QUASI-MOLECULAR, PARTICLE MODELING OF CRACK GENERATION
AND FRACTURE

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Abstract

In this paper a new, particle-type approach is developed for the simulation of crack generation and fracture. Rectangular plates are modeled as particle aggregates and then stressed by using molecular type force formulas. Computer examples which include wedges and holes are described and discussed.

1. Introduction. The study of fracture and crack growth is of interest, for example, to engineers, mathematicians, and geologists (see, e.g., [1] - [14], [17], [19] - [27] , [29] - [31]). Most studies, whether experimental, theoretical, or numerical, have emphasized brittle materials, tensile forces, and stress concentration factors near crack tips. However, interest is also manifest in crack propagation rates, energy release rates, branching, temperature dependence, compressive and impulsive force effects, and effects of impurities and fatigue. In theoretical modeling, materials are usually assumed to behave linearly and to be continuous, homogeneous, and isotropic.

In this paper, we will initiate a new, computer oriented, quasi-molecular approach ([15] , [18]) to the study of crack and fracture generation. The models will not require the severe constraints imposed on continuous models, will allow for highly nonlinear behavior, and will be more consistent with the knowledge that the phenomena to be studied occur on the atomic and molecular levels. Though the method will be described in complete generality, we will, however, apply it specifically to phenomena related to crack generation due to tensile forces.

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 [15]. 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 [15] .

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 [16]. Extensions and modifications for the examples which follow can be developed easily from it.

4. Examples. Let us begin by considering a flat, rectangular sheet which is to be stressed on top and on bottom. We assume first that the sheet has a large interior crack.

As shown in Figure 1, the sheet is approximated by a set of one hundred forty six particles P_1 - P_{146} . The exact coordinates of the particles, in the XY system shown in Figure 2, are given in the TABLE. The distance between each particle and any adjacent particle is unity, though this is not apparent from the figures because the units on the coordinate axes are slightly different. All particles are assigned unit masses and zero initial velocities.

The neighbors of any given particle are defined to be those particles which are adjacent to the given particle in the usual numerical sense. For example, in the given mosaic, the neighbors of P_1 are P_2 and P_{15} ; those of P_3 are P_2 , P_4 , P_{16} , P_{17} ; those of P_{15} are P_1 , P_2 , P_{16} , P_{28} , P_{29} ; those of P_{17} are P_3 , P_4 , P_{16} , P_{18} , P_{30} , P_{31} ; those of P_{28} are P_{15} , P_{29} , P_{42} ; those of P_{47} are P_{33} , P_{34} , P_{46} , P_{48} , P_{60} ; those of P_{61} are P_{48} , P_{49} , P_{62} , P_{74} ; those of P_{73} are P_{60} , P_{72} , P_{85} , P_{86} ; those of P_{111} are P_{97} , P_{98} , P_{110} , P_{112} , P_{124} , P_{125} ; and those of P_{140} are P_{126} , P_{127} , P_{139} , P_{141} .

Throughout, the parameter choices in (3.1)-(3.5) are $p = 4$, $q = 6$, $G = H = 1$, $\Delta t = 10^{-4}$.

Since all initial data and parameters are now fixed, we proceed to apply tensile forces in the following way. At each time step, that is, every 10^{-4} time units, the particles P_1 - P_{14} are relocated so that their X coordinates remain the same, their Y coordinates

Figure 1. Particle configuration.

Figure 2. Coordinate system.

