Particle Simulation of Compression Waves

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Abstract

Compression waves are studied using a quasi-molecular, particle approach. Explosive type disturbances are simulated to generate such waves, which propagate by the interaction of each particle with its immediate neighbors. Obstacles to wave motions are studied by the introduction of variable densities. Computer examples are described and discussed.

1. Introduction. Compression waves have long been of interest to scientists and engineers (see, e.g., refs. [1]-[4] and the numerous additional references contained therein). These waves have important roles in, for example, studies of acoustics, seismology, gas dynamics, and stress analysis. The propagation of such waves, unlike electromagnetic waves, is the direct result of molecular interaction. For this reason, we will describe and apply a new particle approach to compression wave simulation which is based on classical molecular mechanics [5]. Computer examples will be described and discussed.

2. Classical Molecular Mechanics. For purposes of intuition, it will be important to review, first, how molecules interact. Within a larger body, molecules interact only locally, that is, only with their nearest neighbors. This interaction is of the following general nature [5]. If two molecules are pushed together they repel each other, if pulled apart they attract each other, and mutual repulsion is of a greater order of magnitude than is mutual attraction. Mathematically, this behavior is often formulated as follows. The magnitude F of the force $\vec{F}$ between two molecules which are locally r units apart is of the form

$$(2.1) \quad F = - \frac{G}{r^p} + \frac{H}{r^q} \quad ,$$

where, typically,

$$(2.2) \quad G > 0, H > 0, q > p \geq 7 \quad .$$

The major problem in any simulation of a physical body is that there are too many component molecules to incorporate into the model. The classical mathematical approach is to replace the large, but finite, number of molecules by an infinite set of points. In so doing, the rich physics of molecular interaction is lost because every point always has an infinite number of neighbors which are arbitrarily close. A viable computer alternative is to replace the large number of molecules by a much smaller number of particles and then readjust the parameters in (2.1) to compensate. It is this latter approach which we will follow.

3. A General Computer Algorithm. The general idea outlined in Section 2 can be implemented easily in the following constructive fashion [6] .

Consider N particles P_i , $i=1,2,\dots,N$. For $\Delta t > 0$, let $t_k = k \Delta t$, $k=0,1,2,\dots$. For each of $i=1,2,\dots,N$, let m_i denote the mass of P_i , and let P_i at t_k be located at $\vec{r}_{i,k} = (x_{i,k}, y_{i,k}, z_{i,k})$, have velocity $\vec{v}_{i,k} = (v_{i,k,x}, v_{i,k,y}, v_{i,k,z})$, and have acceleration $\vec{a}_{i,k} = (a_{i,k,x}, a_{i,k,y}, a_{i,k,z})$. Let position, velocity, and acceleration be related by the recursion formulas

$$(3.1) \quad \vec{v}_{i,\frac{1}{2}} = \vec{v}_{i,0} + \frac{1}{2} (\Delta t) \vec{a}_{i,0} \quad (\text{starter formula})$$

$$(3.2) \quad \vec{v}_{i,k+\frac{1}{2}} = \vec{v}_{i,k-\frac{1}{2}} + (\Delta t) \vec{a}_{i,k}, \quad k=1,2,3,\dots$$

$$(3.3) \quad \vec{r}_{i,k+1} = \vec{r}_{i,k} + (\Delta t) \vec{v}_{i,k+\frac{1}{2}}, \quad k=0,1,2,\dots$$

At t_k , let the force acting on P_i be $\vec{F}_{i,k} = (F_{i,k,x}, F_{i,k,y}, F_{i,k,z})$. We relate force and acceleration by the dynamical equation

$$(3.4) \quad \vec{F}_{i,k} = m_i \vec{a}_{i,k}.$$

As soon as the precise structure of $\vec{F}_{i,k}$ is given, the motion of each P_i will be determined explicitly and recursively by

(3.1)-(3.4) from given initial data. The force $\vec{F}_{i,k}$ is described now as follows. Assume first that P_j is a neighbor of P_i . Then, let $\vec{r}_{ij,k}$ be the vector from P_i to P_j at time t_k , so that $r_{ij,k} = |\vec{r}_{i,k} - \vec{r}_{j,k}|$ is the distance between the two particles.

Then the force $\vec{F}_{ij,k}$ on P_i exerted by P_j at time t_k is assumed to be

$$(3.5) \quad \vec{F}_{ij,k} = \left[\left[-\frac{G}{(r_{ij,k})^p} + \frac{H}{(r_{ij,k})^q} \right] \frac{\vec{r}_{ji,k}}{r_{ij,k}} \right],$$

in consistency with (2.1). Next, suppose that P_j is not a neighbor of P_i . Then we define the force on P_i exerted by P_j to be

$$(3.6) \quad \vec{F}_{ij,k} = \vec{0}.$$

Finally, the total force $\vec{F}_{i,k}$ on P_i at t_k is defined by

$$(3.7) \quad \vec{F}_{i,k} = \sum_{\substack{j=1 \\ j \neq i}}^N \vec{F}_{ij,k}.$$

For the convenience of the reader, a basic, two dimensional, FORTRAN program of the above algorithm is given in the Appendix of Greenspan [7]. Extensions and modifications for the examples which follow can be developed easily from it.

Throughout the discussion in the present paper, the parameter choices in (3.1)-(3.5) are $N = 295$, $p = 4$, $q = 6$, $G = H = m_i m_j$, $\Delta t = 10^{-4}$ sec. Usually, we will take all the masses to be unity, in which case $G = H = 1$. However, later examples will require the introduction of two different mass constants, which is the reason why G and H are chosen as indicated.

