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Abstract

A new particle approach for the study of solids is developed. The basic forces included are gravity and interparticle attraction and repulsion. Triangular and rectangular bodies are generated on the UNIVAC 1110 and various gross physical properties are verified.

1. INTRODUCTION

In recent years, the development of digital computer technology has led to the approximate solution of a broad spectrum of previously unsolved problems in mathematics and physics (see, e.g., [1]-[6] and the numerous additional references contained therein). In addition, new types of models, called particle models, have emerged and have proved to be viable because the resolution of their dynamical equations requires only the capability to do arithmetic at high speeds (see, e.g., [7]-[9] and the references contained therein).

In this paper we will direct attention to the construction of particle type solids which include both gravity and intermolecular type forces. Only the latter type forces had been considered previously for solids because their enormous magnitudes in the bonding process precluded the necessity to include gravity ([8], p. 75-76). However, in subsequent research, we wish to explore phenomena in which gravity is important. This is the case, for example, in the analysis of a melting solid, a changing portion of which is always liquid. It is also the case in various structural type problems and in a broad spectrum of free boundary problems.

In the present paper the emphasis will be on the computer methodology for generating particle solids of the above type. Specific physical applications using the solids so generated will be described in later papers.

2. Basic Definitions and Formulas.

For positive time step Δt, let $t_k = k\Delta t$, $k = 0,1,2,\ldots$. For $i = 1,2,\ldots,N$, 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 ([8], p. 107):

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

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

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

If $\vec{F}_{i,k}$ is the force acting an 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

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

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_{ij} (coefficient matrix of attraction), H_{ij} (coefficient matrix of repulsion), β_{ij} (exponent matrix of attraction) and α_{ij} (exponent matrix of repulsion) be determined by P_i and P_j subject to the constraints $G_{ij} \geq 0$, $H_{ij} \geq 0$, $\alpha_{ij} \geq \beta_{ij} \geq 2$ (see [10]). Then the force $(\bar{F}_{i,k,x}, \bar{F}_{i,k,y})$ exerted on P_i by P_j is given by

$$(2.5)\qquad \bar{F}_{i,k,x} = \left[\frac{-G_{ij}\, m_i\, m_j}{r_{ij,k}{}^{\beta_{ij}}} + \frac{H_{ij}\, m_i\, m_j}{r_{ij,k}{}^{\alpha_{ij}}}\right] \frac{x_{i,k} - x_{j,k}}{r_{ij,k}}$$

$$(2.6)\qquad \bar{F}_{i,k,y} = \left[\frac{-G_{ij}\, m_i\, m_j}{r_{ij,k}{}^{\beta_{ij}}} + \frac{H_{ij}\, m_i\, m_j}{r_{ij,k}{}^{\alpha_{ij}}}\right] \frac{y_{i,k} - y_{j,k}}{r_{ij,k}} \quad .$$

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

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

Finally, we include gravity into the model by

$$(2.8)\qquad F_{i,k,x} = F^*_{i,k,x} \quad ; \quad F_{i,k,y} = F^*_{i,k,y} - 32m_i .$$

The formulation (2.1)-(2.8) is explicit and economical, though nonconservative. Conservation of energy and momenta can be achieved [8], but only through an implicit, less economical approach.

3. Triangular Building Blocks

Later, a solid will be treated as a cohesive set of particles $P_1, P_2, \ldots, P_N$ which are arranged in triangular building blocks, at each vertex of which is located a particle of the given set ([8], p. 75). Moreover, these triangles will be almost, but not quite, congruent because, as in solid state physics, the particles will exhibit small vibrations in p˙ice. Let us begin, then, by showing how to construct a reasonable first approximation for a single triangular building block. Later we will show how to program a computer to generate any solid by using this basic configuration.

As shown in Figure 3.1, let P_1, P_2, P_3 be located at the vertices of an ~~equilateral~~ isosceles triangle in which $|P_1 P_2| = |P_1 P_3| = r$. In order to develop a strong, three particle bond, we will neglect all time dependences at present so that, for example, r, d, and h, as shown in Figure 3.1, are constant and satisfy

$$h^2 + d^2 = r^2 \quad .$$

Now, if P_1, P_2 and P_3 were strongly bonded, then all forces on these particles would be close to zero in magnitude. These forces, from (2.8), are, in general, given by

$$(3.1)\qquad F_x(P_1) = \frac{-G_{12}\, m_1\, m_2}{r_{12}{}^{\beta_{12}}}\,\frac{x_1-x_2}{r_{12}} + \frac{H_{12}\, m_1\, m_2}{r_{12}{}^{\alpha_{12}}}\,\frac{x_1-x_2}{r_{12}} - \frac{G_{13}\, m_1\, m_3}{r_{13}{}^{\beta_{13}}}\,\frac{x_1-x_3}{r_{13}} + \frac{H_{13}\, m_1\, m_3}{r_{13}{}^{\alpha_{13}}}\,\frac{x_1-x_3}{r_{13}}$$

$$(3.2)\qquad F_x(P_2) = \frac{-G_{21}\, m_1\, m_2}{r_{12}{}^{\beta_{21}}}\,\frac{x_2-x_1}{r_{12}} + \frac{H_{21}\, m_1\, m_2}{r_{12}{}^{\alpha_{21}}}\,\frac{x_2-x_1}{r_{12}} - \frac{G_{23}\, m_2\, m_3}{r_{23}{}^{\beta_{23}}}\,\frac{x_2-x_3}{r_{23}} + \frac{H_{23}\, m_2\, m_3}{r_{23}{}^{\alpha_{23}}}\,\frac{x_2-x_3}{r_{23}}$$