TABLE

i	x	y	i	x	y	i	x	y
1	-6.50000	-4.330	60	-1.50000	-0.866	120	-6.00000	3.464
2	-5.50000	-4.330	61	0.50000	-0.866	121	-5.00000	3.464
3	-4.50000	-4.330	62	1.50000	-0.866	122	-4.00000	3.464
4	-3.50000	-4.330	63	2.50000	-0.866	123	-3.00000	3.464
5	-2.50000	-4.330	64	3.50000	-0.866	124	-2.00000	3.464
6	-1.50000	-4.330	65	4.50000	-0.866	125	-1.00000	3.464
7	-0.50000	-4.330	66	5.50000	-0.866	126	0.00000	3.464
8	0.50000	-4.330	67	6.50000	-0.866	127	1.00000	3.464
9	1.50000	-4.330	68	-6.00000	0.000	128	2.00000	3.464
0	2.50000	-4.330	69	-5.00000	0.000	129	3.00000	3.464
1	3.50000	-4.330	70	-4.00000	0.000	130	4.00000	3.464
2	4.50000	-4.330	71	-3.00000	0.000	131	5.00000	3.464
3	5.50000	-4.330	72	-2.00000	0.000	132	6.00000	3.464
4	6.50000	-4.330	73	-1.00000	0.000	133	-6.50000	4.330
5	-6.00000	-3.464	74	1.00000	0.000	134	-5.50000	4.330
6	-5.00000	-3.464	75	2.00000	0.000	135	-4.50000	4.330
7	-4.00000	-3.464	76	3.00000	0.000	136	-3.50000	4.330
8	-3.00000	-3.464	77	4.00000	0.000	137	-2.50000	4.330
9	-2.00000	-3.464	78	5.00000	0.000	138	-1.50000	4.330
0	-1.00000	-3.464	79	6.00000	0.000	139	-0.50000	4.330
1	0.00000	-3.464	80	-6.50000	0.866	140	0.50000	4.330
2	1.00000	-3.464	81	-5.50000	0.866	141	1.50000	4.330
3	2.00000	-3.464	82	-4.50000	0.866	142	2.50000	4.330
4	3.00000	-3.464	83	-3.50000	0.866	143	3.50000	4.330
5	4.00000	-3.464	84	-2.50000	0.866	144	4.50000	4.330
6	5.00000	-3.464	85	-1.50000	0.866	145	5.50000	4.330
7	6.00000	-3.464	86	-0.50000	0.866	146	6.50000	4.330
8	-6.50000	-2.598	87	1.50000	0.866			
9	-5.50000	-2.598	88	2.50000	0.866			
0	-4.50000	-2.598	89	3.50000	0.866			
1	-3.50000	-2.598	90	4.50000	0.866			
2	-2.50000	-2.598	91	5.50000	0.866			
3	-1.50000	-2.598	92	6.50000	0.866			
4	-0.50000	-2.598	93	-6.00000	1.732			
5	0.50000	-2.598	94	-5.00000	1.732			
6	1.50000	-2.598	95	-4.00000	1.732			
7	2.50000	-2.598	96	-3.00000	1.732			
8	3.50000	-2.598	97	-2.00000	1.732			
9	4.50000	-2.598	98	-1.00000	1.732			
0	5.50000	-2.598	99	0.00000	1.732			
1	6.50000	-2.598	100	1.00000	1.732			
2	-6.00000	-1.732	101	2.00000	1.732			
3	-5.00000	-1.732	102	3.00000	1.732			
4	-4.00000	-1.732	103	4.00000	1.732			
5	-3.00000	-1.732	104	5.00000	1.732			
6	-2.00000	-1.732	105	6.00000	1.732			
7	-1.00000	-1.732	106	-6.50000	2.598			
8	0.00000	-1.732	107	-5.50000	2.598			
9	1.00000	-1.732	108	-4.50000	2.598			
0	2.00000	-1.732	109	-3.50000	2.598			
1	3.00000	-1.732	110	-2.50000	2.598			
2	4.00000	-1.732	111	-1.50000	2.598			
3	5.00000	-1.732	112	-0.50000	2.598			
4	6.00000	-1.732	113	0.50000	2.598			
5	-6.50000	-0.866	114	1.50000	2.598			
6	-5.50000	-0.866	115	2.50000	2.598			
7	-4.50000	-0.866	116	3.50000	2.598			
8	-3.50000	-0.866	117	4.50000	2.598			
9	-2.50000	-0.866	118	5.50000	2.598			
			119	6.50000	2.598			

are decreased by 0.0000001, and their velocities are set to zero. The particles P_{133} - P_{146} are treated similarly with the exception that their Y coordinates are increased by 0.0000001. In this fashion, the top and bottom rows are stretched. Each remaining particle reacts to this stretching process by interacting with its neighbors in accordance with (3.1)-(3.5). Finally, we impose an elastic limit L in the following way. If and when a particle and one of its neighbors move a distance apart which is greater than L , then the force between these particles is set to zero and their bond is considered to be broken thereafter, thereby simulating the generation of a crack.

For $L = 1.004$, Figures 3-7 show the developing force field throughout the sheet at the times $T = 1, 2, 5, 11, 16$, i.e., after 10000, 20000, 50000, 110000, 160000 time steps, respectively. In these figures, the force field is represented by vectors emanating from the centers of the particles. Figure 3 reveals the stress effect being transmitted to the interior of the sheet. Though this transmission occurs in a relatively short time, the fact that it is not instantaneous is significant, as will be shown later in the application of an impulsive force. Figure 4 shows that at $T = 2$ the maximum stress is now at the ends of the large crack. By the time $T = 5$, as shown in Figure 5, the greatest stress around the large crack has now shifted to the sides of the crack. At $T = 11$, one now finds that the directions of the forces around the sides of the large crack are changing significantly. Finally, at $T = 16$, as shown in Figure 7, one sees clearly from the force field that a hairline crack has now developed on the lower left

and upper right sides of the large crack. And, indeed, the computer output does show that the distances $|P_{60}P_{72}|$, $|P_{60}P_{73}|$, $|P_{74}P_{87}|$, $|P_{75}P_{87}|$ are now greater than 1.004.