4. Particle Simulation of a Rectangular Body. To begin, let us consider the particle configuration shown in Figure 4.1. The particles P_i , $i = 1, 2, \dots, 295$, shown there are arranged in a large rectangular figure which has been constructed from a triangular mosaic. The mosaic triangles are regular, with edge length unity, and the particles lie on the vertices. The numbering is in a sequential pattern from left to right on each row and increasing vertically upward with the rows. On any row, the number to the left is the number of the leftmost particle of that row, while the number to the right is the number of the rightmost particle of the row. The distance between two consecutive rows is, approximately, 0.866. The coordinates of P_1 and P_{16} are set at $(-7.5, 0)$ and $(7.5, 0)$, which then fixes the coordinates of all the particles. Thus, for example, the coordinates of P_6 , P_{32} , P_{48} , P_{62} , P_{173} , P_{278} and P_{287} are, respectively, $(-2.5, 0)$, $(-7.5, 1.732)$, $(-7, 2.598)$, $(7, 2.598)$, $(-6, 9.526)$, $(6, 14.722)$, $(-0.5, 15.588)$. A complete listing of the particle numbers and coordinates is given in Appendix B of Greenspan [7].

Initially, all masses are set at unity and all velocities at zero.

Fig. 4.1. Initial Particle Configuration.

5. Explosion Simulation. In order to simulate compression waves in the particle arrangement shown in Figure 4.1, we will show now how to generate initial data for an internal explosion. The explosion center is chosen to be near the top, at the point (0,15.299). In Figure 4.1, this point is the centroid of the three particles P_{272} , P_{287} , P_{288} , where P_{272} is the highest particle on the Y axis and P_{287} , P_{288} are the closest particles to P_{272} on the very top row. Our objective is to reset the velocities of particles within a circular region about (0,15.299) so that their directions are outward and their magnitudes vary in a $1/r^2$ fashion from this central point. This will be done in three ways, as follows:

Case 1. Reset the velocities of P_{240} - P_{242} , P_{255} - P_{258} , P_{270} - P_{274} so that

$$(5.1) \quad v_{i,0,x} = \frac{0.05}{x_1^2 + (y_1 - 15.299)^2} \frac{x_1}{(x_1^2 + (y_1 - 15.299)^2)^{\frac{1}{2}}}$$

$$(5.2) \quad v_{i,0,y} = \frac{0.05}{x_1^2 + (y_1 - 15.299)^2} \frac{y_1 - 15.299}{(x_1^2 + (y_1 - 15.299)^2)^{\frac{1}{2}}}$$

The resulting velocity field, magnified by the factor 1500, is shown in Figure 5.1. (Note that throughout the remainder of the paper velocity fields will always be displayed using the magnification factor 1500. This is necessary for far field displays later. Note also that to accommodate the vector fields to be displayed, it will be convenient to take the unit distance on the Y axis to be slightly larger than the unit distance on the X axis.)

Case 2. Repeat Case 1, but also reset the velocities of P_{285} , P_{286} ,

P_{289} , P_{290} by (5.1)-(5.2). The resulting velocity field is shown in Figure 5.2.

Case 3. Repeat Case 1 but also reset the velocities of $P_{285} - P_{290}$ by (5.1)-(5.2). The resulting velocity field is shown in Figure 5.3.

Fig. 5.1. Explosion Model - Case I

Fig. 5.2. Explosion Model - Case II

Fig. 5.3. Explosion Model - Case III

Fig. 6.1. Case I. $T = 3$.

6. Compression Wave Simulation. Since all force parameters have been defined, and since all initial data have been given, there remains only one matter to be decided before compression waves can be simulated. We must define, precisely, which particles are the neighbors of any given particle. This will be done as follows. For any particle P_i in Figure 4.1, its neighbors, for all time, are defined to be those particles whose initial distance to P_i is unity. Thus, for example, the neighbors of P_6 are P_5, P_7, P_{21}, P_{22} ; those of P_{17} are $P_1, P_2, P_{18}, P_{32}, P_{33}$; those of P_{32} are P_{17}, P_{33}, P_{48} ; those of P_{65} are $P_{49}, P_{50}, P_{64}, P_{66}, P_{80}, P_{81}$; and those of P_{295} are P_{279}, P_{294} . This definition and the indexing used in Figure 4.1 allow a simple programming routine for force calculations.

Let us turn now to the generation of compression waves. Throughout, configuration stability is maintained by fixing the particles P_1 and P_{16} for all time at their initial positions $(-7.5, 0), (7.5, 0)$.

Figures 6.1-6.12 show the velocity field development from Figure 5.1 for Case 1. Figure 6.2 shows the initial development of concentration and rarefaction at time $T = 4$. Figure 6.4 shows clearly at $T = 6$ the emergence, from the complex interactions now present in the explosion area, of a second wave front. From Figure 6.4 we can approximate the resulting wave length to be 5.2 units. Figure 6.5 shows not only the advance of the wave fronts but indicates circulation areas, due to reflection, in the upper left and right hand corners. Using wave front positions in Figure 6.3 at $T = 5$ and Figure 6.6 at $T = 8$, we now approximate the wave speed to be 1.44 units per second. By the time $T = 9$, shown in Figure 6.7,

the wave front has reached the bottom of the rectangle. Figures 6.8-6.12 show the reflection pattern. In Figures 6.11 - 6.12, concentration and rarefaction layers have emerged which are somewhat similar to a standing wave pattern.

The computer results for Cases 2 and 3 are similar, but do increase in complexity. Figures 6.13 and 6.14 show the emergence of the second wave at $T = 8$ for Case 2 and Case 3, respectively, in analogy with Figure 6.6 for Case 1. Figures 6.15 and 6.16 show the reflection patterns at time $T = 13$ for Cases 2 and 3, respectively, in analogy with Figure 6.11 for Case 1.

As a by-product of the above simulation, one can also observe small surface waves. Figures 6.1-6.12 indicate the wave pattern on the very top row. For the most volatile case, that is, Case 3, Figure 6.17 shows the actual particle positions through $T = 20$. The surface wave speed is, approximately, 1.25 units per second.

Fig. 6.2. Case I, $T = 4$.

Fig. 6.3. Case I - $T = 5$.

Fig. 6.4. Case I- $T = 6$

Fig. 6.5. Case I - $T = 7$.

Fig. 6.6. Case I - $T = 8$.