$$(3.3)\qquad F_x(P_3) = \frac{-G_{31}\, m_1\, m_3}{r_{13}{}^{\beta_{31}}}\,\frac{x_3-x_1}{r_{13}} + \frac{H_{31}\, m_1\, m_3}{r_{13}{}^{\alpha_{31}}}\,\frac{x_3-x_1}{r_{13}} - \frac{G_{32}\, m_2\, m_3}{r_{23}{}^{\beta_{32}}}\,\frac{x_3-x_2}{r_{23}} + \frac{H_{32}\, m_2\, m_3}{r_{23}{}^{\alpha_{32}}}\,\frac{x_3-x_2}{r_{23}}$$

$$(3.4)\qquad F_y(P_1) = \frac{-G_{12}\, m_1\, m_2}{r_{12}{}^{\beta_{12}}}\,\frac{y_1-y_2}{r_{12}} + \frac{H_{12}\, m_1\, m_2}{r_{12}{}^{\alpha_{12}}}\,\frac{y_1-y_2}{r_{12}} - \frac{G_{13}\, m_1\, m_3}{r_{13}{}^{\beta_{13}}}\,\frac{y_1-y_3}{r_{13}} + \frac{H_{13}\, m_1\, m_3}{r_{13}{}^{\alpha_{13}}}\,\frac{y_1-y_3}{r_{13}} - 32m_1$$

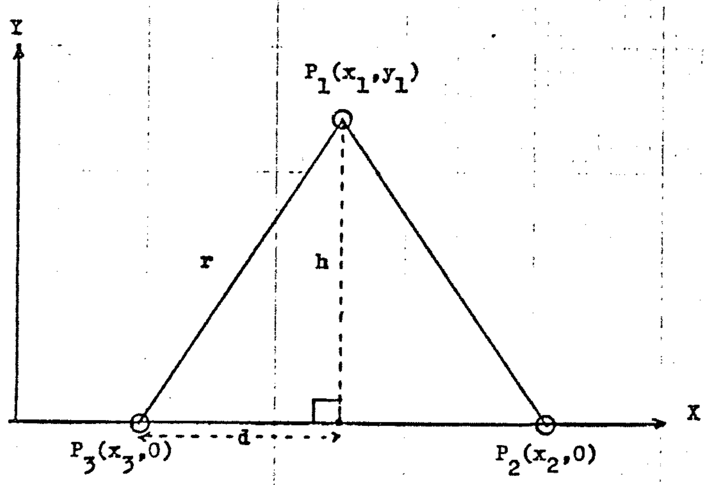

FIGURE 3.1

(3.5) $$F_y(P_2) = \frac{-G_{21}\, m_1\, m_2}{r_{12}^{\beta_{21}}}\ \frac{y_2-y_1}{r_{12}} + \frac{H_{21}\, m_1\, m_2}{r_{12}^{\alpha_{21}}}\ \frac{y_2-y_1}{r_{12}} - \frac{G_{23}\, m_2\, m_3}{r_{23}^{\beta_{23}}}\ \frac{y_2-y_3}{r_{23}} + \frac{H_{23}\, m_2\, m_3}{r_{23}^{\alpha_{23}}}\ \frac{y_2-y_3}{r_{23}} - 32m_2$$

(3.6) $$F_y(P_3) = \frac{-G_{31}\, m_1\, m_3}{r_{13}^{\beta_{31}}}\ \frac{y_3-y_1}{r_{13}} + \frac{H_{31}\, m_1\, m_3}{r_{13}^{\alpha_{31}}}\ \frac{y_3-y_1}{r_{13}} - \frac{G_{32}\, m_2\, m_3}{r_{23}^{\beta_{32}}}\ \frac{y_3-y_2}{r_{23}} + \frac{H_{32}\, m_2\, m_3}{r_{23}^{\alpha_{32}}}\ \frac{y_3-y_2}{r_{23}} - 32m_3 \ .$$

Since we will be interested later in homogeneous solids, let us continue under the assumptions that various parameters are constants and, in particular, set

(3.7) $m_i \equiv m_j \equiv m$

(3.8) $G_{ij} \equiv G$

(3.9) $H_{ij} \equiv H$

(3.10) $\alpha_{ij} \equiv \alpha$

(3.11) $\beta_{ij} \equiv \beta$.

Next, let us for clarity consider the particle parameter choices

(3.12) $\alpha = 6,\ \beta = 4,\ d = 0.6,\ h = 0.8,\ r = 1.0,$

the reasoning being completely analogous for other sets of choices. Then, (3.7)-(3.12) imply with regard to (3.1)-(3.6) that

(3.13) $F_x(P_1) = 0$

(3.14) $F_x(P_2) = -G\, m^2(.6) + H\, m^2\, (.6) - \frac{G\, m^2}{(1.2)^4} + \frac{H\, m^2}{(1.2)^6}$

(3.15) $F_x(P_3) = -\ F_x(P_2)$

(3.16) $F_y(P_1) = 2\,[-G\, m^2(.8) + H\, m^2(.8)]\ -32m$

(3.17) $F_y(P_2) = -G\, m^2(-.8) + H\, m^2(-.8)\ -32m$

(3.18) $F_y(P_3) = F_y(P_2)$.

