A NEW COMPUTER-ORIENTED APPROACH TO
MOLECULAR MECHANICS

by

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

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ABSTRACT

A new dynamical theory for atomic and molecular dynamics is formulated and discussed. The associated nonlinear differential system is derived from general atomic and molecular stability properties and from aspects of modern particle theory, especially as it relates to the structure of the electron. Computer experiments are described for developing a new model of the water molecule.

1. Introduction. Modeling of fundamental, natural phenomena, like those associated with, say, living cell metabolism, requires a methodology for analyzing dynamical interactions within and between atoms and molecules. Quantum mechanical methodology has been successful in energy calculation, in spectroscopy, and in aspects of solid state physics. However, quantum dynamics of wave functions has proved to be distinctly unsuccessful for all but the most simplistic phenomena (3), (10), (12). For this reason, various combinations of quantum mechanical and classical methods have been devised recently. Levine and Bernstein (9), for example, determine energies from Schroedinger's equation and then scattering trajectories from Newton's equations. Kirschenbaum and Wilets (8) incorporate Heisenberg and Pauli principles into classical n-body models. Greenspan (4) assumes energy to be known and incorporates a local repulsion term into classical equations to prevent electron capture by a nucleus.

In this paper we will make a distinct departure from all existing methods, and, in the spirit of Einstein's thinking, develop a new approach to atomic and molecular dynamics which is entirely deterministic. We will make two fundamental assumptions. First, we assume that each atom or molecule under consideration is stable, that is, it neither collapses nor explodes. Experimentally, this is valid for most atoms and molecules which are isolated from radiation and from other atoms and molecules (3). Second, we assume that for any given set of like particles, say electrons, or helium atoms, or water molecules, any two particles of the set have

substructures which are either identical to or are mirror images of each other. From this assumption it follows, for example, that the electrostatic force between a pair of identical electrons need not be the same as that between a mirror image pair.

To illustrate the value of the approach and the way it lends itself to computer experimentation, we will describe related computations for developing a new model of the ground state water molecule. Relativistic effects, which are small (3), will not be considered in the present paper. The H_2O molecule was selected because of its fundamental importance in science and because most of its individual and group properties still elude theoretical explanation (1), (2), (11).

In the final section, we will show, heuristically, that our approach is consistent with the particle-wave assumption of quantum mechanics.

2. General Formulas. Electrons and nuclei will be treated as point sources. Given n particles P_i , $i = 1, 2, \dots, n$, let m_i and e_i be the mass, measured in grams, and the charge, measured in esu units, respectively, of P_i for each value of i . For positive grid size Δt and $t_k = k \Delta t$, $k = 0, 1, 2, \dots$, let P_i at time t_k be located at $\vec{r}_{i,k} = (x_{i,k}, y_{i,k}, z_{i,k})$, measured in cm, have velocity $\vec{v}_{i,k} = (v_{i,k,x}, v_{i,k,y}, v_{i,k,z})$, measured in cm/sec, and have acceleration $\vec{a}_{i,k} = (a_{i,k,x}, a_{i,k,y}, a_{i,k,z})$, measured in cm/sec². If the force $\vec{F}_{i,k} = (F_{i,k,x}, F_{i,k,y}, F_{i,k,z})$ acts on P_i at t_k , then we assume the dynamical relationship (5):

$$(2.1) \quad \vec{F}_{i,k} = m_i \vec{a}_{i,k}, \quad i = 1, 2, \dots, n; \quad k = 0, 1, 2, \dots$$

Let us consider first a Coulombic type component in $\vec{F}_{i,k}$ in (2.1). For this purpose, let $\vec{F}_{ij,k}^{(1)}$, the electrostatic force exerted on P_i by P_j , be

$$\vec{F}_{ij,k}^{(1)} = \frac{e_i e_j}{(r_{ij,k})^{2+\alpha_{ij}}} \frac{\vec{r}_{ji,k}}{r_{ij,k}},$$

where $\vec{r}_{ij,k}$ is the vector from P_i to P_j at time t_k . Then the total electrostatic force $\vec{F}_{i,k}^{(1)}$ on P_i due to all the other particles is

$$(2.2) \quad \vec{F}_{i,k}^{(1)} = \sum_{\substack{j=1 \\ j \neq i}}^n \vec{F}_{ij,k}^{(1)}.$$