Figure 8 shows at $T=18$ the relatively rapid growth of the hairline cracks from the central area of the configuration and, in addition, the development of additional hairline cracks at the lower left and upper right.

For our second example, let us reconsider the first example with only one change. Instead of moving the points P_1-P_{14} and $P_{133}-P_{146}$ a distance 0.0000001 every time step, let us move them 0.00001. The resulting simulation corresponds to an impulsive force, that is, one which does not allow sufficient time for its effect to be transmitted to the interior. By the time $T=1.6$, both the top and the bottom have been pulled off from the larger configuration. Figure 9 shows the force field at the time $T=1.5$, just prior to the fracture.

For our third example, we will show that the concept of an impulsive force is relative by considering a more flexible material than that considered in the two examples above. For this purpose, we consider the same parameters as in the second example, but with only one change, that is, the elastic limit is set to $L=1.3$. With such a limit the sheet should show extensive stretching. Figures 10-12, at times 2.1, 4.1, and 5.6, respectively, show exactly this behavior. Moreover, the development of the force field is

entirely similar to that shown in Figures 3-7, with the newly developed cracks in Figure 12 at the same places as in Figure 7. It must be indicated immediately that the force field in Figure 12 is approximately ten times greater in magnitude than that shown in Figure 7, but that rescaling for illustrative purposes has concealed this fact.

As a fourth, and final, example, we consider a modification of the sheet shown in Figure 1. The three particles P_7 , P_8 , P_{21} are reset to fill in the large central crack, thus resulting in a sheet with a wedge on the bottom, as shown in Figure 13. The configuration is now stretched right and left by moving the right and left boundary particles a distance 0.0000001 every time step. For the elastic limit $L=1.0015$, Figures 14-17 show the developing force field throughout the sheet at the respective times $T=2, 4, 5, 5.2$. Figures 17 and 18 show the force field and the crack development at $T=5.2$.

Figure 3. Example 1 at $T = 1$.

Figure 4. Example 1 at $T = 2$.

Figure 5. Example 1 at $T = 5$.

Figure 6. Example 1 at $T = 11$.

Figure 7. Example 1 at $T = 16$.

Figure 8. Example 1 at $T=18$.

Figure 9. Example 2 at $T = 1.5$.

Figure 10. Example 3 at $T = 2.1$.

Figure 11. Example 3 at $T = 4.1$.

Figure 12. Example 3 at $T = 5.6$.

Figure 13. Wedge configuration.

Figure 14. Example 4 at $T=2$.

Figure 15. Example 4 at $T=4$.

Figure 16. Example 4 at $T=5$.

Figure 17. Example 4 at $T=5.2$.

Figure 18. Example 4 at $T=5.2$.

5. Remarks. A variety of examples similar to those of Section 4 were run in addition. No significant qualitative differences resulted. Of course, quantitative results for specific materials should be established next. The approach contemplated will follow that of Reeves and Greenspan for aluminum bars [28] .

Initial calculations for simulating the effects of compressive forces indicate that a more general approach than that of this paper is required. The concept of a neighbor as defined in Section 4 must be extended to allow for complex motions which can occur under compression.

Another variable worth considering in future calculations is temperature. Clearly, the application of tensile forces, for example, to stretch a sheet increases the energy of the particles of the sheet. When the temperature of the sheet increases to a value above that of the surrounding medium, the sheet will transfer energy to that medium. Mathematically, this could be implemented by damping the particle velocities. However, the implementation of this idea does not appear to be trivial because preliminary calculations indicate a high degree of sensitivity to choices of damping factors.

Finally, we remark that the development of vector and parallel computers makes our approach most attractive, since on such machines the calculations for all the particles can be done simultaneously at each time step.

References

1. J. D. Achenbach, "Wave propagation, elastodynamic stress intensity factors and fractures", in Theoretical and Applied Mechanics, Proc. 14th IUTAM Congress, North Holland, Amsterdam, 1976, p. 71.
2. J. C. Amazigo and J. W. Hutchinson, "Crack-tip fields in steady crack growth with linear strain-hardening", J. Mech. Phys. Solids, 25, 1977, p. 81.
3. E. G. Bombolakis, "Photoelastic study of initial stages of brittle fracture in compression", Int. J. Tectonophys., 6, 1968, p. 461.
4. K. B. Broberg, "Crack-growth criteria in non-linear fracture mechanics", J. Mech. Phys. Solids, 19, 1971, p. 407.
5. B. Budiansky and J. R. Rice, "Conservation laws and energy release rates", J. Appl. Mech., 40, 1973, p. 201.
6. R. Burridge (Editor), Fracture Mechanics, Amer. Math. Soc., Providence, R.I., 1978.
7. G. P. Cherepanov, Mechanics of Brittle Fracture (in Russian), Publishing House "Hauka", Moscow, 1972.
8. J. Congleton and N. J. Petch, "Crack-branching", Phil. Mag., 16, 1967, p. 749.
9. B. Cotterell, "Brittle fracture in compression", Int. J. Fracture Mech., 8, 1972, p. 195.
10. S. Das and K. Aki, "Fault plane with barriers: a versatile earthquake model", J. Geophys. Res., 82, 1977, p. 5658.