If, as shown in Figure 3.1, we now assume that P_2 and P_3 are fully supported below, which will be implemented later by strongly damped reflection, then the forces $F_y(P_2)$ and $F_y(P_3)$ in (3.17) and (3.18) will be of no consequence. Thus, we concentrate only on parameter choices which result in each of (3.13)-(3.16) being zero. Hence, we need only consider $F_x(P_2) = 0$ and $F_y(P_1) = 0$, or equivalently,

$$-[(1.2)^2 + (.6)\ (1.2)^6]\ G + [1 + (.6)\ (1.2)^6]\ H = 0$$

$$-\ G \qquad + H = \frac{20}{m}\ ,$$

the solution of which, in terms of m, is given by

(3.19) $\quad G = \frac{1395.7952}{11m}\ , \quad H = G + \frac{20}{m}\ .$

Thus, as a particular example, for unit mass and for G and H rounded to integers which are divisible by five, one has from (3.19)

(3.20) $\quad m = 1,\ G = 125,\ H = 145\ .$

From (3.19) and (3.20), one can construct additional approximations like

(3.21) $\quad m = \frac{1}{5}\ ,\ G = 625,\ H = 725$

(3.22) $\quad m = \frac{1}{20},\ G = 2500,\ H = 2900.$

4. A Triangular Solid

In order to show how to construct solids, we will restrict attention to two-dimensional configurations only and will always call these bodies. Triangular building blocks will be used in the construction of bodies. All the ideas to be developed extend in a natural way dimensionwise.

For simplicity and clarity, in this section we will consider only a triangular shaped body, so that, beginning with N = 28, let the particles

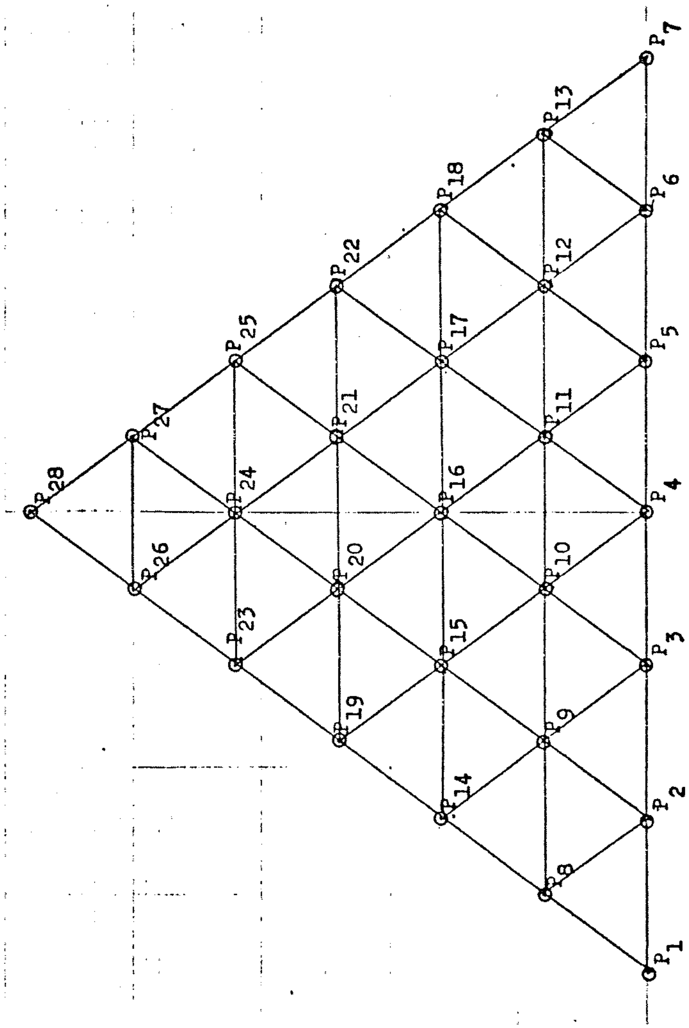

FIGURE 4.1

P_1-P_{28} be arranged as shown in Figure 4.1. The triangular building blocks each have base length 1.2 and equal arm length 1.0. The initial positions are given precisely in Table 1 and all initial velocities are taken to be zero.

TABLE 1 - Initial Positions of Particles P_i : Triangular Body

i	$x_{i,0}$	$y_{i,0}$	i	$x_{i,0}$	$y_{i,0}$	i	$x_{i,0}$	$y_{i,0}$	i	$x_{i,0}$	$y_{i,0}$
1	-3.6	0.0	8	-3.0	0.8	15	-1.2	1.6	22	1.8	2.4
2	-2.4	0.0	9	-1.8	0.8	16	0.0	1.6	23	-1.2	3.2
3	-1.2	0.0	10	-0.6	0.8	17	1.2	1.6	24	0.0	3.2
4	0.0	0.0	11	0.6	0.8	18	2.4	1.6	25	1.2	3.2
5	1.2	0.0	12	1.8	0.8	19	-1.8	2.4	26	-0.6	4.0
6	2.4	0.0	13	3.0	0.8	20	-.6	2.4	27	0.6	4.0
7	3.6	0.0	14	-2.4	1.6	21	.6	2.4	28	0.0	4.8

Let us fix the parameters by (3.7)-(3.12) and (3.22), so that each building block whose base is on the X axis should be a bonded unit. It is not to be implied, however, that the entire body is in equilibrium, nor that the remaining building blocks are bonded units, since the discussion of Section 3 followed from severe restrictions. Nevertheless, each of the remaining building blocks is supported by blocks beneath it, and the bonding constants H and G are sufficiently large so that the effect of gravity due to the total mass of the body should not be too great. Thus, if our intuition is correct, the body should be close to an equilibrium state. Our method of achieving such a desired state, which has already been shown to be viable in the study of liquids ([11], [12]), will be to let the particles interact according to (2.1)-(2.8) and to converge to

equilibrium by themselves. There is, of course, no hope of finding an analytical solution of this n-body problem.