Unfortunately, even if (2.1) were the only force we wished to consider, and it is not, the numerical solution of (2.1) in the present units yields severe computational underflow and overflow problems. So, before proceeding further, let us make the following changes of variables (4) :

$$(2.3) \quad M_i = 10^{28} m_i$$

$$(2.4) \quad E_i = 10^{10} e_i / 4.80236$$

$$(2.5) \quad \vec{R} = (X, Y, Z) = 10^{12} (x, y, z) = 10^{12} \vec{r}$$

$$(2.6) \quad T = 10^{22} t.$$

In the new variables, $M(\text{electron}) = 9.1085$, $M(\text{proton}) = 16742$, $E(\text{electron}) = -1$, $E(\text{proton}) = 1$. Velocities and accelerations transform as follows:

$$(2.7) \quad \vec{V} = (dX/dT, dY/dT, dZ/dT) = 10^{-10} (dx/dt, dy/dt, dz/dt) = 10^{-10} \vec{v}$$

$$(2.8) \quad \vec{A} = (d^2X/dT^2, d^2Y/dT^2, d^2Z/dT^2) = 10^{-32} (d^2x/dt^2, d^2y/dt^2, d^2z/dt^2) = 10^{-32} \vec{a}.$$

The particular dynamical form

$$\vec{F}_{i,k}^{(1)} = m_i \vec{a}_{i,k}$$

of (2.1) transforms into

$$(2.9) \quad M_i \frac{d^2 \vec{R}_{i,k}}{dT^2} = (4.80286)^2 \sum_{\substack{j=1 \\ j \neq i}}^n \frac{E_i E_j}{(R_{ij,k})^{2+\beta_{ij}}} \frac{\vec{R}_{ji,k}}{R_{ij,k}},$$

where

$$(R_{ij,k})^{2+\beta_{ij}} = (R_{ij,k})^{2+\alpha_{ij}} (10)^{-12 \alpha_{ij}}.$$

Since the numerical solution of (2.9) can be generated readily by any of the currently popular methods for initial value problems, we now modify (2.9) as follows to include additional effects. We will consider it in the more general form

$$(2.10) \quad M_i \frac{d^2 \vec{R}_{i,k}}{dT^2} = (4.80286)^2 \sum_{\substack{j=1 \\ j \neq i}}^n E_i E_j \left(\frac{1 + A_{ij,k}}{(R_{ij,k})^{2+\beta_{ij}}} \right) \frac{\vec{R}_{ji,k}}{R_{ij,k}},$$

where $A_{ij,k}$ will, in general, be related to the boundedness of the molecule. Since the actual structure of the $A_{ij,k}$ depends on the

5

molecule under consideration, we will deal with it more specifically in the next section in connection with a new water molecule model.

3. A Water Molecule Model. We formulate now a dynamical model of the water molecule which consists of only seven particles, that is, an O nucleus, two H nuclei, and four electrons. The reason we can do so is as follows. Extensive preliminary calculations with larger models (6) yielded the following phenomenon consistently. Of the six second ring electrons from the O atom and the two electrons from the H atoms, four were invariably oscillating close to the O nucleus while the other four were invariably oscillating far from the O nucleus. Such a phenomenon follows from a kinetic energy transfer which results whenever any electron comes between the O nucleus and a second electron (4), (6). The four electron model follows by absorbing both the inner ring O electrons and the four oscillating near the O nucleus into the O nucleus.

Thus, let P_1 represent the O nucleus, let P_2, P_3 represent H nuclei, and let P_4, P_5, P_6, P_7 represent electrons. Since six electrons have been absorbed into P_1 , it follows readily that

$$(3.1) \quad E_1 = 2, E_2 = E_3 = 1, E_4 = E_5 = E_6 = E_7 = -1.$$

By assuming also that neutron and proton masses are approximately equal, it follows that

$$(3.2) \quad M_1 = 267584, M_2 = M_3 = 16724, M_4 = M_5 = M_6 = M_7 = 9.1085.$$

The initial positions and velocities of P_1 - P_7 were derived from a more extensive eight-electron model (6) at a time when four of the electrons were oscillating near the O nucleus and are given by