11. G. T. Dvorak and H. C. Tang, "The influence of material properties in dynamic fracture toughness of steels", Eng. Fracture Mech., 5, 1973, p. 91.
12. G. D. Fearnehough and R. W. Nichols, "Fracture mechanism considerations in the Charpy impact test", Int. J. Fracture Mech., 4, 1968, p. 245.
13. S. W. Freeman (Editor), Fracture Mechanics Applied to Brittle Materials, ASTM, Philadelphia, 1979.
14. L. B. Freund, "Stress intensity factor calculations based on a conservation integral", Int. J. of Solids and Structures, 14, 1978, p. 241.
15. D. Greenspan, Arithmetic Applied Mathematics, Pergamon, Oxford, 1980.
16. D. Greenspan, "Quasi-molecular , particle modeling of crack generation and fracture", TR 208, Dept. Math., Univ. Texas at Arlington, 1984.
17. R. W. Hertzberg, Deformation and Fracture Mechanics of Engineering Materials, Wiley, N.Y., 1976.
18. R. W. Hockney and J. W. Eastwood, Computer Simulation Using Particles, McGraw-Hill, N.Y., 1981.
19. J. A. Hudson, M. P. Hardy and C. Fairhurst, "The failure of rock beams: Part I - Theoretical studies", Int. J. Rock Mech. Min. Sci., 10, 1973, p. 69.
20. M. F. Kanninen, "A critical appraisal of solution techniques in dynamic fracture mechanics", in Numerical Methods in Fracture Mechanics, Univ. Coll. of Swansea, Swansea, UK, 1978.

21. F. Kerkhof, Bruchvorange in Glasern, Verlage der Deutschen Glastetechnischen Gesellschaft, Frankfurt, 1970.
22. J. K. Knowles and E. Sternberg, "On a class of conservation laws in linearized and finite elastostatics", Arch. Rat. Mech. and Anal., 44, 1972, p. 187.
23. A. S. Kobayashi, B. G. Wade and D. E. Maiden, "Photoelastic investigation on the crack-arrest capability of a hole", Exp. Mech., 12, 1972, p. 32.
24. H. Kolsky, Stress Waves in Solids, Dover, N.Y., 1964.
25. H. Liebowitz (Editor), Fracture, an Advanced Treatise, Academic, N.Y., 1968.
26. R. Madariago, "Dynamics of an expanding circular fault", Bull. Seism. Soc. Amer., 65, 1976, p. 163.
27. N. Perrone and S. N. Alturi (Editors), Nonlinear and Dynamic Fracture Mechanics, ASME, N.Y., 1979.
28. W. R. Reeves and D. Greenspan, "An analysis of stress wave propagation in slender bars using a discrete particle approach", Applied Math. Modelling, 6, 1982, p. 185.
29. R. L. Sierakowski, G. E. Nevill, C. A. Ross and E. R. Jones, "Dynamic compressive strength and failure of steel reinforced epoxy composites", J. Comp. Mat., 5, 1971, p. 362.
30. G. C. Sih (Editor), Dynamic Crack Propagation, Noordhoff, Leiden, 1973.
31. I. N. Sneddon and M. Lowengrub, Crack Problems in the Classical Theory of Elasticity, Wiley, N.Y., 1969.
32. S. P. Timoshenko and J. N. Goodier, Theory of Elasticity, 3rd Ed., McGraw Hill, N.Y., 1970.