There remains, however, a final consideration before the calculations are executed. We will assume that the body is supported by the X-axis, and this will be implemented as follows. If any particle P_i falls below the X-axis at time t_k, then it is reflected and its velocity reset in the following manner: $x_{i,k} \to x_{i,k}$; $y_{i,k} \to -y_{i,k}$; $v_{i,k,x} \to 0$, $v_{i,k,y} \to (.1) v_{i,k,y}$. With this modification, then, particles P_1-P_{28} were allowed to interact with $\Delta t = 10^{-4}$ in accordance with (2.1)-(2.8) and with initial positions those of Table 1 and initial velocities all zero.

The first results were interesting, but not satisfying. By time t_{10000} all the particles had fallen to the X-axis and the body had gone through a transformation like honey, in which it had deformed gradually into a flat surface. The problem was that gravity was overcoming the interparticle forces of attraction and repulsion. To remedy this situation, since interparticle forces increase with m^2 while gravity increases only with m, the mass was increased to $\frac{1}{4}$, so that (3.22) was replaced by

$$m = \frac{1}{4},\ G = 2500,\ H = 2900 \quad .$$

The calculations were repeated and this time a configuration like that in Figure 3.1 did result. However, to test that the body was cohesive, particle P_{19} was removed. Two thousand further iterations resulted in P_{23}, P_{26} and P_{28} sliding down to replace P_{19}, P_{23} and P_{26}, respectively. Thus, the body simulated a pile of sand. To remedy this situation the mass was increased to unity, so that (3.22) was replaced by

$$(4.1) \qquad m = 1,\ G = 2500,\ H = 2900$$

and the calculations were repeated again. The results now simulated a gravitational collapse in which each particle showed exceptionally strong attraction to all other particles. Indeed, the entire body initially rose upward and gradually settled down into a triangular body similar to, but smaller than, that shown in Figure 3.1. To test that the resulting body was cohesive, particle P_{19} was removed again. Two thousand further iterations showed that P_1, P_8 and P_{14} had moved up the side of the triangle while P_{23}, P_{26}, and P_{28} had moved down, thereby filling in the void left by P_{19}. Thus, the resulting body was cohesive, but not in the way one would expect a large solid body to be. The problem was that P_1 and P_{28}, for example, were attracting each other very strongly, whereas, for a large body, this would not happen, since interparticle forces decay rapidly with increasing r.

There are then two possible ways to remedy this last problem. One can take N much larger than 28. In this way the distance between the furthest separated particles increases and the resulting interparticle force becomes negligible. To economize, however, the following alternative was used with N = 28. We merely set $\bar{F}_{i,k,x}$ and $\bar{F}_{i,k,y}$ in (2.5) and (2.6) equal to zero if $|P_i P_j| > 1.5$, thus keeping these forces local. With this modification and with (4.1), the calculations were repeated again and were finally successful. To describe the results, we let $K(t_k) = K_k$ be the system's kinetic energy at t_k. K_k will be used as a measure of the body's relative state of equilibrium, since an absolute state is not attainable directly on a computer.

By time t_{10000}, the system kinetic energy had decreased, in an oscillatory fashion, which is indicated by the sequence: $K_{500} = 436$, $K_{1000} = 487$, $K_{1500} = 211$, $K_{2000} = 345$, $K_{2500} = 234$, $K_{3000} = 371$, $K_{3500} = 302$, $K_{4000} = 237$, $K_{4500} = 153$, $K_{5000} = 192$, $K_{5500} = 195$, $K_{6000} = 230$, $K_{6500} = 122$, $K_{7000} = 91$, $K_{7500} = 94$, $K_{8000} = 78$, $K_{8500} = 108$, $K_{9000} = 80$, $K_{9500} = 51$, $K_{10000} = 74$. The resulting body is shown in Fig 4.2 and all positions and velocities are recorded in Table 2. Particle oscillations showed changes in position corrdinates in only the third decimal place. Removal of particle P_{19} resulted in no additional structural change in two thousand additional time steps.

The FORTRAN program used is given in the Appendix of [13] so that the interested reader can reproduce all the above results.