$$\vec{R}_{1,0} = (26.39, 0, 0)$$

$$\vec{R}_{2,0} = (5862.71, 5350.89, 5350.89)$$

$$\vec{R}_{3,0} = (5862.71, -5350.89, -5350.89)$$

$$\vec{R}_{4,0} = (-15491.27, 3676.16, 1649.70)$$

$$\vec{R}_{5,0} = (-15491.27, -3676.16, -1649.70)$$

$$\vec{R}_{6,0} = (-15491.27, 1649.70, 3676.16)$$

$$\vec{R}_{7,0} = (-15491.27, -1649.70, -3676.16)$$

$$\vec{V}_{1,0} = (0.0000003, 0, 0)$$

$$\vec{V}_{2,0} = (0.0000476, 0.0000412, 0.0000412)$$

$$\vec{V}_{3,0} = (0.0000476, -0.0000412, -0.0000412)$$

$$\vec{V}_{4,0} = (0.0005566, 0.0007202, -0.0125138)$$

$$\vec{V}_{5,0} = (0.0005566, -0.0007202, 0.0125138)$$

$$\vec{V}_{6,0} = (0.0005566, -0.0125138, 0.0007202)$$

$$\vec{V}_{7,0} = (0.0005566, 0.0125138, -0.0007202) .$$

From these initial data, the motions of P_1 - P_7 can be approximated readily from (2.10) with $i=1,2,\dots,7$. We assume, of course, that $\vec{F}_{ij,k} = -\vec{F}_{ji,k}$, so that the $A_{ij,k}$ in (2.10) need be defined only for $i < j$. These are now given as follows. If $i=1$ and $j=4,5,6,7$, set $\beta_{ij} = 0$ and

$$(3.13) \quad A_{ij,k} = - \left(\frac{s_1}{R_{ij,k}} \right)^{p_1} + \left(\frac{R_{ij,k}}{s_2} \right)^{p_2} ,$$

where

$$(3.14) \quad s_1 \leq 4500, \quad s_2 \geq 12000 .$$

In (3.13), the term with exponent p_1 preserves the domain of the

inner electrons, even though these have been absorbed into the nucleus. The term with exponent p_2 preserves the boundedness of the molecule by limiting the radii of the electrons. If $i=1$ and $j=2,3$, set $\beta_{ij}=0$ and

$$(3.15) \quad A_{ij,k} = - \left(\frac{R_{ij,k}}{s_3} \right)^{p_3}, \quad s_3 \geq 5000,$$

which, again, preserves the boundedness of the molecule, but by limiting the nuclei radii. Note that both (3.13) and (3.15) limit only radial motions. Neither limits angular motions. If

$i=2$ and $j=3$, set $A_{ij,k}=0$ and

$$(3.16) \quad \beta_{ij} = p_4 > 0.$$

If $i=2$ and $j=4,5$, set $A_{ij,k}=0$ and

$$(3.17) \quad \beta_{ij} = p_5 > 0.$$

If $i=3$ and $j=6,7$, set $A_{ij,k}=0$ and use (3.17). If $i=4,5$

and $j=6,7$, set $A_{ij,k}=0$ and use (3.17). If $i=2$ and $j=6,7$, set $A_{ij,k}=0$ and

$$(3.18) \quad \beta_{ij} = -p_5 < 0.$$

If $i=3$ and $j=4,5$, set $A_{ij,k}=0$ and use (3.18). If $i=4$ and $j=5$

set $A_{ij,k}=0$ and use (3.18). If $i=6$ and $j=7$, set $A_{ij,k}=0$

and use (3.18). Thus, all particle interactions are now defined completely in terms of the parameters $p_1, p_2, p_3, p_4, p_5, s_1, s_2$ and s_3 .

Next, let us give an example of a specific computation. Fix the parameters by

$$(3.19) \quad p_1=4, p_2=8, p_3=4, p_4=1/4, p_5=1/16, s_1=1250, s_2=20000, s_3=9800.$$

Using double precision with $\Delta T=2.0$, and rounding to two decimal

places in position and seven in velocity every 240000 iterations, we have recorded in Figures 1 and 2 the variations of the bond length R and the bond angle θ over the first radial oscillation of the H nuclei. For simplicity, the graphs utilize the time τ , where $T = 960000\tau$. The period is about $\tau = 52.5$, or $T = (5.04)10^7$, which, from (2.6), is $(5.04)10^{-15}$ sec. The average altitude in Figure 1 is 9977 units, or, in xyz coordinates, $0.9977 \text{ \AA}$. The average bond angle in Figure 2 is 104.28° . These results are in excellent agreement with experiment. The computer program used is provided in the Appendix of Greenspan (7).

