QUASI-MOLECULAR, PARTICLE MODELING OF CRACK GENERATION AND FRACTURE

by

Donald Greenspan

Department of Mathematics
University of Texas at Arlington
Arlington, Texas 76019

TR. #208
Quasi-Molecular, Particle Modeling of Crack Generation and Fracture

by

Donald Greenspan

TR 208

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

\[
F = -\frac{G}{r^p} + \frac{H}{r^q},
\]

where, typically,

\[
(2.2) \quad G > 0, \ H > 0, \ p \geq 7
\]

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 $P_i$, $i=1,2,\ldots,N$. For $\Delta t > 0$, let $t_k = k \Delta t$, $k = 0,1,2,\ldots$. For each of $i=1,2,\ldots,N$, 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

\begin{align}
(3.1) & \quad \vec{v}_{i,0} = \vec{v}_{i,0} + \frac{1}{2} (\Delta t) \vec{a}_{i,0} \quad \text{(starter formula)} \\
(3.2) & \quad \vec{v}_{i,k} = \vec{v}_{i,k-1} + (\Delta t) \vec{a}_{i,k}, \quad k = 1,2,3,\ldots \\
(3.3) & \quad \vec{r}_{i,k} = \vec{r}_{i,k} + (\Delta t) \vec{v}_{i,k}, \quad k = 0,1,2,\ldots \\
\end{align}

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

\begin{equation}
(3.4) \quad \vec{F}_{i,k} = m_i \vec{a}_{i,k} 
\end{equation}

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

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

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

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

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.
<p>| | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>-6.50000</td>
<td>-4.330</td>
<td></td>
</tr>
<tr>
<td>-2.50000</td>
<td>-2.50000</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>0.50000</td>
<td></td>
</tr>
<tr>
<td></td>
<td>1.50000</td>
<td></td>
</tr>
<tr>
<td></td>
<td>2.50000</td>
<td></td>
</tr>
<tr>
<td></td>
<td>3.50000</td>
<td></td>
</tr>
<tr>
<td></td>
<td>4.50000</td>
<td></td>
</tr>
<tr>
<td>-4.00000</td>
<td>-2.00000</td>
<td></td>
</tr>
<tr>
<td>-6.00000</td>
<td>-4.00000</td>
<td></td>
</tr>
<tr>
<td>-8.00000</td>
<td>-6.00000</td>
<td></td>
</tr>
</tbody>
</table>

**Table 8**
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 $P = 1$. 
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 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


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,
1P6,F1,F2,F3,F4,F5,F6,F7,F8,F9,F10,F11,F12,F13,F14,F15,F16,F17,
R1,R2,R3,R4,R5,R6,R7,R8,R9,R10,R11,R12,R13,R14,R15,R16,R17,
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,F9.5)
9978 FORMAT (2X,I6,F9.5)
9979 FORMAT (2X,I6,F9.5)
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)=X3(I)
Y(I,1)=Y0(I)
VX(I,1)=VX(I)
VY(I,1)=VY(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.

APPENDIX
CONTINUE

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 .EQ. 75) GO TO 7003
IF (I .EQ. 149) GO TO 7019

ACX(I)=0.
GO TO 77

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

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
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 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)
FY4 = F4*(Y(I, 1) - Y(I + 13, 1))/ R4
FY5 = F5*(X(I, 1) - X(I + 14, 1))/ R5
FY6 = F6*(Y(I, 1) - Y(I + 14, 1))/ R5
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 + 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 - 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 + 13) * (-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 + 13, 1))/ R3
FY3 = F3*(Y(I, 1) - Y(I + 13, 1))/ R3
ACY(I) = FX1 + FX2 + FX3
ACY(I) = FY1 + FY2 + FY3
ACY(I) = ACY(I - 1)
ACY(I) = ACY(I - 1)
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
ACY(I) = FX1 + FX2 + FX3
ACY(I) = FY1 + FY2 + FY3
ACY(I) = FY1 + FY2 + FY3
ACY(I) = ACY(I - 1)
ACY(I) = ACY(I - 1)
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, LT, 76) GO TO 7986
```fortran
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)-0.000001
       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)+0.0001*ACY(I)
       Y(I,2)=Y(I,1)+0.0001*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)
       GO TO 7123

7123  CONTINUE

8043  K=K+1
       IF (MOD(K,KPRINT),GT,0) GO TO 82
       DO 810 1=1,149
       WRITE (5,81) K,1,X(I,2),Y(I,2),VX(I,2),VY(I,2)

81  FORMAT (5X,112,15,2F13.6,2F13.6)
       WRITE (99,10) X(I,2),Y(I,2),ACX(I),ACY(I)

810  CONTINUE
       DO 7394 1=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+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
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+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
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-13, 1))**2+(Y(I, 1)-Y(I-13, 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