Fig. 6.7. Case I - $T = 9$.

Fig. 6.8. Case I - $T = 10$.

Fig. 6.9. Case I - $T = 11$.

Fig. 6.10. Case I - $T = 12$.

Fig. 6.11. Case I - $T = 13$.

Fig. 6.12. Case I - $T = 14$.

Fig. 6.13. Case II - $T = 8$.

Fig. 6.14. Case III, $T = 8$.

Fig. 6.15. Case II - $T = 13$.

Fig. 6.16. Case III, $T = 13$.

Fig. 6.17. Surface Waves.

7. Diffraction and Reflection. In this section, we will examine some simple diffraction and reflection effects. Concentration will be on the initial configuration of Case 2, as shown in Figure 6.2. Let us first place a flat, wall-type obstacle in the wave path, as shown in Figure 7.1. This is simulated by resetting the masses of P_{161} - P_{166} equal to M , where $M > 1$.

For the case $M = 2$, Figure 7.1 at $T = 4$ shows a small amount of reflection and a relatively large amount of transmission. For $M = 10$, Figures 7.2 - 7.6 show an increase in reflection and a decrease in transmission. In addition, Figure 7.4 shows cumulative effects from separated wave fronts to the left and right of the wall. For $M = 200$, Figures 7.7-7.12 show a relatively large reflection with only a small amount of transmission. The wave separation process is especially clear in Figures 7.9-7.10, while small effects in the shadow region appear in Figures 7.11-7.12.

The difference in surface effects at the top of the configuration due to reflection are apparent by comparison of Figures 7.6 and 7.12 with Figure 6.13, in which there is no obstacle. Large velocities due to reflection are observed at P_{286} - P_{289} in Figures 7.6 and 7.12. It is also interesting to note the relatively large velocity due to reflection at P_{272} in Figures 7.5 and 7.11.

Figures 7.13-7.18 show the diffraction and reflection patterns around a triangular obstacle, simulated by setting $M = 200$ for P_{163} , P_{164} and P_{179} .

Fig. 7.1. $M = 2$, $T = 4$.

Fig. 7.2. $M = 10$, $T = 4$.

Fig. 7.3. $M = 10$, $T = 5$.

Fig. 7.4. $M = 10$, $T = 6$.

Fig. 7.5. $M = 10$, $T = 7$.

Fig. 7.6. $M = 10$, $T = 8$.

Fig. 7.7. $M = 200$, $T = 3$.

Fig. 7.8. $M = 200$, $T = 4$.

Fig. 7.9. $M = 200$, $T = 5$.

Fig. 7.10. $M = 200$, $T = 6$.

Fig. 7.11. $M = 200$, $T = 7$.

Fig. 7.12. $M = 200$, $T = 8$.

Fig. 7.13. $M = 200$, $T = 3$.

Fig. 7.14. $M = 200$, $T = 4$.

Fig. 7.15. $M = 200$, $T = 5$.

Fig. 7.16. $M = 200$, $T = 6$.

Fig. 7.17. $M = 200$, $T = 7$.

Fig. 7.18. $M = 200$, $T = 8$.

8. Remarks. Note first that since compression waves are molecular phenomena, particle modeling using molecular type formulas is a natural method of simulation. Such an approach even includes the nonlinear effects omitted by continuum linearization. In the future, the need to increase the number of particles in each model should be greatly facilitated by the development of vector and parallel technology.

Next, note that, of the large number of calculations which were only surveyed in Sections 6-7, the choice of formulas like (5.1)-(5.2), but with 0.05 replaced by constants larger than 2, resulted invariably in wave motion along only two rays. These waves did not have the general spherical structure of the ones presented in our examples and imply the existence of a wave condition relating the speed of the wave, the nature of the transmitting medium, the speed of sound, and, perhaps, the time step. We have not been able to deduce such a relationship as yet.

Finally, note that with sufficient resources, it is possible to redo all the calculations in an implicit fashion so that all the conservation laws of continuum mechanics remain valid [6]. The approach we have used is, however, far more economical.

References

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      DOUBLE PRECISION X0(295),Y0(295),VX0(295),VY0(295),
      1X(295,2),Y(295,2),VX(295,2),VY(295,2),
      1ACX(295),ACY(295),F1,F2,F3,F4,F5,
      1F6,FX1,FX2,FX3,FX4,FX5,FX6,FY1,FY2,FY3,FY4,FY5,FY6,
      1R1,R2,R3,R4,R5,R6,R11,R22,R33,R44,R55,R66,PMASS(295)
      OPEN (UNIT=7,FILE='WAVE2.DAT',DEVICE='DSK')
      OPEN (UNIT=21,FILE='WAVE2.DAT')
      OPEN (UNIT=5,DEVICE='DPT',FILE='WAVE2.PRT',ACCESS='SEQUOUT')
      OPEN (UNIT=99,FILE='WAVE2.FIG')
      KPRINT=10000
      NMI=294
      K=1
      DO 4 I=1,295
      X(I,1)=0.
      Y(I,1)=0.
      VX(I,1)=0.
      VY(I,1)=0.
      X(I,2)=0.
      Y(I,2)=0.
      VX(I,2)=0.
      VY(I,2)=0.
      ACX(I)=0.
      ACY(I)=0.
4      CONTINUE
      DO 7 I=1,295
      IF (I.LE.68) GO TO 5
      IF (I.LE.113) GO TO 6
      IF (I.LE.158) GO TO 5
      IF (I.LE.295) GO TO 6
5      PMASS(I)=1.0
      GO TO 7
6      PMASS(I)=1.0
7      CONTINUE
      READ (21,10) (X0(I),Y0(I),VX0(I),VY0(I),I=1,295)
10      FORMAT (2F12.5,2F12.5)
11      DO 20 I=1,295
      WRITE (5,15) I,X0(I),Y0(I),VX0(I),VY0(I)
15      FORMAT (5X,15,2F12.5,2F12.5)
20      CONTINUE
      DO 30 I=1,295
      X(I,1)=X0(I)
      Y(I,1)=Y0(I)
      VX(I,1)=VX0(I)
      VY(I,1)=VY0(I)
30      CONTINUE
      GO TO 71
65      DO 70 I=1,295
      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
      DO 701 I=1,295
      ACX(I)=0.
      ACY(I)=0.
701      CONTINUE