The above example was one of a large variety of similar calculations using parameters selected from

$$p_1 = 4, 8$$

$$p_2 = 8$$

$$p_3 = 4, 8$$

$$p_4 = 1/4, 1/8, 1/16$$

$$p_5 = 0, 1/2, 1/4, 1/8, 1/16, 1/32$$

$$s_1 = 1000, 1250, 1300, 2500, 3000, 4000, 5000$$

$$s_2 = 9000, 9600, 10000, 10500, 12000, 14000, 18000, 20000, \\ 21250, 22500, 23000$$

$$s_3 = 8000, 8500, 9000, 9400, 9600, 9800, 9850, 10200, 11000, 12000$$

The majority of these calculations, however, resulted in the bond angle exceeding acceptable bounds (1), (11). In general, all the calculations were exceptionally sensitive to all the input parameters. The reason is that the masses of the particles are so vastly different that an element of stiffness enters all the

calculations. Perhaps the parameter of greatest interest in the s (3.19) is S_2 . With $S_2 = 20000$, the maximum electron radial distance is, approximately, 29500 units. Only slight variations of this parameter result in dramatic effects on the motions of the H nuclei. Thus, a fine tuning of the parameters in (3.19) is anticipated if the oscillations in Figures 1 and 2 are to continue for all time. An alternative to these extensive computations would be to proceed directly to a full eight electron model, in which case total energy is known correctly (6). Also, a qualitative analysis of system (2.10) would be of value, but the system is so highly nonlinear that the development of such an analysis seems quite difficult.

4. Remarks. It is our purpose now to show, heuristically, that our approach is consistent with the particle-wave assumption of quantum mechanics. Recall that the basic double slit experiments for electrons, for example, yield, under special conditions (3), particle distributions like those shown in Figure 3. Such a

Figure 3. Electron distribution in special double slit experiments.

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Figure 3. Electron distribution in special double slit experiments.

distribution pattern can be interpreted reasonably as a wave interference pattern. However, it is also possible that, under the same special conditions, the electrons, because they fall into the two classes of identical and mirror image types, separate out. Should such a separation process occur, the resulting distribution could be the same as that shown in Figure 3. From this point of view, the resulting model would be deterministic. Thus, the question of whether a model which is consistent with Figure 3 is probabilistic or deterministic follows from the assumptions one makes about the mechanisms which caused the distribution. The quantum mechanical particle-wave assumption has been exceptionally valuable, but it has failed in dynamics and in approximating the energies of nuclei. Our approach in this paper is a first attempt to develop a viable alternative for such extant problems.

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C THIS IS THE WATER MOLECULE H2OIP2.
C IT HAS ONLY 7 PARTICLES AND WAS DERIVED FROM H2OZ69.
C THE NUCLEUS AND FIRST TWO (INNER) ELECTRONS ARE TREATED AS A POINT SOURCE.
  DOUBLE PRECISION XU(7),YU(7),ZU(7),VXU(7),VYU(7),VZU(7),
  1X(7,2),Y(7,2),Z(7,2),VX(7,2),VY(7,2),VZ(7,2),
  1ACX(7),ACY(7),ACZ(7),R2,R,FX,FY,FZ,F,ECHARG(7),PMASS(7),
  1R18,R110,R810,XKE,COS,XKEPE,XPE,RMIN,R3,RES(7)
  OPEN (UNIT=7,FILE='H2OIP2.OUT',DEVICE='DSK')
  OPEN (UNIT=21,FILE='H2OIP2.DAT')
  OPEN (UNIT=5,DEVICE='LPT',FILE='H2OIP2.PRT',ACCESS='SEQUOUT')
  KPRINT=20000
  NM1=6
  K=1
  COS=0.
  DO 4 I=1,7
    X(I,1)=0.
    Y(I,1)=0.
    Z(I,1)=0.
    VX(I,1)=0.
    VY(I,1)=0.
    VZ(I,1)=0.
    X(I,2)=0.
    Y(I,2)=0.
    Z(I,2)=0.
    VX(I,2)=0.
    VY(I,2)=0.
    VZ(I,2)=0.
    ACX(I)=0.
    ACY(I)=0.
    ACZ(I)=0.
C ECHARG(1) INCLUDES 8 PROTONS AND 6 ELECTRONS.
4  CONTINUE
  ECHARG(1)=2.
  ECHARG(2)=1.0
  ECHARG(3)=1.0
  ECHARG(4)=-1.
  ECHARG(5)=-1.
  ECHARG(6)=-1.
  ECHARG(7)=-1.
  PMASS(1)=267584.
  PMASS(2)=16724.0
  PMASS(3)=16724.0
  PMASS(4)=9.1085
  PMASS(5)=9.1085
  PMASS(6)=9.1085
  PMASS(7)=9.1085
  READ (21,10) (XU(I),YU(I),ZU(I),VXU(I),VYU(I),VZU(I),I=1,7)
  GO TO 11
7  REWIND 21
  READ (21,10) (XU(I),YU(I),ZU(I),VXU(I),VYU(I),VZU(I),I=1,7)
  READ (21,10) (XU(I),YU(I),ZU(I),VXU(I),VYU(I),VZU(I),I=1,7)
  GO TO 11
8  REWIND 21
  READ (21,10) (XU(I),YU(I),ZU(I),VXU(I),VYU(I),VZU(I),I=1,7)
  READ (21,10) (XU(I),YU(I),ZU(I),VXU(I),VYU(I),VZU(I),I=1,7)
  READ (21,10) (XU(I),YU(I),ZU(I),VXU(I),VYU(I),VZU(I),I=1,7)
  GO TO 11
9  REWIND 21
  READ (21,10) (XU(I),YU(I),ZU(I),VXU(I),VYU(I),VZU(I),I=1,7)
  READ (21,10) (XU(I),YU(I),ZU(I),VXU(I),VYU(I),VZU(I),I=1,7)

```