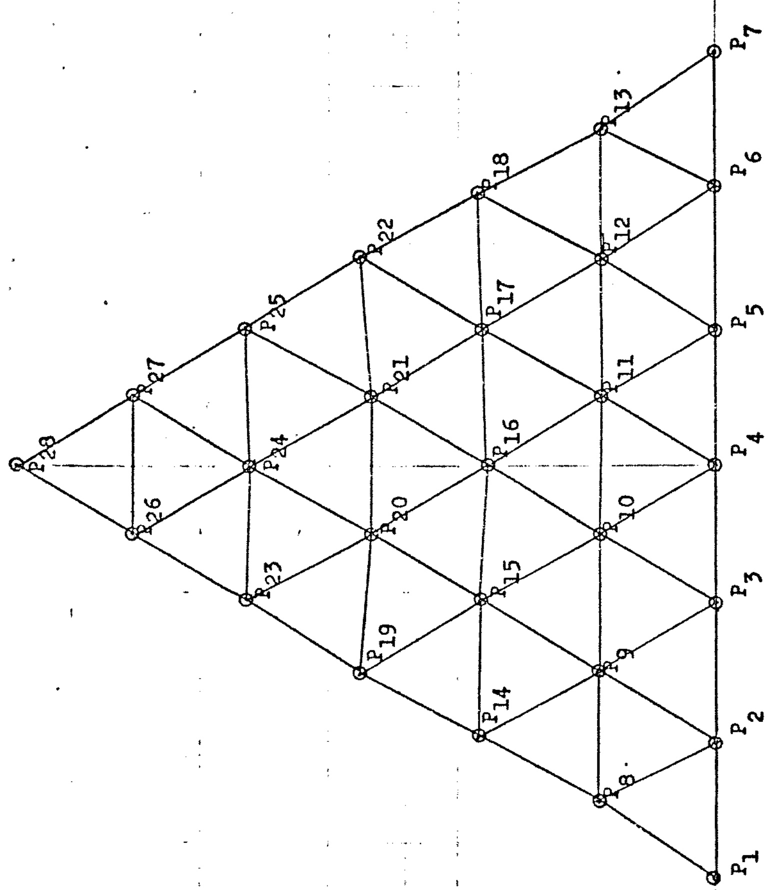

FIGURE 4.2

TABLE 2 - Equilibrium Positions and Velocities of Particles P_i : Triangular Body

i	x	y	v_x	v_y
1	-3.2652	0.0000	0.0000	0.0005
2	-2.1924	0.0000	0.0000	0.0065
3	-1.0895	0.0000	0.0000	0.0018
4	0.0000	0.0000	0.0000	0.0016
5	1.0895	0.0000	0.0000	0.0018
6	2.1924	0.0000	0.0000	0.0065
7	3.2652	0.0000	0.0000	0.0005
8	-2.6754	0.8909	-0.9437	1.0055
9	-1.6310	0.8990	2.0010	3.7973
10	-.5445	0.9032	4.1844	-0.9128
11	.5445	0.9032	-4.1844	-0.9128
12	1.6310	0.8990	-2.0010	3.7973
13	2.6754	0.8909	0.9437	1.0055
14	-2.1366	1.8374	0.9267	0.4191
15	-1.0763	1.8146	-2.5412	-2.1506
16	0.0000	1.7923	0.0000	-1.5731
17	1.0763	1.8146	2.5412	-2.1506
18	2.1366	1.8374	-0.9267	0.4191
19	-1.6674	2.7530	-0.9468	0.6165
20	-0.5441	2.6879	-1.8075	2.1719
21	0.5441	2.6879	1.8075	2.1719
22	1.6674	2.7530	0.9468	0.6165
23	-1.0877	3.6478	0.2061	-2.6777
24	0.0000	3.6174	0.0000	0.4901
25	1.0877	3.6478	-0.2061	-2.6777
26	-0.5536	4.5068	-0.5620	0.7410
27	0.5536	4.5068	0.5620	0.7410
28	0.0000	5.4351	0.0000	-2.8452

5. Other Solids

In this section we will discuss two bodies which are not triangular in shape. The first example will be a simple one to verify another desirable physical property of our models. The second example will be a more complex one with another set of force parameters. The computational details are entirely analogous to those described in Section 4.

For N = 8, consider the eight particles $P_1, P_2, P_3, \ldots, P_8$ with respective initial positions (-3.6,0), (-2.4,0), (-3,0.8), (-1.8,0.8), (-2.4,1.6), (-1.2,1.6), (-1.8,2.4), (-0.6,2.4), as shown in Figure 5.1 (a) and with all initial velocities equal to zero. All parameter choices are the same as in Section 4, with m, G and H determined by (4.1) and with inter-particle forces restricted to distances less than 1.5. As is apparent from the figure, the center of gravity is not supported, so that the body must fall. Up to t_{4500}, the body showed both oscillatory particle motions toward an equilibrium position and a small initial gross falling motion. Figures 5.1 (b)-(g) show the most rapid part of the fall at every 500 time steps from t_{4500} through t_{7000} and verify that the body retains its cohesive structure throughout the motion.

As a last example, we let N = 46 and we will construct a rectangular shaped body. The initial positions are given in Table 3 and the initial velocities are all taken to be zero. All parameter choices are the same as in Section 4 with the following exceptions.