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71

DD 77 1=1,295

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IF (1.EQ.1) GO TO 7008
IF (1.LE.15) GO TO 7001
IF (1.EQ.16) GO TO 7008
IF (1.EQ.17) GO TO 7002
IF (1.LE.30) GO TO 7003
IF (1.EQ.31) GO TO 7004
IF (1.EQ.32) GO TO 7005
IF (1.LE.46) GO TO 7003
IF (1.EQ.47) GO TO 7006
IF (1.EQ.48) GO TO 7002
IF (1.LE.61) GO TO 7003
IF (1.EQ.62) GO TO 7004
IF (1.EQ.63) GO TO 7005
IF (1.LE.77) GO TO 7003
IF (1.EQ.78) GO TO 7006
IF (1.EQ.79) GO TO 7002
IF (1.LE.92) GO TO 7003
IF (1.EQ.93) GO TO 7004
IF (1.EQ.94) GO TO 7005
IF (1.LE.108) GO TO 7003
IF (1.EQ.109) GO TO 7006
IF (1.EQ.110) GO TO 7002
IF (1.LE.123) GO TO 7003
IF (1.EQ.124) GO TO 7004
IF (1.EQ.125) GO TO 7005
IF (1.LE.139) GO TO 7003
IF (1.EQ.140) GO TO 7006
IF (1.EQ.141) GO TO 7002
IF (1.LE.154) GO TO 7003
IF (1.EQ.155) GO TO 7004
IF (1.EQ.156) GO TO 7005
IF (1.LE.170) GO TO 7003
IF (1.EQ.171) GO TO 7006
IF (1.EQ.172) GO TO 7002
IF (1.LE.185) GO TO 7003
IF (1.EQ.186) GO TO 7004
IF (1.EQ.187) GO TO 7005
IF (1.LE.201) GO TO 7003
IF (1.EQ.202) GO TO 7006
IF (1.EQ.203) GO TO 7002
IF (1.LE.216) GO TO 7003
IF (1.EQ.217) GO TO 7004
IF (1.EQ.218) GO TO 7005
IF (1.LE.232) GO TO 7003
IF (1.EQ.233) GO TO 7006
IF (1.EQ.234) GO TO 7002
IF (1.LE.247) GO TO 7003
IF (1.EQ.248) GO TO 7004
IF (1.EQ.249) GO TO 7005
IF (1.LE.263) GO TO 7003
IF (1.EQ.264) GO TO 7006
IF (1.EQ.265) GO TO 7002
IF (1.LE.278) GO TO 7003
IF (1.EQ.279) GO TO 7004
IF (1.EQ.280) GO TO 7011
IF (1.LE.294) GO TO 7007
IF (1.EQ.295) GO TO 7012

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7001 R11=(X(1,1)-X(1-1,1))*2+(Y(1,1)-Y(1-1,1))*2

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R22=(X(1,1)-X(1+1,1))*2+(Y(1,1)-Y(1+1,1))*2
R33=(X(1,1)-X(1+15,1))*2+(Y(1,1)-Y(1+15,1))*2
R44=(X(1,1)-X(1+16,1))*2+(Y(1,1)-Y(1+16,1))*2
R1=DSORT(R11)
R2=DSORT(R22)
R3=DSORT(R33)
R4=DSORT(R44)
F1=PMASS(1)*PMASS(1-1)*(-1.+1./(R11))/(R11**2)
F2=PMASS(1)*PMASS(1+1)*(-1.+1./(R22))/(R22**2)
F3=PMASS(1)*PMASS(1+15)*(-1.+1./(R33))/(R33**2)
F4=PMASS(1)*PMASS(1+16)*(-1.+1./(R44))/(R44**2)
FX1=F1*(X(1,1)-X(1-1,1))/R1
FY1=F1*(Y(1,1)-Y(1-1,1))/R1
FX2=F2*(X(1,1)-X(1+1,1))/R2
FY2=F2*(Y(1,1)-Y(1+1,1))/R2
FX3=F3*(X(1,1)-X(1+15,1))/R3
FY3=F3*(Y(1,1)-Y(1+15,1))/R3
FX4=F4*(X(1,1)-X(1+16,1))/R4
FY4=F4*(Y(1,1)-Y(1+16,1))/R4
ACX(1)=FX1+FX2+FX3+FX4
ACY(1)=FY1+FY2+FY3+FY4
GO TO 77

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7002 R11=(X(1,1)-X(1-16,1))*2+(Y(1,1)-Y(1-16,1))*2
R22=(X(1,1)-X(1-15,1))*2+(Y(1,1)-Y(1-15,1))*2
R33=(X(1,1)-X(1+1,1))*2+(Y(1,1)-Y(1+1,1))*2
R44=(X(1,1)-X(1+15,1))*2+(Y(1,1)-Y(1+15,1))*2
R55=(X(1,1)-X(1+16,1))*2+(Y(1,1)-Y(1+16,1))*2
R1=DSORT(R11)
R2=DSORT(R22)
R3=DSORT(R33)
R4=DSORT(R44)
R5=DSORT(R55)
F1=PMASS(1)*PMASS(1-16)*(-1.+1./(R11))/(R11**2)
F2=PMASS(1)*PMASS(1-15)*(-1.+1./(R22))/(R22**2)
F3=PMASS(1)*PMASS(1+1)*(-1.+1./(R33))/(R33**2)
F4=PMASS(1)*PMASS(1+15)*(-1.+1./(R44))/(R44**2)
F5=PMASS(1)*PMASS(1+16)*(-1.+1./(R55))/(R55**2)
FX1=F1*(X(1,1)-X(1-16,1))/R1
FY1=F1*(Y(1,1)-Y(1-16,1))/R1
FX2=F2*(X(1,1)-X(1-15,1))/R2
FY2=F2*(Y(1,1)-Y(1-15,1))/R2
FX3=F3*(X(1,1)-X(1+1,1))/R3
FY3=F3*(Y(1,1)-Y(1+1,1))/R3
FX4=F4*(X(1,1)-X(1+15,1))/R4
FY4=F4*(Y(1,1)-Y(1+15,1))/R4
FX5=F5*(X(1,1)-X(1+16,1))/R5
FY5=F5*(Y(1,1)-Y(1+16,1))/R5
ACX(1)=FX1+FX2+FX3+FX4+FX5
ACY(1)=FY1+FY2+FY3+FY4+FY5
GO TO 77