```

ACX(1)=0.
ACY(1)=0.
ACZ(1)=0.
701 CONTINUE
71 DO 77 I=1,6
    IP1=I+1
    DO 76 J=IP1,7
        R2=(X(I,1)-X(J,1))**2+(Y(I,1)-Y(J,1))**2+(Z(I,1)-Z(J,1))**2
        R=DSQRT(R2)
        IF (I.EQ.1.AND.J.GE.4) GO TO 721
        IF (I.EQ.1.AND.J.LE.3) GO TO 722
        IF (I.LE.3.AND.J.LE.3) GO TO 7243
        IF (I.EQ.2.AND.J.LE.5) GO TO 723
        IF (I.EQ.2.AND.J.GE.6) GO TO 7223
        IF (I.EQ.3.AND.J.LE.5) GO TO 7223
        IF (I.EQ.3.AND.J.GE.6) GO TO 723
        IF (I.LE.5.AND.J.LE.5) GO TO 7223
        IF (I.LE.5.AND.J.GE.6) GO TO 723
        IF (I.GE.6.AND.J.GE.6) GO TO 7223
C WE NOW PRESERVE THE FIRST ELECTRON RING OF THE O NUCLEUS.
721 F=ECHARG(I)*ECHARG(J)*23.06746*(1.-(1./((R/1250.))**4))+
    1(1./((20000./R)**8)))/(R2*R)
    GO TO 727
C WE NOW, FOR VARIATION, USE A SWITCHING TYPE FUNCTION FOR STABILITY.
722 IF (R.GT.5000.) GO TO 7272
    F=ECHARG(I)*ECHARG(J)*23.06746/(R2*R)
    GO TO 727
7272 F=ECHARG(I)*ECHARG(J)*23.06746*(1.-(1./((9800./R)**4)))/
    1(R2*R)
    GO TO 727
7223 R3=R**(1/16)
    F=ECHARG(I)*ECHARG(J)*23.06746*R3/(R2*R)
    GO TO 727
7243 R3=R**(1/4)
    F=ECHARG(I)*ECHARG(J)*23.06746/(R2*R3*R)
    GO TO 727
723 R3=R**(1/16)
    F=ECHARG(I)*ECHARG(J)*23.06746/(R2*R3*R)
727 FX=F*(X(I,1)-X(J,1))
    FY=F*(Y(I,1)-Y(J,1))
    FZ=F*(Z(I,1)-Z(J,1))
75 ACX(I)=ACX(I)+FX
    ACX(J)=ACX(J)-FX
    ACY(I)=ACY(I)+FY
    ACY(J)=ACY(J)-FY
    ACZ(I)=ACZ(I)+FZ
    ACZ(J)=ACZ(J)-FZ
76 CONTINUE
77 CONTINUE
    DO 770 I=1,7
        ACX(I)=ACX(I)/PMASS(I)
        ACY(I)=ACY(I)/PMASS(I)
        ACZ(I)=ACZ(I)/PMASS(I)
770 CONTINUE
79 DO 80 I=1,7
    VX(I,2)=VX(I,1)+2.0*ACX(I)
    VY(I,2)=VY(I,1)+2.0*ACY(I)
    VZ(I,2)=VZ(I,1)+2.0*ACZ(I)
    X(I,2)=X(I,1)+2.0*VX(I,2)
    Y(I,2)=Y(I,1)+2.0*VY(I,2)

```