APPENDIX

C THIS IS THE 2D FRACTURE PROGRAM. TENSILE FORCES ARE UP ON
 C BOTTOM, DOWN ON TOP. THE GIVEN PLATE HAD 149 PARTICLES, OF
 C WHICH 3 ARE GIVEN ZERO MASS TO MAKE A CRACK. ALL OTHER
 C MASSES ARE 1. FORCE IS LIKE $-1/R^{**4}+1./R^{**6}$. CRACK IS AT
 C A SLANT. 100000 STEPS TAKES ABOUT 3 HOURS.

```
DOUBLE PRECISION XO(149),YO(149),VXO(149),VYO(149),
1X(149,2),Y(149,2),VX(149,2),VY(149,2),
1ACX(149),ACY(149),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(149)
OPEN (UNIT=7,FILE='FRAC16.OUT',DEVICE='DSK')
OPEN (UNIT=21,FILE='FRAC16.DAT')
OPEN (UNIT=5,DEVICE='LPT',FILE='FRAC16.PRT',ACCESS='SEQOUT')
OPEN (UNIT=99,FILE='FRAC16.FIG')
KPRINT=10000
```

```
9976 FORMAT (2X,I6,F9.5)
9977 FORMAT (2X,I6,6F9.5)
9978 FORMAT (2X,I6,5F9.5)
9979 FORMAT (2X,I6,3F9.5)
```

```
NM1=148
K=1
DO 4 I=1,149
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.
PMASS(I)=1.
```

```
4 CONTINUE
PMASS(61)=0.
PMASS(75)=0.
PMASS(89)=0.
READ (21,10) (XO(I),YO(I),VXO(I),VYO(I),I=1,149)
```

```
10 FORMAT (2F12.5,2F12.5)
11 DO 20 I=1,149
WRITE (5,15) I,XO(I),YO(I),VXO(I),VYO(I)
15 FORMAT (5X,I5,2F12.5,2F12.5)
20 CONTINUE
```

```
DO 30 I=1,149
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=1,149
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=1,149
ACX(I)=0.
ACY(I)=0.
```

701 CONTINUE

71 DO 77 I=1,149

IF (I.LE.14) GO TO 7001

IF (I.EQ.15) GO TO 7002

IF (I.LT.27) GO TO 7003

IF (I.EQ.27) GO TO 7004

IF (I.EQ.28) GO TO 7005

IF (I.LT.41) GO TO 7003

IF (I.EQ.41) GO TO 7006

IF (I.EQ.42) GO TO 7002

IF (I.LT.54) GO TO 7003

IF (I.EQ.54) GO TO 7004

IF (I.EQ.55) GO TO 7005

IF (I.LT.68) GO TO 7003

IF (I.EQ.68) GO TO 7006

IF (I.EQ.69) GO TO 7002

IF (I.LE.75) GO TO 7003

IF (I.LE.149) GO TO 7019

7001 ACX(I)=0.

ACY(I)=0.

GO TO 77

7002 R11=(X(I,1)-X(I-14,1))**2+(Y(I,1)-Y(I-14,1))**2

R22=(X(I,1)-X(I-13,1))**2+(Y(I,1)-Y(I-13,1))**2

R33=(X(I,1)-X(I+1,1))**2+(Y(I,1)-Y(I+1,1))**2

R44=(X(I,1)-X(I+13,1))**2+(Y(I,1)-Y(I+13,1))**2

R55=(X(I,1)-X(I+14,1))**2+(Y(I,1)-Y(I+14,1))**2

R1=DSQRT(R11)

R2=DSQRT(R22)

R3=DSQRT(R33)

R4=DSQRT(R44)

R5=DSQRT(R55)

F1=PMASS(I)*PMASS(I-14)*(-1.+1./(R11))/(R11**2)

IF (R1.GT.1.004) F1=0.

F2=PMASS(I)*PMASS(I-13)*(-1.+1./(R22))/(R22**2)

IF (R2.GT.1.004) F2=0.

F3=PMASS(I)*PMASS(I+1)*(-1.+1./(R33))/(R33**2)

IF (R3.GT.1.004) F3=0.

F4=PMASS(I)*PMASS(I+13)*(-1.+1./(R44))/(R44**2)

IF (R4.GT.1.004) F4=0.

F5=PMASS(I)*PMASS(I+14)*(-1.+1./(R55))/(R55**2)

IF (R5.GT.1.004) F5=0.