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7003 R11=(X(1,1)-X(1-16,1))*2+(Y(1,1)-Y(1-16,1))*2
R22=(X(1,1)-X(1-15,1))*2+(Y(1,1)-Y(1-15,1))*2
R33=(X(1,1)-X(1-1,1))*2+(Y(1,1)-Y(1-1,1))*2
R44=(X(1,1)-X(1+1,1))*2+(Y(1,1)-Y(1+1,1))*2
R55=(X(1,1)-X(1+15,1))*2+(Y(1,1)-Y(1+15,1))*2
R66=(X(1,1)-X(1+16,1))*2+(Y(1,1)-Y(1+16,1))*2
R1=DSORT(R11)
R2=DSORT(R22)
R3=DSORT(R33)
R4=DSORT(R44)

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R5=DSQRT(R55)
R6=DSQRT(R66)
F1=PMASS(1)*PMASS(1-10)*(-1.+1./(R11))/ (R11**2)
F2=PMASS(1)*PMASS(1-15)*(-1.+1./(R22))/ (R22**2)
F3=PMASS(1)*PMASS(1-1)*(-1.+1./(R33))/ (R33**2)
F4=PMASS(1)*PMASS(1+1)*(-1.+1./(R44))/ (R44**2)
F5=PMASS(1)*PMASS(1+15)*(-1.+1./(R55))/ (R55**2)
F6=PMASS(1)*PMASS(1+16)*(-1.+1./(R66))/ (R66**2)
FX1=F1*(X(1,1)-X(1-16,1))/R1
FY1=F1*(Y(1,1)-Y(1-16,1))/R1
FX2=F2*(X(1,1)-X(1-15,1))/R2
FY2=F2*(Y(1,1)-Y(1-15,1))/R2
FX3=F3*(X(1,1)-X(1-1,1))/R3
FY3=F3*(Y(1,1)-Y(1-1,1))/R3
FX4=F4*(X(1,1)-X(1+1,1))/R4
FY4=F4*(Y(1,1)-Y(1+1,1))/R4
FX5=F5*(X(1,1)-X(1+15,1))/R5
FY5=F5*(Y(1,1)-Y(1+15,1))/R5
FX6=F6*(X(1,1)-X(1+16,1))/R6
FY6=F6*(Y(1,1)-Y(1+16,1))/R6
ACX(1)=FX1+FX2+FX3+FX4+FX5+FX6
ACY(1)=FY1+FY2+FY3+FY4+FY5+FY6
GO TO 77

7004  R11=(X(1,1)-X(1-16,1))**2+(Y(1,1)-Y(1-16,1))**2
      R22=(X(1,1)-X(1-15,1))**2+(Y(1,1)-Y(1-15,1))**2
      R33=(X(1,1)-X(1-1,1))**2+(Y(1,1)-Y(1-1,1))**2
      R44=(X(1,1)-X(1+1,1))**2+(Y(1,1)-Y(1+1,1))**2
      R55=(X(1,1)-X(1+15,1))**2+(Y(1,1)-Y(1+15,1))**2
      R66=(X(1,1)-X(1+16,1))**2+(Y(1,1)-Y(1+16,1))**2
R1=DSQRT(R11)
R2=DSQRT(R22)
R3=DSQRT(R33)
R4=DSQRT(R44)
R5=DSQRT(R55)
R6=DSQRT(R66)
F1=PMASS(1)*PMASS(1-16)*(-1.+1./(R11))/ (R11**2)
F2=PMASS(1)*PMASS(1-15)*(-1.+1./(R22))/ (R22**2)
F3=PMASS(1)*PMASS(1-1)*(-1.+1./(R33))/ (R33**2)
F4=PMASS(1)*PMASS(1+1)*(-1.+1./(R44))/ (R44**2)
F5=PMASS(1)*PMASS(1+15)*(-1.+1./(R55))/ (R55**2)
F6=PMASS(1)*PMASS(1+16)*(-1.+1./(R66))/ (R66**2)
FX1=F1*(X(1,1)-X(1-16,1))/R1
FY1=F1*(Y(1,1)-Y(1-16,1))/R1
FX2=F2*(X(1,1)-X(1-15,1))/R2
FY2=F2*(Y(1,1)-Y(1-15,1))/R2
FX3=F3*(X(1,1)-X(1-1,1))/R3
FY3=F3*(Y(1,1)-Y(1-1,1))/R3
FX4=F4*(X(1,1)-X(1+1,1))/R4
FY4=F4*(Y(1,1)-Y(1+1,1))/R4
FX5=F5*(X(1,1)-X(1+15,1))/R5
FY5=F5*(Y(1,1)-Y(1+15,1))/R5
ACX(1)=FX1+FX2+FX3+FX4+FX5
ACY(1)=FY1+FY2+FY3+FY4+FY5
GO TO 77

7005  R11=(X(1,1)-X(1-15,1))**2+(Y(1,1)-Y(1-15,1))**2
      R22=(X(1,1)-X(1+1,1))**2+(Y(1,1)-Y(1+1,1))**2
      R33=(X(1,1)-X(1+16,1))**2+(Y(1,1)-Y(1+16,1))**2
R1=DSQRT(R11)
R2=DSQRT(R22)
R3=DSQRT(R33)
F1=PMASS(1)*PMASS(1-15)*(-1.+1./(R11))/ (R11**2)
F2=PMASS(1)*PMASS(1+1)*(-1.+1./(R22))/ (R22**2)
F3=PMASS(1)*PMASS(1+16)*(-1.+1./(R33))/ (R33**2)

```