```

READ (21,10) (X0(I),Y0(I),Z0(I),VX0(I),VY0(I),VZ0(I),I=1,7)
READ (21,10) (X0(I),Y0(I),Z0(I),VX0(I),VY0(I),VZ0(I),I=1,7)
GO TO 11
  REWIND 21
READ (21,10) (X0(I),Y0(I),Z0(I),VX0(I),VY0(I),VZ0(I),I=1,7)
READ (21,10) (X0(I),Y0(I),Z0(I),VX0(I),VY0(I),VZ0(I),I=1,7)
READ (21,10) (X0(I),Y0(I),Z0(I),VX0(I),VY0(I),VZ0(I),I=1,7)
READ (21,10) (X0(I),Y0(I),Z0(I),VX0(I),VY0(I),VZ0(I),I=1,7)
READ (21,10) (X0(I),Y0(I),Z0(I),VX0(I),VY0(I),VZ0(I),I=1,7)
GO TO 11
  REWIND 21
READ (21,10) (X0(I),Y0(I),Z0(I),VX0(I),VY0(I),VZ0(I),I=1,7)
READ (21,10) (X0(I),Y0(I),Z0(I),VX0(I),VY0(I),VZ0(I),I=1,7)
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READ (21,10) (X0(I),Y0(I),Z0(I),VX0(I),VY0(I),VZ0(I),I=1,7)
READ (21,10) (X0(I),Y0(I),Z0(I),VX0(I),VY0(I),VZ0(I),I=1,7)
READ (21,10) (X0(I),Y0(I),Z0(I),VX0(I),VY0(I),VZ0(I),I=1,7)
READ (21,10) (X0(I),Y0(I),Z0(I),VX0(I),VY0(I),VZ0(I),I=1,7)
READ (21,10) (X0(I),Y0(I),Z0(I),VX0(I),VY0(I),VZ0(I),I=1,7)
READ (21,10) (X0(I),Y0(I),Z0(I),VX0(I),VY0(I),VZ0(I),I=1,7)
READ (21,10) (X0(I),Y0(I),Z0(I),VX0(I),VY0(I),VZ0(I),I=1,7)
GO TO 11
  REWIND 21
READ (21,10) (X0(I),Y0(I),Z0(I),VX0(I),VY0(I),VZ0(I),I=1,7)
READ (21,10) (X0(I),Y0(I),Z0(I),VX0(I),VY0(I),VZ0(I),I=1,7)
READ (21,10) (X0(I),Y0(I),Z0(I),VX0(I),VY0(I),VZ0(I),I=1,7)
READ (21,10) (X0(I),Y0(I),Z0(I),VX0(I),VY0(I),VZ0(I),I=1,7)
READ (21,10) (X0(I),Y0(I),Z0(I),VX0(I),VY0(I),VZ0(I),I=1,7)
READ (21,10) (X0(I),Y0(I),Z0(I),VX0(I),VY0(I),VZ0(I),I=1,7)
READ (21,10) (X0(I),Y0(I),Z0(I),VX0(I),VY0(I),VZ0(I),I=1,7)
READ (21,10) (X0(I),Y0(I),Z0(I),VX0(I),VY0(I),VZ0(I),I=1,7)
  FORMAT (3F12.2,3F12.7)
  DO 20 I=1,7
    WRITE (5,15) I,PMASS(I),ECHARG(I),X0(I),Y0(I),Z0(I),VX0(I),
    1VY0(I),VZ0(I)
    FORMAT (5X,15,8F13.5)
    CONTINUE
  DO 30 I=1,7
    X(I,1)=X0(I)
    Y(I,1)=Y0(I)
    Z(I,1)=Z0(I)
    VX(I,1)=VX0(I)
    VY(I,1)=VY0(I)
    VZ(I,1)=VZ0(I)
    CONTINUE
  GO TO 71
  DO 70 I=1,7
    X(I,1)=X(I,2)
    Y(I,1)=Y(I,2)
    Z(I,1)=Z(I,2)
    VX(I,1)=VX(I,2)
    VY(I,1)=VY(I,2)
    VZ(I,1)=VZ(I,2)
    CONTINUE
  DO 701 I=1,7

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