FX1=F1*(X(I,1)-X(I-14,1))/R1

FY1=F1*(Y(I,1)-Y(I-14,1))/R1

FX2=F2*(X(I,1)-X(I-13,1))/R2

FY2=F2*(Y(I,1)-Y(I-13,1))/R2

FX3=F3*(X(I,1)-X(I+1,1))/R3

FY3=F3*(Y(I,1)-Y(I+1,1))/R3

FX4=F4*(X(I,1)-X(I+13,1))/R4

FY4=F4*(Y(I,1)-Y(I+13,1))/R4

FX5=F5*(X(I,1)-X(I+14,1))/R5

FY5=F5*(Y(I,1)-Y(I+14,1))/R5

ACX(I)=FX1+FX2+FX3+FX4+FX5

ACY(I)=FY1+FY2+FY3+FY4+FY5

GO TO 77

7003 R11=(X(I,1)-X(I-14,1))**2+(Y(I,1)-Y(I-14,1))**2

R22=(X(I,1)-X(I-13,1))**2+(Y(I,1)-Y(I-13,1))**2

R33=(X(I,1)-X(I-1,1))**2+(Y(I,1)-Y(I-1,1))**2

R44=(X(I,1)-X(I+1,1))**2+(Y(I,1)-Y(I+1,1))**2

R55=(X(I,1)-X(I+13,1))**2+(Y(I,1)-Y(I+13,1))**2

R66=(X(I,1)-X(I+14,1))**2+(Y(I,1)-Y(I+14,1))**2

```

R1=DSQRT(R11)
R2=DSQRT(R22)
R3=DSQRT(R33)
R4=DSQRT(R44)
R5=DSQRT(R55)
R6=DSQRT(R66)
F1=PMASS(I)*PMASS(I-14)*(-1.+1./(R11))/(R11**2)
IF (R1.GT.1.004) F1=0.
F2=PMASS(I)*PMASS(I-13)*(-1.+1./(R22))/(R22**2)
IF (R2.GT.1.004) F2=0.
F3=PMASS(I)*PMASS(I-1)*(-1.+1./(R33))/(R33**2)
IF (R3.GT.1.004) F3=0.
F4=PMASS(I)*PMASS(I+1)*(-1.+1./(R44))/(R44**2)
IF (R4.GT.1.004) F4=0.
F5=PMASS(I)*PMASS(I+13)*(-1.+1./(R55))/(R55**2)
IF (R5.GT.1.004) F5=0.
F6=PMASS(I)*PMASS(I+14)*(-1.+1./(R66))/(R66**2)
IF (R6.GT.1.004) F6=0.
FX1=F1*(X(I,1)-X(I-14,1))/R1
FY1=F1*(Y(I,1)-Y(I-14,1))/R1
FX2=F2*(X(I,1)-X(I-13,1))/R2
FY2=F2*(Y(I,1)-Y(I-13,1))/R2
FX3=F3*(X(I,1)-X(I-1,1))/R3
FY3=F3*(Y(I,1)-Y(I-1,1))/R3
FX4=F4*(X(I,1)-X(I+1,1))/R4
FY4=F4*(Y(I,1)-Y(I+1,1))/R4
FX5=F5*(X(I,1)-X(I+13,1))/R5
FY5=F5*(Y(I,1)-Y(I+13,1))/R5
FX6=F6*(X(I,1)-X(I+14,1))/R6
FY6=F6*(Y(I,1)-Y(I+14,1))/R6
ACX(I)=FX1+FX2+FX3+FX4+FX5+FX6
ACY(I)=FY1+FY2+FY3+FY4+FY5+FY6
GO TO 77

```

```

7004  R11=(X(I,1)-X(I-14,1))**2+(Y(I,1)-Y(I-14,1))**2
      R22=(X(I,1)-X(I-13,1))**2+(Y(I,1)-Y(I-13,1))**2
      R33=(X(I,1)-X(I-1,1))**2+(Y(I,1)-Y(I-1,1))**2
      R44=(X(I,1)-X(I+13,1))**2+(Y(I,1)-Y(I+13,1))**2
      R55=(X(I,1)-X(I+14,1))**2+(Y(I,1)-Y(I+14,1))**2
R1=DSQRT(R11)
R2=DSQRT(R22)
R3=DSQRT(R33)
R4=DSQRT(R44)
R5=DSQRT(R55)
F1=PMASS(I)*PMASS(I-14)*(-1.+1./(R11))/(R11**2)
IF (R1.GT.1.004) F1=0.
F2=PMASS(I)*PMASS(I-13)*(-1.+1./(R22))/(R22**2)
IF (R2.GT.1.004) F2=0.
F3=PMASS(I)*PMASS(I-1)*(-1.+1./(R33))/(R33**2)
IF (R3.GT.1.004) F3=0.
F4=PMASS(I)*PMASS(I+13)*(-1.+1./(R44))/(R44**2)
IF (R4.GT.1.004) F4=0.
F5=PMASS(I)*PMASS(I+14)*(-1.+1./(R55))/(R55**2)
IF (R5.GT.1.004) F5=0.
FX1=F1*(X(I,1)-X(I-14,1))/R1
FY1=F1*(Y(I,1)-Y(I-14,1))/R1
FX2=F2*(X(I,1)-X(I-13,1))/R2
FY2=F2*(Y(I,1)-Y(I-13,1))/R2
FX3=F3*(X(I,1)-X(I-1,1))/R3
FY3=F3*(Y(I,1)-Y(I-1,1))/R3
FX4=F4*(X(I,1)-X(I+13,1))/R4

```

FY4=F4*(Y(I,1)-Y(I+13,1))/R4

FX5=F5*(X(I,1)-X(I+14,1))/R5

FY5=F5*(Y(I,1)-Y(I+14,1))/R5

ACX(I)=FX1+FX2+FX3+FX4+FX5

ACY(I)=FY1+FY2+FY3+FY4+FY5

GO TO 77

7005 R11=(X(I,1)-X(I-13,1))*2+(Y(I,1)-Y(I-13,1))*2

R22=(X(I,1)-X(I+1,1))*2+(Y(I,1)-Y(I+1,1))*2

R33=(X(I,1)-X(I+14,1))*2+(Y(I,1)-Y(I+14,1))*2

R1=DSQRT(R11)

R2=DSQRT(R22)

R3=DSQRT(R33)

F1=PMASS(I)*PMASS(I-13)*(-1.+1./(R11))/(R11**2)

IF (R1.GT.1.004) F1=0.