```

FX1=F1*(X(1,1)-X(1-15,1))/R1
FY1=F1*(Y(1,1)-Y(1-15,1))/R1
FX2=F2*(X(1,1)-X(1+1,1))/R2
FY2=F2*(Y(1,1)-Y(1+1,1))/R2
FX3=F3*(X(1,1)-X(1+16,1))/R3
FY3=F3*(Y(1,1)-Y(1+16,1))/R3
ACX(1)=FX1+FX2+FX3
ACY(1)=FY1+FY2+FY3
GO TO 77

```

```

7006 R11=(X(1,1)-X(1-16,1))*2+(Y(1,1)-Y(1-16,1))*2
R22=(X(1,1)-X(1-1,1))*2+(Y(1,1)-Y(1-1,1))*2
R33=(X(1,1)-X(1+15,1))*2+(Y(1,1)-Y(1+15,1))*2
R1=DSQRT(R11)
R2=DSQRT(R22)
R3=DSQRT(R33)
F1=PMASS(1)*PMASS(1-16)*(-1.+1./(R11))/(R11*2)
F2=PMASS(1)*PMASS(1-1)*(-1.+1./(R22))/(R22*2)
F3=PMASS(1)*PMASS(1+15)*(-1.+1./(R33))/(R33*2)
FX1=F1*(X(1,1)-X(1-16,1))/R1
FY1=F1*(Y(1,1)-Y(1-16,1))/R1
FX2=F2*(X(1,1)-X(1-1,1))/R2
FY2=F2*(Y(1,1)-Y(1-1,1))/R2
FX3=F3*(X(1,1)-X(1+15,1))/R3
FY3=F3*(Y(1,1)-Y(1+15,1))/R3
ACX(1)=FX1+FX2+FX3
ACY(1)=FY1+FY2+FY3
GO TO 77

```

```

7011 R11=(X(1,1)-X(1+1,1))*2+(Y(1,1)-Y(1+1,1))*2
R33=(X(1,1)-X(1-15,1))*2+(Y(1,1)-Y(1-15,1))*2
R1=DSQRT(R11)
R3=DSQRT(R33)
F1=PMASS(1)*PMASS(1+1)*(-1.+1./(R11))/(R11*2)
F3=PMASS(1)*PMASS(1-15)*(-1.+1./(R33))/(R33*2)
FX1=F1*(X(1,1)-X(1+1,1))/R1
FY1=F1*(Y(1,1)-Y(1+1,1))/R1
FX3=F3*(X(1,1)-X(1-15,1))/R3
FY3=F3*(Y(1,1)-Y(1-15,1))/R3
ACX(1)=FX1+FX3
ACY(1)=FY1+FY3
GO TO 77

```

```

7007 R11=(X(1,1)-X(1-16,1))*2+(Y(1,1)-Y(1-16,1))*2
R22=(X(1,1)-X(1-15,1))*2+(Y(1,1)-Y(1-15,1))*2
R33=(X(1,1)-X(1-1,1))*2+(Y(1,1)-Y(1-1,1))*2
R44=(X(1,1)-X(1+1,1))*2+(Y(1,1)-Y(1+1,1))*2
R1=DSQRT(R11)
R2=DSQRT(R22)
R3=DSQRT(R33)
R4=DSQRT(R44)
F1=PMASS(1)*PMASS(1-16)*(-1.+1./(R11))/(R11*2)
F2=PMASS(1)*PMASS(1-15)*(-1.+1./(R22))/(R22*2)
F3=PMASS(1)*PMASS(1-1)*(-1.+1./(R33))/(R33*2)
F4=PMASS(1)*PMASS(1+1)*(-1.+1./(R44))/(R44*2)
FX1=F1*(X(1,1)-X(1-16,1))/R1
FY1=F1*(Y(1,1)-Y(1-16,1))/R1
FX2=F2*(X(1,1)-X(1-15,1))/R2
FY2=F2*(Y(1,1)-Y(1-15,1))/R2
FX3=F3*(X(1,1)-X(1-1,1))/R3
FY3=F3*(Y(1,1)-Y(1-1,1))/R3
FX4=F4*(X(1,1)-X(1+1,1))/R4
FY4=F4*(Y(1,1)-Y(1+1,1))/R4

```



