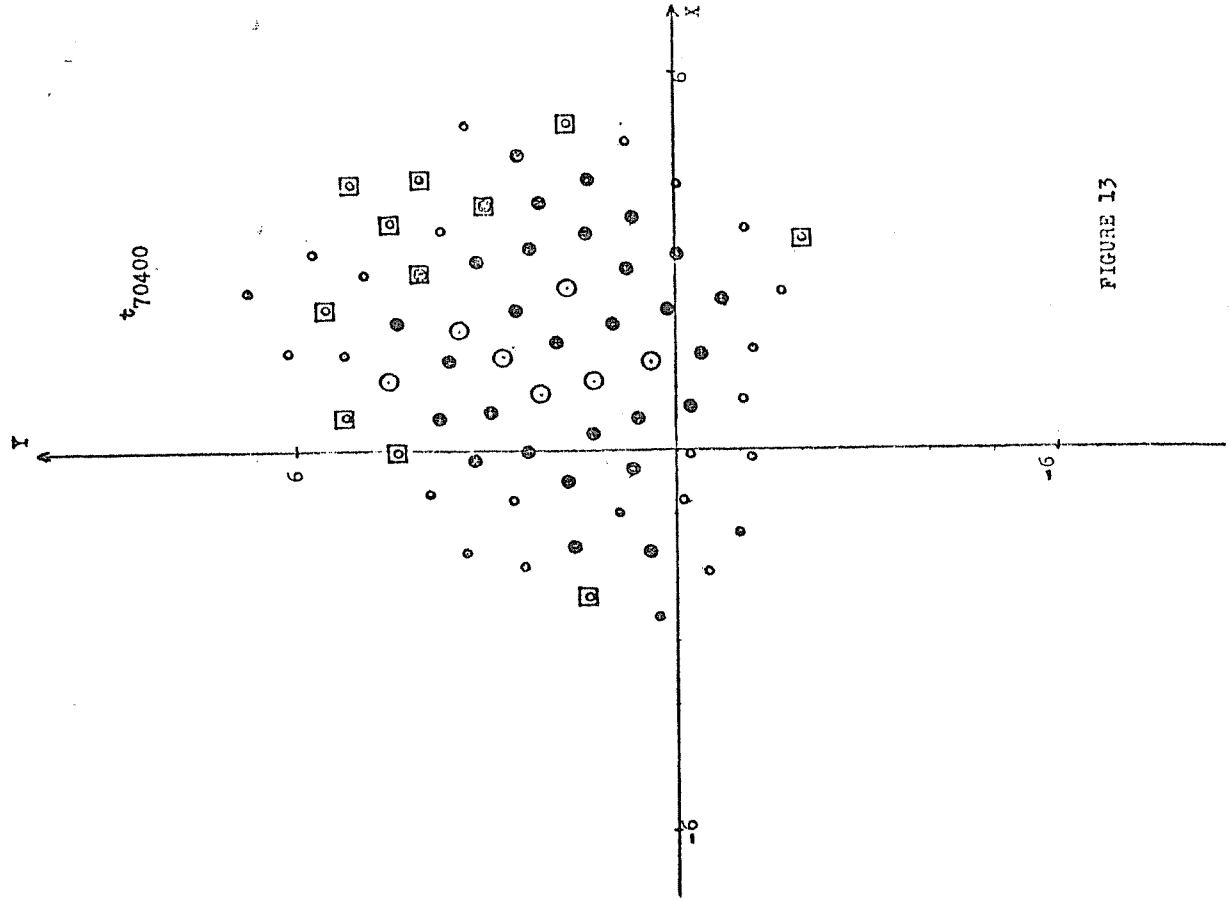


FIGURE 13

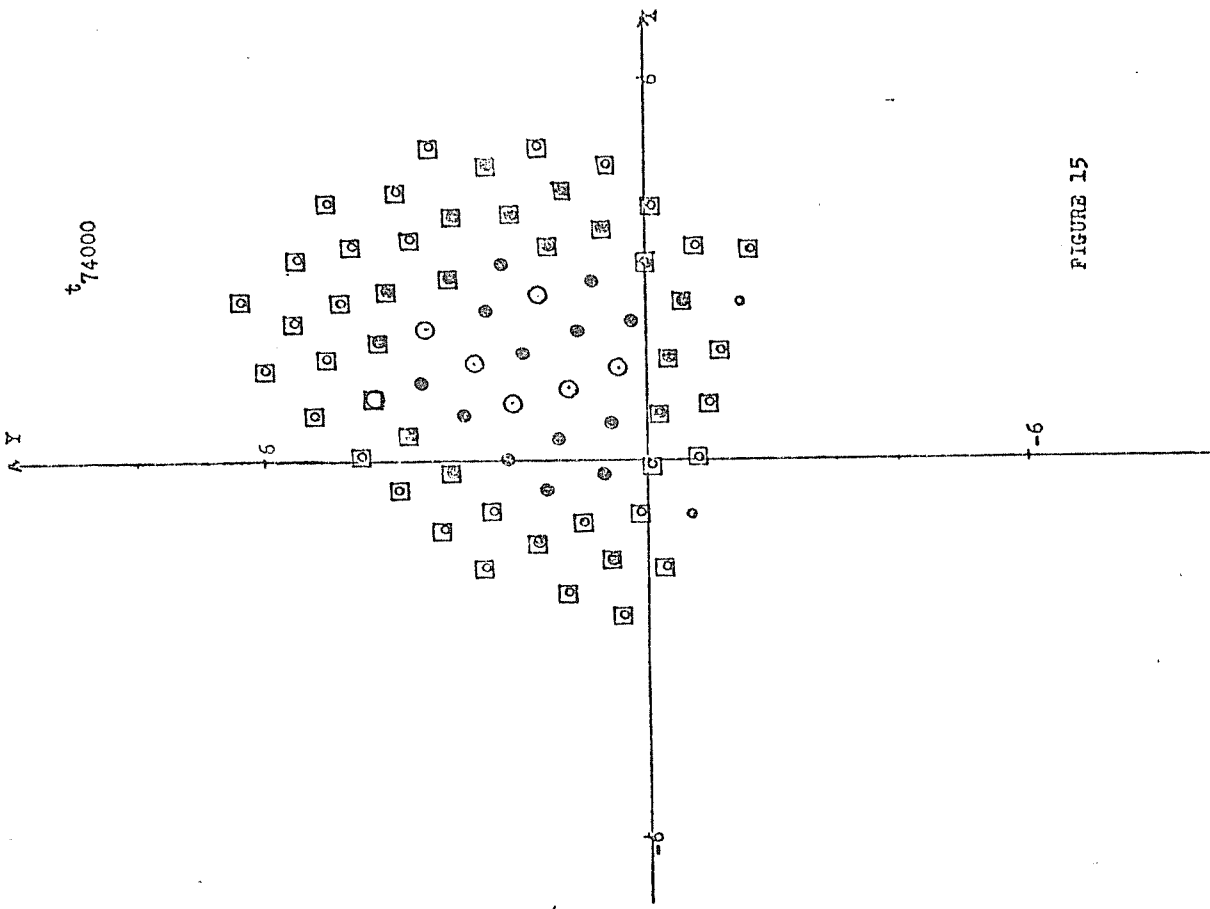


FIGURE 15

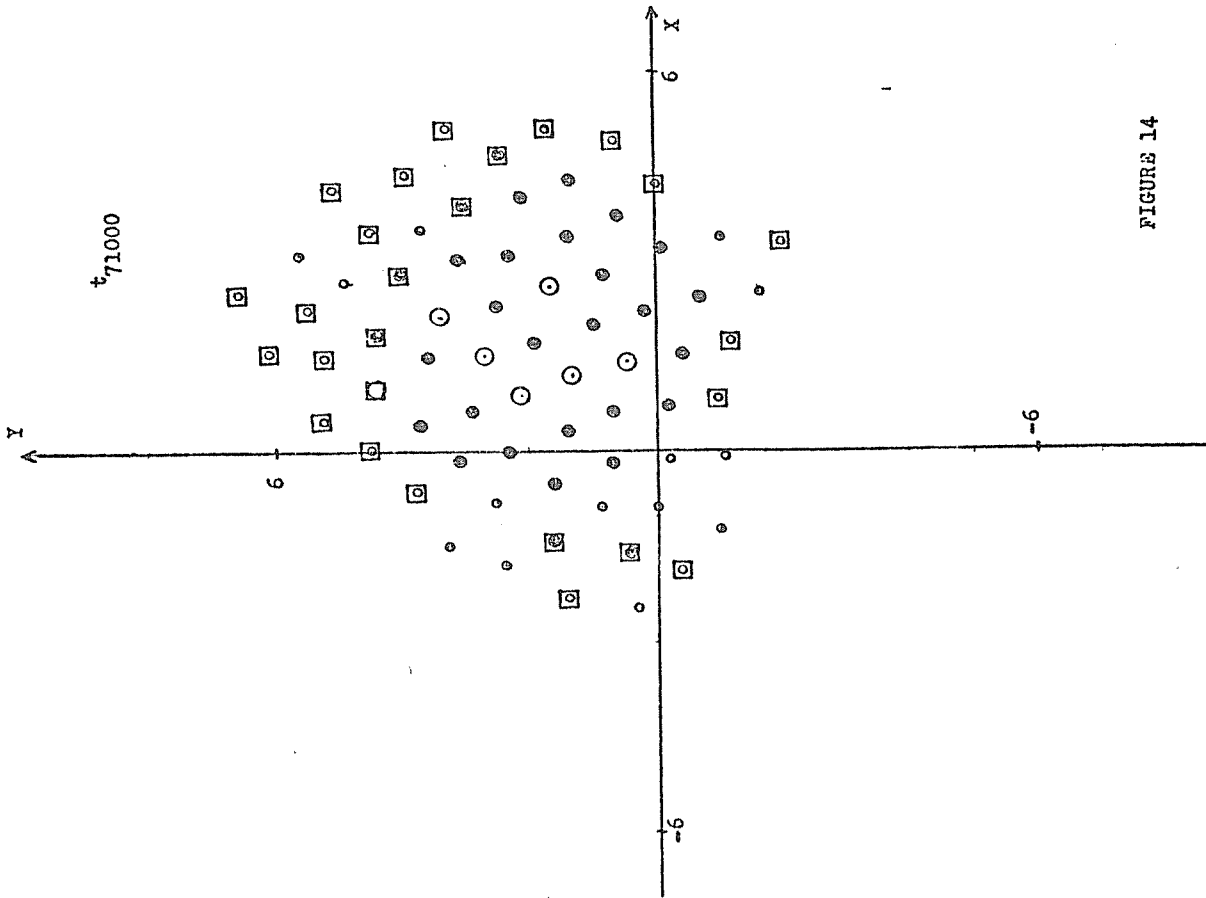


FIGURE 14

4. Concluding Remarks

We have shown in this paper how a new type of modeling, which relies heavily on high-speed computations, can yield results which are suggestive of natural phenomena involving interactions of particles of differing masses. Of basic importance is a natural, self-reorganizing property of any particle system so modeled. Extensions of the computer examples of Section 3 are now planned. For example, for the very last example, N will be increased, D decreased, a larger variation of masses will be given, δ will be made to vary in the range $-1 < \delta < 1$, and the concepts of outer particle and temperature will be refined.

In this way, it is hoped that one can develop a realistic model of the evolution of a planet.

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