F2=PMASS(I)*PMASS(I+1)*(-1.+1./(R22))/(R22**2)

IF (R2.GT.1.004) F2=0.

F3=PMASS(I)*PMASS(I+14)*(-1.+1./(R33))/(R33**2)

IF (R3.GT.1.004) F3=0.

FX1=F1*(X(I,1)-X(I-13,1))/R1

FY1=F1*(Y(I,1)-Y(I-13,1))/R1

FX2=F2*(X(I,1)-X(I+1,1))/R2

FY2=F2*(Y(I,1)-Y(I+1,1))/R2

FX3=F3*(X(I,1)-X(I+14,1))/R3

FY3=F3*(Y(I,1)-Y(I+14,1))/R3

ACX(I)=FX1+FX2+FX3

ACY(I)=FY1+FY2+FY3

GO TO 77

7006 R11=(X(I,1)-X(I-14,1))*2+(Y(I,1)-Y(I-14,1))*2

R22=(X(I,1)-X(I-1,1))*2+(Y(I,1)-Y(I-1,1))*2

R33=(X(I,1)-X(I+13,1))*2+(Y(I,1)-Y(I+13,1))*2

R1=DSQRT(R11)

R2=DSQRT(R22)

R3=DSQRT(R33)

F1=PMASS(I)*PMASS(I-14)*(-1.+1./(R11))/(R11**2)

IF (R1.GT.1.004) F1=0.

F2=PMASS(I)*PMASS(I-1)*(-1.+1./(R22))/(R22**2)

IF (R2.GT.1.004) F2=0.

F3=PMASS(I)*PMASS(I+13)*(-1.+1./(R33))/(R33**2)

IF (R3.GT.1.004) F3=0.

FX1=F1*(X(I,1)-X(I-14,1))/R1

FY1=F1*(Y(I,1)-Y(I-14,1))/R1

FX2=F2*(X(I,1)-X(I-1,1))/R2

FY2=F2*(Y(I,1)-Y(I-1,1))/R2

FX3=F3*(X(I,1)-X(I+13,1))/R3

FY3=F3*(Y(I,1)-Y(I+13,1))/R3

ACX(I)=FX1+FX2+FX3

ACY(I)=FY1+FY2+FY3

GO TO 77

7019 ACX(I)=-ACX(150-I)

ACY(I)=-ACY(150-I)

77 CONTINUE

DO 7123 I=1,149

IF (I.LT.15) GO TO 7985

IF (I.LT.28) GO TO 7986

IF (I.EQ.28) GO TO 7986

IF (I.LT.41) GO TO 7986

IF (I.EQ.41) GO TO 7986

IF (I.LT.55) GO TO 7986

IF (I.EQ.55) GO TO 7986

IF (I.LT.68) GO TO 7986

```

      IF (I.EQ.68) GO TO 7986
      IF (I.LE.75) GO TO 7986
      IF (I.LE.149) GO TO 7988
7986   VX(I,2)=VX(I,1)+0.0001*ACX(I)
      VY(I,2)=VY(I,1)+0.0001*ACY(I)
      X(I,2)=X(I,1)+0.0001*VX(I,2)
      Y(I,2)=Y(I,1)+0.0001*VY(I,2)
      GO TO 7123
7985   X(I,2)=X(I,1)
      Y(I,2)=Y(I,1)-0.0000001
      VX(I,2)=0.
      VY(I,2)=0.
      GO TO 7123
7987   X(I,2)=X(I,1)
      VX(I,2)=0.
      VY(I,2)=VY(I,1)+.0001*ACY(I)
      Y(I,2)=Y(I,1)+.0001*VY(I,2)
      GO TO 7123
7988   X(I,2)=-X(150-I,2)
      Y(I,2)=-Y(150-I,2)
      VX(I,2)=-VX(150-I,2)
      VY(I,2)=-VY(150-I,2)
7123   CONTINUE
8043   K=K+1
      IF (MOD(K,KPRINT).GT.0) GO TO 82
      DO 810 I=1,149
      WRITE (5,81) K,I,X(I,2),Y(I,2),VX(I,2),VY(I,2)
81     FORMAT (5X,I12,15,2F13.6,2F13.6)
      WRITE (99,10) X(I,2),Y(I,2),ACX(I),ACY(I)
810    CONTINUE
      DO 7394 I=1,149
      IF (I.LE.14) GO TO 1231
      IF (I.EQ.15) GO TO 1232
      IF (I.LT.27) GO TO 1233
      IF (I.EQ.27) GO TO 1234
      IF (I.EQ.28) GO TO 1235
      IF (I.LT.41) GO TO 1233
      IF (I.EQ.41) GO TO 1236
      IF (I.EQ.42) GO TO 1232
      IF (I.LT.54) GO TO 1233
      IF (I.EQ.54) GO TO 1234
      IF (I.EQ.55) GO TO 1235
      IF (I.LT.68) GO TO 1233
      IF (I.EQ.68) GO TO 1236
      IF (I.EQ.69) GO TO 1232
      IF (I.LE.75) GO TO 1233
      IF (I.LE.149) GO TO 7394
1231   R1=0.
      WRITE (5,9976) I,R1
      GO TO 7394
1232   R11=(X(I,1)-X(I-14,1))**2+(Y(I,1)-Y(I-14,1))**2
      R22=(X(I,1)-X(I-13,1))**2+(Y(I,1)-Y(I-13,1))**2
      R33=(X(I,1)-X(I+1,1))**2+(Y(I,1)-Y(I+1,1))**2
      R44=(X(I,1)-X(I+13,1))**2+(Y(I,1)-Y(I+13,1))**2
      R55=(X(I,1)-X(I+14,1))**2+(Y(I,1)-Y(I+14,1))**2
      R1=DSQRT(R11)
      R2=DSQRT(R22)
      R3=DSQRT(R33)
      R4=DSQRT(R44)
      R5=DSQRT(R55)