```

ACX(1)=FX1+FX2+FX3+FX4
ACY(1)=FY1+FY2+FY3+FY4
GO TO 77
7012  R22=(X(1,1)-X(1-1,1))**2+(Y(1,1)-Y(1-1,1))**2
      R44=(X(1,1)-X(1-16,1))**2+(Y(1,1)-Y(1-16,1))**2
      R2=DSQRT(R22)
      R4=DSQRT(R44)
      F2=PMASS(1)*PMASS(1-1)*(-1.+1./(R22))/(R22**2)
      F4=PMASS(1)*PMASS(1-16)*(-1.+1./(R44))/(R44**2)
      FX2=F2*(X(1,1)-X(1-1,1))/R2
      FY2=F2*(Y(1,1)-Y(1-1,1))/R2
      FX4=F4*(X(1,1)-X(1-16,1))/R4
      FY4=F4*(Y(1,1)-Y(1-16,1))/R4
      ACX(1)=FX2+FX4
      ACY(1)=FY2+FY4
      GO TO 77
7008  ACX(1)=0.
      ACY(1)=0.
      GO TO 77
7009  R22=(X(1,1)-X(1+1,1))**2+(Y(1,1)-Y(1+1,1))**2
      R44=(X(1,1)-X(1+16,1))**2+(Y(1,1)-Y(1+16,1))**2
      R2=DSQRT(R22)
      R4=DSQRT(R44)
      F2=PMASS(1)*PMASS(1+1)*(-1.+1./(R22))/(R22**2)
      F4=PMASS(1)*PMASS(1+16)*(-1.+1./(R44))/(R44**2)
      FX2=F2*(X(1,1)-X(1+1,1))/R2
      FY2=F2*(Y(1,1)-Y(1+1,1))/R2
      FX4=F4*(X(1,1)-X(1+16,1))/R4
      FY4=F4*(Y(1,1)-Y(1+16,1))/R4
      ACX(1)=FX2+FX4
      ACY(1)=FY2+FY4
      GO TO 77
7010  R11=(X(1,1)-X(1-1,1))**2+(Y(1,1)-Y(1-1,1))**2
      R33=(X(1,1)-X(1+15,1))**2+(Y(1,1)-Y(1+15,1))**2
      R1=DSQRT(R11)
      R3=DSQRT(R33)
      F1=PMASS(1)*PMASS(1-1)*(-1.+1./(R11))/(R11**2)
      F3=PMASS(1)*PMASS(1+15)*(-1.+1./(R33))/(R33**2)
      FX1=F1*(X(1,1)-X(1-1,1))/R1
      FY1=F1*(Y(1,1)-Y(1-1,1))/R1
      FX3=F3*(X(1,1)-X(1+15,1))/R3
      FY3=F3*(Y(1,1)-Y(1+15,1))/R3
      ACX(1)=FX1+FX3
      ACY(1)=FY1+FY3
77    CONTINUE
DO 7100 I=1,295
  ACX(1)=ACX(1)/PMASS(1)
  ACY(1)=ACY(1)/PMASS(1)
7100  CONTINUE
DO 7123 I=1,295
7986  VX(1,2)=VX(1,1)+0.0001*ACX(1)
      VY(1,2)=VY(1,1)+0.0001*ACY(1)
      X(1,2)=X(1,1)+0.0001*VX(1,2)
      Y(1,2)=Y(1,1)+0.0001*VY(1,2)
7123  CONTINUE
8043  K=K+1
      IF (MOD(K,KPRINT).GT.0) GO TO 82
      DO 810 I=1,295
C THE NEXT C SHOULD BE REMOVED WHEN PRINT IS DESIRED.
      WRITE (5,81) K,I,X(1,2),Y(1,2),VX(1,2),VY(1,2)