(5.1) $m = 1,\ G = 2540,\ H = 2940;\ \alpha = 10,\ \beta = 7.$

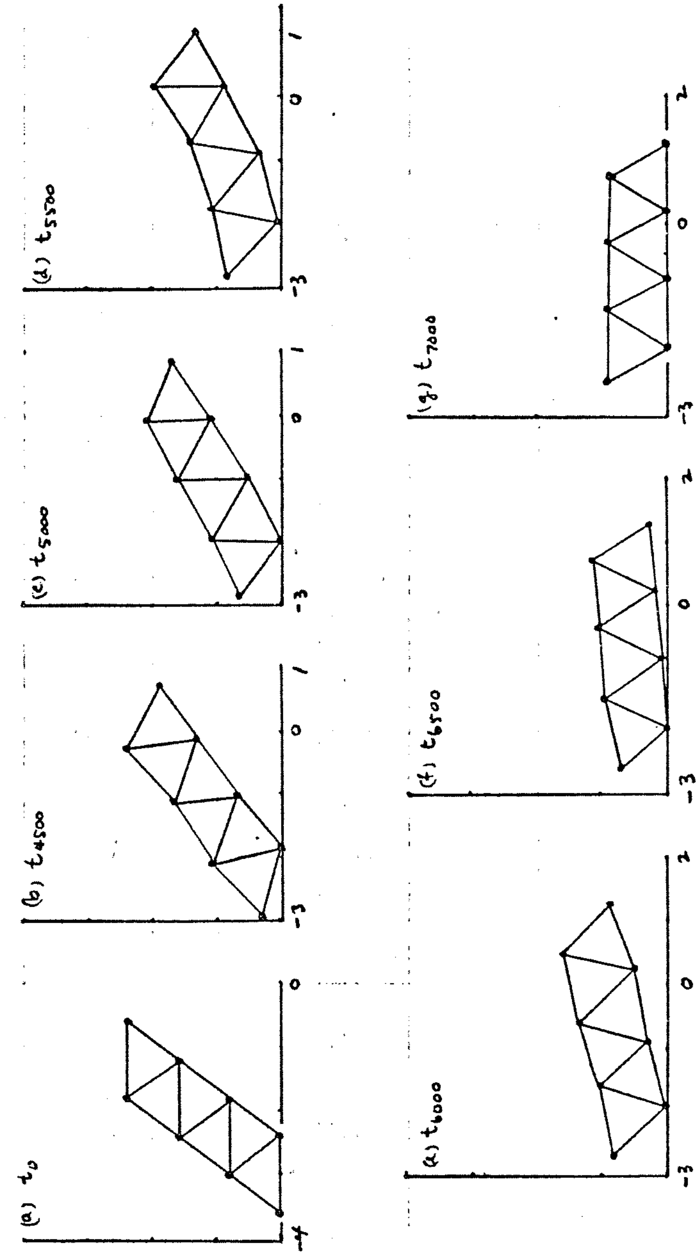

FIGURE 5.1

The body was then allowed, as in Section 3, to find an equilibrium position, and this is shown in Figure 5.2 after 32000 time steps, with the positions and velocities listed precisely in Table 4. Though most position coordinates were changing in the third decimal place only, a few still showed changed in the second.