```

```
WRITE (5,9978) I,R1,R2,R3,R4,R5
```

```
GO TO 7394
```

```
1233 R11=(X(I,1)-X(I-14,1))**2+(Y(I,1)-Y(I-14,1))**2
      R22=(X(I,1)-X(I-13,1))**2+(Y(I,1)-Y(I-13,1))**2
      R33=(X(I,1)-X(I-1,1))**2+(Y(I,1)-Y(I-1,1))**2
      R44=(X(I,1)-X(I+1,1))**2+(Y(I,1)-Y(I+1,1))**2
      R55=(X(I,1)-X(I+13,1))**2+(Y(I,1)-Y(I+13,1))**2
      R66=(X(I,1)-X(I+14,1))**2+(Y(I,1)-Y(I+14,1))**2
```

```
R1=DSQRT(R11)
```

```
R2=DSQRT(R22)
```

```
R3=DSQRT(R33)
```

```
R4=DSQRT(R44)
```

```
R5=DSQRT(R55)
```

```
R6=DSQRT(R66)
```

```
WRITE (5,9977) I,R1,R2,R3,R4,R5,R6
```

```
GO TO 7394
```

```
1234 R11=(X(I,1)-X(I-14,1))**2+(Y(I,1)-Y(I-14,1))**2
      R22=(X(I,1)-X(I-13,1))**2+(Y(I,1)-Y(I-13,1))**2
      R33=(X(I,1)-X(I-1,1))**2+(Y(I,1)-Y(I-1,1))**2
      R44=(X(I,1)-X(I+13,1))**2+(Y(I,1)-Y(I+13,1))**2
      R55=(X(I,1)-X(I+14,1))**2+(Y(I,1)-Y(I+14,1))**2
```

```
R1=DSQRT(R11)
```

```
R2=DSQRT(R22)
```

```
R3=DSQRT(R33)
```

```
R4=DSQRT(R44)
```

```
R5=DSQRT(R55)
```

```
WRITE (5,9978) I,R1,R2,R3,R4,R5
```

```
GO TO 7394
```

```
1235 R11=(X(I,1)-X(I-13,1))**2+(Y(I,1)-Y(I-13,1))**2
      R22=(X(I,1)-X(I+1,1))**2+(Y(I,1)-Y(I+1,1))**2
      R33=(X(I,1)-X(I+14,1))**2+(Y(I,1)-Y(I+14,1))**2
```

```
R1=DSQRT(R11)
```

```
R2=DSQRT(R22)
```

```
R3=DSQRT(R33)
```

```
WRITE (5,9979) I,R1,R2,R3
```

```
GO TO 7394
```

```
1236 R11=(X(I,1)-X(I-14,1))**2+(Y(I,1)-Y(I-14,1))**2
      R22=(X(I,1)-X(I-1,1))**2+(Y(I,1)-Y(I-1,1))**2
      R33=(X(I,1)-X(I+13,1))**2+(Y(I,1)-Y(I+13,1))**2
```

```
R1=DSQRT(R11)
```

```
R2=DSQRT(R22)
```

```
R3=DSQRT(R33)
```

```
WRITE (5,9979) I,R1,R2,R3
```

```
7394 CONTINUE
```

```
82 IF (K,LT,50000) GO TO 65
```

```
102 WRITE (7,10) (X(I,2),Y(I,2),VX(I,2),VY(I,2),I=1,
```

```
1149)
```

```
STOP
```

```
END
```