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```
81      FORMAT (5X,11Z,15,2F13.6,2F13.6)
      WRITE (99,10) X(1,2),Y(1,2),VX(1,2),VY(1,2)
810     CONTINUE
82      IF (K.LT.20000) GO TO 65
102     WRITE (7,10) (X(1,2),Y(1,2),VX(1,2),VY(1,2),I=1,
1295)
      STOP
      END
```

APPENDIX B - INITIAL DATA

i	x _i	y _i			
1	-7.50000	0.00000	60	5.00000	2.59800
2	-6.50000	0.00000	61	6.00000	2.59800
3	-5.50000	0.00000	62	7.00000	2.59800
4	-4.50000	0.00000	63	-7.50000	3.46400
5	-3.50000	0.00000	64	-6.50000	3.46400
6	-2.50000	0.00000	65	-5.50000	3.46400
7	-1.50000	0.00000	66	-4.50000	3.46400
8	-0.50000	0.00000	67	-3.50000	3.46400
9	0.50000	0.00000	68	-2.50000	3.46400
10	1.50000	0.00000	69	-1.50000	3.46400
11	2.50000	0.00000	70	-0.50000	3.46400
12	3.50000	0.00000	71	0.50000	3.46400
13	4.50000	0.00000	72	1.50000	3.46400
14	5.50000	0.00000	73	2.50000	3.46400
15	6.50000	0.00000	74	3.50000	3.46400
16	7.50000	0.00000	75	4.50000	3.46400
17	-7.00000	0.86600	76	5.50000	3.46400
18	-6.00000	0.86600	77	6.50000	3.46400
19	-5.00000	0.86600	78	7.50000	3.46400
20	-4.00000	0.86600	79	-7.00000	4.33000
21	-3.00000	0.86600	80	-6.00000	4.33000
22	-2.00000	0.86600	81	-5.00000	4.33000
23	-1.00000	0.86600	82	-4.00000	4.33000
24	0.00000	0.86600	83	-3.00000	4.33000
25	1.00000	0.86600	84	-2.00000	4.33000
26	2.00000	0.86600	85	-1.00000	4.33000
27	3.00000	0.86600	86	0.00000	4.33000
28	4.00000	0.86600	87	1.00000	4.33000
29	5.00000	0.86600	88	2.00000	4.33000
30	6.00000	0.86600	89	3.00000	4.33000
31	7.00000	0.86600	90	4.00000	4.33000
32	-7.50000	1.73200	91	5.00000	4.33000
33	-6.50000	1.73200	92	6.00000	4.33000
34	-5.50000	1.73200	93	7.00000	4.33000
35	-4.50000	1.73200	94	-7.50000	5.19600
36	-3.50000	1.73200	95	-6.50000	5.19600
37	-2.50000	1.73200	96	-5.50000	5.19600
38	-1.50000	1.73200	97	-4.50000	5.19600
39	-0.50000	1.73200	98	-3.50000	5.19600
40	0.50000	1.73200	99	-2.50000	5.19600
41	1.50000	1.73200	100	-1.50000	5.19600
42	2.50000	1.73200	101	-0.50000	5.19600
43	3.50000	1.73200	102	0.50000	5.19600
44	4.50000	1.73200	103	1.50000	5.19600
45	5.50000	1.73200	104	2.50000	5.19600
46	6.50000	1.73200	105	3.50000	5.19600
47	7.50000	1.73200	106	4.50000	5.19600
48	-7.00000	2.59800	107	5.50000	5.19600
49	-6.00000	2.59800	108	6.50000	5.19600
50	-5.00000	2.59800	109	7.50000	5.19600
51	-4.00000	2.59800	110	-7.00000	6.06200
52	-3.00000	2.59800	111	-6.00000	6.06200
53	-2.00000	2.59800	112	-5.00000	6.06200
54	-1.00000	2.59800	113	-4.00000	6.06200
55	0.00000	2.59800	114	-3.00000	6.06200
56	1.00000	2.59800	115	-2.00000	6.06200
57	2.00000	2.59800	116	-1.00000	6.06200
58	3.00000	2.59800	117	0.00000	6.06200
59	4.00000	2.59800	118	1.00000	6.06200
			119	2.00000	6.06200

120	3.00000	6.06200	180	1.00000	9.52600
121	4.00000	6.06200	181	2.00000	9.52600
122	5.00000	6.06200	182	3.00000	9.52600
123	6.00000	6.06200	183	4.00000	9.52600
124	7.00000	6.06200	184	5.00000	9.52600
125	-7.50000	6.92800	185	6.00000	9.52600
126	-6.50000	6.92800	186	7.00000	9.52600
127	-5.50000	6.92800	187	-7.50000	10.39200
128	-4.50000	6.92800	188	-6.50000	10.39200
129	-3.50000	6.92800	189	-5.50000	10.39200
130	-2.50000	6.92800	190	-4.50000	10.39200
131	-1.50000	6.92800	191	-3.50000	10.39200
132	-0.50000	6.92800	192	-2.50000	10.39200
133	0.50000	6.92800	193	-1.50000	10.39200
134	1.50000	6.92800	194	-0.50000	10.39200
135	2.50000	6.92800	195	0.50000	10.39200
136	3.50000	6.92800	196	1.50000	10.39200
137	4.50000	6.92800	197	2.50000	10.39200
138	5.50000	6.92800	198	3.50000	10.39200
139	6.50000	6.92800	199	4.50000	10.39200
140	7.50000	6.92800	200	5.50000	10.39200
141	-7.00000	7.79400	201	6.50000	10.39200
142	-6.00000	7.79400	202	7.50000	10.39200
143	-5.00000	7.79400	203	-7.00000	11.25800
144	-4.00000	7.79400	204	-6.00000	11.25800
145	-3.00000	7.79400	205	-5.00000	11.25800
146	-2.00000	7.79400	206	-4.00000	11.25800
147	-1.00000	7.79400	207	-3.00000	11.25800
148	0.00000	7.79400	208	-2.00000	11.25800
149	1.00000	7.79400	209	-1.00000	11.25800
150	2.00000	7.79400	210	0.00000	11.25800
151	3.00000	7.79400	211	1.00000	11.25800
152	4.00000	7.79400	212	2.00000	11.25800
153	5.00000	7.79400	213	3.00000	11.25800
154	6.00000	7.79400	214	4.00000	11.25800
155	7.00000	7.79400	215	5.00000	11.25800
156	-7.50000	8.66000	216	6.00000	11.25800
157	-6.50000	8.66000	217	7.00000	11.25800
158	-5.50000	8.66000	218	-7.50000	12.12400
159	-4.50000	8.66000	219	-6.50000	12.12400
160	-3.50000	8.66000	220	-5.50000	12.12400
161	-2.50000	8.66000	221	-4.50000	12.12400
162	-1.50000	8.66000	222	-3.50000	12.12400
163	-0.50000	8.66000	223	-2.50000	12.12400
164	0.50000	8.66000	224	-1.50000	12.12400
165	1.50000	8.66000	225	-0.50000	12.12400
166	2.50000	8.66000	226	0.50000	12.12400
167	3.50000	8.66000	227	1.50000	12.12400
168	4.50000	8.66000	228	2.50000	12.12400
169	5.50000	8.66000	229	3.50000	12.12400
170	6.50000	8.66000	230	4.50000	12.12400
171	7.50000	8.66000	231	5.50000	12.12400
172	-7.00000	9.52600	232	6.50000	12.12400
173	-6.00000	9.52600	233	7.50000	12.12400
174	-5.00000	9.52600	234	-7.00000	12.99000
175	-4.00000	9.52600	235	-6.00000	12.99000
176	-3.00000	9.52600	236	-5.00000	12.99000
177	-2.00000	9.52600	237	-4.00000	12.99000
178	-1.00000	9.52600	238	-3.00000	12.99000
179	0.00000	9.52600	239	-2.00000	12.99000

240	-1.00000	12.99000
241	0.00000	12.99000
242	1.00000	12.99000
243	2.00000	12.99000
244	3.00000	12.99000
245	4.00000	12.99000
246	5.00000	12.99000
247	6.00000	12.99000
248	7.00000	12.99000
249	-7.50000	13.85600
250	-6.50000	13.85600
251	-5.50000	13.85600
252	-4.50000	13.85600
253	-3.50000	13.85600
254	-2.50000	13.85600
255	-1.50000	13.85600
256	-0.50000	13.85600
257	0.50000	13.85600
258	1.50000	13.85600
259	2.50000	13.85600
260	3.50000	13.85600
261	4.50000	13.85600
262	5.50000	13.85600
263	6.50000	13.85600
264	7.50000	13.85600
265	-7.00000	14.72200
266	-6.00000	14.72200
267	-5.00000	14.72200
268	-4.00000	14.72200
269	-3.00000	14.72200
270	-2.00000	14.72200
271	-1.00000	14.72200
272	0.00000	14.72200
273	1.00000	14.72200
274	2.00000	14.72200
275	3.00000	14.72200
276	4.00000	14.72200
277	5.00000	14.72200
278	6.00000	14.72200
279	7.00000	14.72200
280	-7.50000	15.58800
281	-6.50000	15.58800
282	-5.50000	15.58800
283	-4.50000	15.58800
284	-3.50000	15.58800
285	-2.50000	15.58800
286	-1.50000	15.58800
287	-0.50000	15.58800
288	0.50000	15.58800
289	1.50000	15.58800
290	2.50000	15.58800
291	3.50000	15.58800
292	4.50000	15.58800
293	5.50000	15.58800
294	6.50000	15.58800
295	7.50000	15.58800