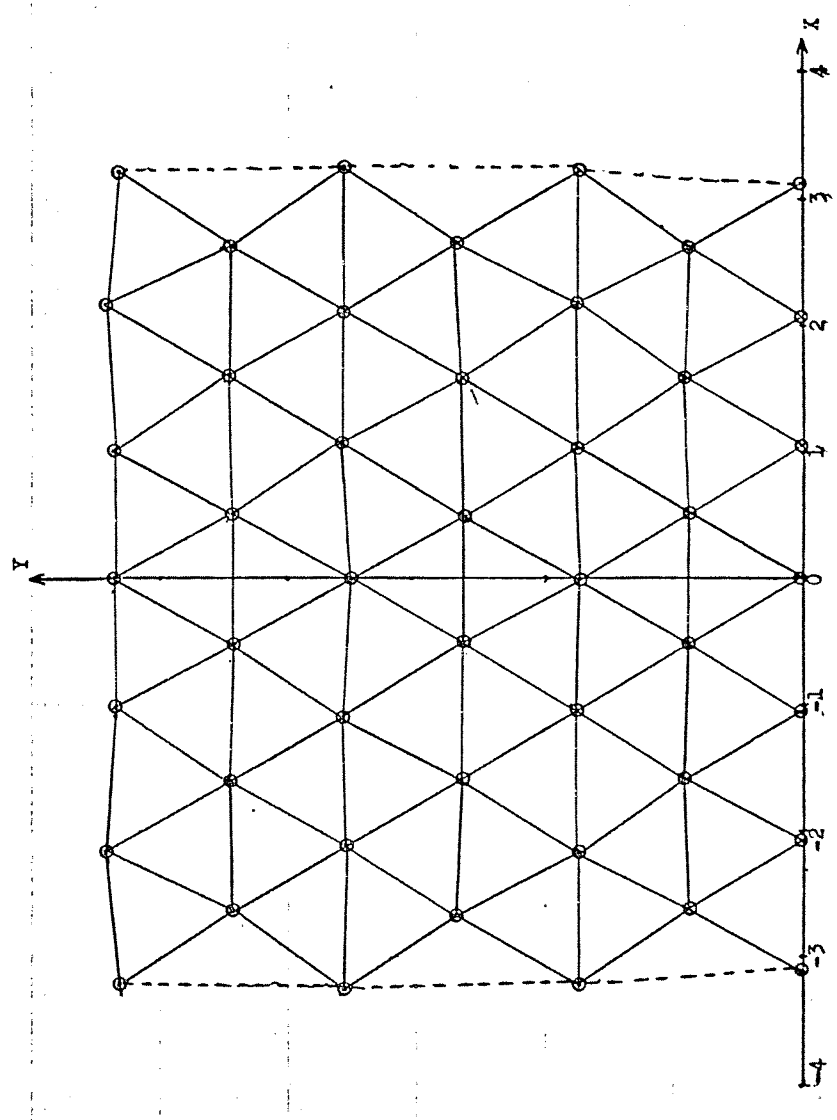

FIGURE 5.2

TABLE 3 - Initial Positions of Particles P_i : Rectangular Body

i	x_i	y_i	i	x_i	y_i	i	x_i	y_i
1	-3.6	0	16	-1.2	1.6	32	2.4	3.2
2	-2.4	0	17	0	1.6	33	3.6	3.2
3	-1.2	0	18	1.2	1.6	34	-3.0	4.0
4	0	0	19	2.4	1.6	35	-1.8	4.0
5	1.2	0	20	3.6	1.6	36	-.6	4.0
6	2.4	0	21	-3.0	2.4	37	.6	4.0
7	3.6	0	22	-1.8	2.4	38	1.8	4.0
8	-3.0	.8	23	-.6	2.4	39	3.0	4.0
9	-1.8	.8	24	.6	2.4	40	-3.6	4.8
10	-.6	.8	25	1.8	2.4	41	-2.4	4.8
11	.6	.8	26	3.0	2.4	42	-1.2	4.8
12	1.8	.8	27	-3.6	3.2	43	0	4.8
13	3.0	.8	28	-2.4	3.2	44	1.2	4.8
14	-3.6	1.6	29	-1.2	3.2	45	2.4	4.8
15	-2.4	1.6	30	0	3.2	46	3.6	4.8
			31	1.2	3.2			

TABLE 4 - Equilibrium Positions and Velocities of Particles P_i : Rectangular Bo

i	x	y	v_x	v_y
1	-3.1286	0.0000	-.0064	-.0143
2	-2.0758	0.0000	-.0027	.0000
3	-1.0569	0.0000	.0025	.0000
4	0.0000	0.0000	.0000	-.0379
5	1.0569	0.0000	-.0025	.0000
6	2.0758	0.0000	.0027	.0000
7	3.1286	0.0000	.0064	-.0143
8	-2.6141	.8925	1.9772	-2.5275
9	-1.5702	.9063	-.2578	-1.6351
10	-.5158	.8806	-.4572	-4.0032
11	.5158	.8806	.4572	-4.0032
12	1.5702	.9063	.2578	-1.6351
13	2.6141	.8925	-1.9772	-2.5275
14	-3.2355	1.7328	.1082	.3596
15	-2.1860	1.7561	-3.4152	1.9154
16	-1.0663	1.7556	4.0996	1.9352
17	.0000	1.7118	.0000	-3.1557
18	1.0663	1.7556	-4.0996	1.9352
19	2.1860	1.7561	3.4152	1.9154
20	3.2355	1.7328	-.1082	.3596
21	-2.6612	2.6948	6.7868	2.4723
22	-1.6000	2.6242	-.9479	-.7837
23	-.4951	2.6327	1.5791	.2733

TABLE 4 - Continued

i	x	y	v_x	v_y
24	.4951	2.6327	-1.5791	.2733
25	1.6000	2.6242	.9479	-.7837
26	2.6612	2.6948	-6.7868	2.4723
27	-3.2632	3.5724	6.3615	1.2408
28	-2.1325	3.5437	-.1162	.8118
29	-1.1082	3.5822	-.5865	-.9931
30	.0000	3.4975	.0000	2.1883
31	1.1082	3.5822	.5865	-.9931
32	2.1325	3.5437	.1162	.8118
33	3.2632	3.5724	-6.3615	1.2408
34	-2.6332	4.4355	.1184	-2.9408
35	-1.6157	4.4688	-6.3966	-1.1250
36	-.5082	4.4248	-.7457	2.3525
37	.5082	4.4248	.7457	2.3525
38	1.6157	4.4688	6.3966	-1.1250
39	2.6332	4.4355	-.1184	-2.9408
40	-3.2233	5.3069	3.3095	-5.0351
41	-2.1720	5.4220	.6164	-3.5682
42	-1.0380	5.3376	.0952	-1.2303
43	.0000	5.3734	.0000	1.7940
44	1.0380	5.3376	-.0952	-1.2303
45	2.1720	5.4220	-.6164	-3.5682
46	3.2233	5.3069	-3.3095	-5.0351

6. Remarks

A large number of other computer examples were run, but each to a lesser extent than those already described. Often the objective was to explore the consequences of changing various parameter sets. It became apparent quickly, however, that unlimited computer time was necessary for a high degree of success in such endeavors. A few of the more interesting results which were obtained are summarized as follows. Increasing Δt to 10^{-3} often yielded physical instability, as did undamped reflection from the X-axis in the Y direction. Variation of α and β from $\alpha = 6$ to $\alpha = 19$ and $\beta = 4$ to $\beta = 16$ were successful to varying degrees, but the set $\alpha = 20$, $\beta = 17$ yielded instability. Finally, the choice of square building blocks invariably resulted in a body's self rearrangement into triangular ones.

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APPENDIX

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C GENERATION OF PARTICLE-SOLID WITH G/R**BETA ATTRACTION, H/R**ALPHA
C REPULSION, AND GRAVITY =-32.  GRAVITY IS INTRODUCED BECAUSE
C WE WISH TO CHANGE STATE FROM SOLID TO LIQUID.  THIS WILL ENABLE US
C TO SOLVE FREE BOUNDARY PROBLEMS LIKE THE STEAM PROBLEM
C FORCES ARE LOCALIZED TO R LT 1.5 BECAUSE N IS RELATIVELY SMALL
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      PARAMETER N=28
      NM1=N-1
      K=1
      KPRINT=250
      H=2900.
      G=2500.
      IALPHA=6
      IBETA=4
C DIMENSION STATEMENT
      DIMENSION PMASS(N),XO(N),YO(N),VXO(N),VYO(N),X(N,2),Y(N,2),
     1VX(N,2),VY(N,2),ACX(N),ACY(N)
C   VARIABLES XO, YO, ETC., HAVE BEEN PUNCHED ON, NOT ZERO
C INITIALIZATION SET TO ZERO AUTOMATICALLY ON 1110
C INITIAL DATA INPUT
      READ 10, (PMASS(I),XO(I),YO(I),VXO(I),VYO(I),I=1,N)
10     FORMAT (5F10.4)
C PRINT INITIAL DATA
      DO 20 I=1,N
      PRINT 15,I,PMASS(I),XO(I),YO(I),VXO(I),VYO(I)
15     FORMAT (5X,I5,5F11.5)
20      CONTINUE
C UPDATE. X(I,1) IS X COORDINATE AT PREVIOUS TIME STEP.  X(I,2) IS X
C  COORDINATE AT PRESENT TIME STEP.  SIMILARLY FOR OTHER VARIABLES.
      DO 30 I=1,N
      X(I,1)=XO(I)
      Y(I,1)=YO(I)
      VX(I,1)=VXO(I)
      VY(I,1)=VYO(I)
30      CONTINUE
       GO TO 71
65      DO 70 I=1,N
      X(I,1)=X(I,2)
      Y(I,1)=Y(I,2)
      VX(I,1)=VX(I,2)
      VY(I,1)=VY(I,2)
70      CONTINUE
C CALCULATION OF ACCELERATIONS IS DONE THROUGH STEP 77.
      DO 701 I=1,N
      ACX(I)=0.
      ACY(I)=0.
701    CONTINUE
71     DO 77 I=1,NM1
      IP1=I+1
      DO 76 J=IP1,N
      R=SQRT((X(I,1)-X(J,1))**2+(Y(I,1)-Y(J,1))**2)
      IF (R.GT.1.5) GO TO 73
      F=(H/R**IALPHA)-(G/R**IBETA)
```

```
      FX=F*(X(I,1)-X(J,1))/R
      FY=F*(Y(I,1)-Y(J,1))/R
      GO TO 75
73     FX=0.
        FY=0.
C ACCUMULATION OF FORCES ON PARTICLE I DUE TO ALL OTHER PARTICLES IS DONE
C IN NEXT FOUR FORMULAS
75     ACX(I)=ACX(I)+FX
      ACX(J)=ACX(J)-FX
      ACY(I)=ACY(I)+FY
      ACY(J)=ACY(J)-FY
76     CONTINUE
77     CONTINUE
C NOTE THAT WE HAVE JUST ACCUMULATED FORCES, NOT ACCELERATIONS - THE ABOVE
C NOTATION, THOUGH MISLEADING, ENABLES US TO SAVE MEMORY LOCATIONS.  WE
C NEXT CALCULATE ONLY THE Y-ACCELERATIONS BECAUSE THE X-ACCELERATIONS AND
C X-FORCES ARE THE SAME DUE TO THE CHOICE OF UNIT MASS.
      DO 770 I=1,N
      ACY(I)=ACY(I)-32.
770     CONTINUE
79     DO 80 I=1,N
      VX(I,2)=VX(I,1)+.0001*ACX(I)
      VY(I,2)=VY(I,1)+.0001*ACY(I)
      X(I,2)=X(I,1)+.0001*VX(I,2)
      Y(I,2)=Y(I,1)+.0001*VY(I,2)
C DAMPED REFLECTION OFF THE WALL IS NOW INTRODUCED.
      IF (Y(I,2).GE.0.0) GO TO 80
      Y(I,2)=-Y(I,2)
      VX(I,2)=0.
      VY(I,2)=-.1*VY(I,2)
80      CONTINUE
800     K=K+1
C PRINT ONLY EVERY KPRINT STEPS
      IF (MOD(K,KPRINT).GT.0) GO TO 82
      IF (MOD(K,KPRINT).LT.0) GO TO 82
      DO 810 I=1,N
      PRINT 81,K,I,X(I,2),Y(I,2),VX(I,2),VY(I,2)
81     FORMAT (5X,2I5,4F20.10)
810      CONTINUE
C CALCULATE TOTAL KE
      ENERGY=0.
      DO 8100 I=1,N
      ENERGY=ENERGY+.5*(VX(I,2)**2+VY(I,2)**2)
8100    CONTINUE
      PRINT 8101, ENERGY
8101   FORMAT (5X,F20.10)
C TERMINATION AFTER A FIXED NUMBER OF STEPS
82     IF (K.LT.5000) GO TO 65
C PUNCH OUTPUT FOR RESTART
      PUNCH 10, (DMASS(I),X(I,2),Y(I,2),VX(I,2),VY(I,2),I=1,N)
      STOP
      END
```