**Supercomputer Simulation of Liquid Drop Formation
on a Solid Surface**

by
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Abstract

Using a molecular dynamics type approach, we show how to simulate the formation of a liquid drop on a solid surface. Application is made to the case in which the liquid is water and the solid is graphite. The dynamical equations are large systems of nonlinear, ordinary differential equations which must be solved numerically. CRAY X-MP/24 simulations and related contact angle calculations are described and discussed.

*Computations performed at the University of Texas Center for High Performance Computing.

1. Introduction

Fluid phenomena which involve large gradients present exceptional theoretical difficulties [1]. This is readily apparent in the study of liquid drops, in which surface tension plays a major role [3], [4]. In this paper we will develop a molecular dynamics type approach to such problems. In particular, we will show how to simulate the formation of a liquid drop, taken to be water, on a horizontal solid surface, taken to be graphite. The related dynamical equations will be large systems of second order, nonlinear, ordinary differential equations which will be solved numerically [6] on a CRAY X-MP/24.

At present, for budgetary reasons and for computational simplicity, attention will be restricted to two dimensional simulations. Nevertheless, all the ideas and methods do extend to three dimensions [10].

2. Local Force Formulas

In order not to be confined to a system of molecules whose volume is prohibitively small [2], we will think in terms of aggregates of molecules, called particles or quasimolecules. The force interaction formulas for particles will be derived in this section by conserving the total mass and the total energy of the original molecular system.

Consider first the system of 823 water particles $P_1, P_2, \dots, P_{823}$ shown in Figure 1. These particles are arranged on a regular triangular mosaic, but in a relatively circular pattern. The edge length of each triangle in the mosaic is 0.0305871 cm, the rationale of which will be explained shortly. The algorithm for generating the positions $\vec{r}(i) = (x(i), y(i))$ and velocity $\vec{v}(i) = (v_x(i), v_y(i))$ for each P_i is given as follows. From the 9500 points with:

$x(1) = -0.6117420, y(1) = -0.7946762, v_x(1) = 0.0, v_y(1) = 10^{-9}$
 $x(42) = -0.5964485, y(42) = -0.7681870, v_x(42) = 10^{-9}, v_y(42) = 0.0$
 $x(i+1) = x(i) + 0.0305871, y(i+1) = y(1), v_x(i+1) = 0.0, v_y(i+1) = v_y(1), i = 1, 2, 3, \dots, 40$
 $x(i+1) = x(i) + 0.0305871, y(i+1) = y(42), v_x(i+1) = v_x(42), v_y(i+1) = 0.0, i = 42, 43, \dots, 80$
 $x(i) = x(i-81), y(i) = y(i-81) + 0.0529784, v_x(i) = -v_x(i-81), v_y(i) = -v_y(i-81), i = 82, 83,$
 $\dots, 9500,$

choose only those which satisfy

$$(2.1) \quad [x(i)]^2 + [y(i)]^2 \leq 0.2123$$

Fig. 1. Initial fluid

These are the 823 points shown in Figure 1. Note that the horizontal radius of this relatively circular set contains 15 particles, so that the radius r is, approximately,

$$(2.2) \quad r = 15(0.0305871) = 0.4588065 \text{ cm.}$$

For the interaction of the particles, we assume a force $\vec{F}_1$, in dynes, between two particles R cm apart, with magnitude F_1 given

$$(2.3) \quad F_1(R) = -\frac{G}{R^3} + \frac{H}{R^5}.$$

From (2.3), then, in ergs,

$$(2.4) \quad \phi_1(R) = -\frac{G}{2R^2} + \frac{H}{4R^4}.$$

For the system shown in Figure 1, we assume that $F_1 = 0$ between two neighbors, so that

$$(2.5) \quad -(0.0305871)^2 G + H = 0.$$

Assuming zero kinetic energy, the total energy E_1 of the particle system is, approximately [7],

$$(2.6) \quad E_1 = 3(823) \left(-\frac{G}{2(0.0305871)^2} + \frac{H}{4(0.0305871)^4} \right)$$

We show next how to use (2.5), (2.6) and conservation of total energy to determine G and H uniquely in (2.3). For actual water molecules, one can use the approximation [8]

$$(2.7) \quad \phi(r) = (1.9646383)10^{-13} \left[\left(\frac{2.725}{r} \right)^{12} - \left(\frac{2.725}{r} \right)^6 \right] \text{ erg,}$$

in which the distance r between two molecules is measured in angstroms. From (2.7), the magnitude of the force $\vec{F}$, in dynes, is

$$(2.8) \quad F(r) = (1.9646383)10^{-5} \left[12 \frac{(2.725)^{12}}{r^{13}} - 6 \frac{(2.725)^6}{r^7} \right]$$

Note, from (2.8), that $F(r) = 0$ implies $r = 3.05871 \text{ \AA}$. (Our choice of 0.0305871 cm for the

construction of Figure 1 was based on this angstrom measurement for the purpose of simplifying later calculations.) We now fill the circle shown in Figure 1 with molecules which are vertices of a regular triangular grid with edge length 3.05871 Å. The number N of molecules which fills the region is, approximately,

$$(2.9) \quad N = \pi \left(\frac{15(0.0305871)}{(3.05871)10^{-8}} \right)^2 \sim (707)10^{12}.$$

Assuming zero kinetic energy, the total energy E of the molecular system is, approximately,

$$(2.10) \quad E = 3(707)10^{12}(1.9646383)10^{-13} \left[\left(\frac{2.725}{3.05871} \right)^{12} - \left(\frac{2.725}{3.05871} \right)^6 \right] \text{erg}$$

or

$$E = -104.1745$$

Equating E_1 and E implies

$$(2.11) \quad -534.4332 G + 285618.8 H = -0.04219299$$

The solution of (2.5) and (2.11) is

$$G = (1.57898)10^{-4}, H = (1.47725)10^{-7},$$

so that (2.3), (2.4) can be given explicitly as

$$(2.12) \quad F_1(R) = -\frac{1.57898}{R^3}10^{-4} + \frac{(1.47725)10^{-7}}{R^5}$$

$$(2.13) \quad \phi_1(R) = -\frac{7.8949}{R^2}10^{-5} + \frac{3.693125}{R^4}10^{-8}$$

Note that (2.13) can be rewritten in the form

$$(2.14) \quad \phi_1(R) = 4\epsilon_1 \left[-\left(\frac{\sigma_1}{R} \right)^2 + \left(\frac{\sigma_1}{R} \right)^4 \right],$$

in which $\epsilon_1 = 0.0421929$, $\sigma_1 = 0.0216284$.

Note also that since the mass of a single water molecule is, approximately, $m = (30.103)10^{-24}$ gr, distributing the total water molecule mass over the 823 particles yields an individual water particle mass M_1 given by

$$(2.15) \quad M_1 = (2.586)10^{-11} \text{ gr.}$$

Using the very same line of reasoning as for water, let us proceed to develop appropriate formulas for graphite. A 5-row, 1003 particle slab of graphite particles is generated using a regular triangular mosaic with edge length 0.03834 cm by the formulas

$$\begin{aligned} x(1) &= -3.834, y(1) = 0.0, x(202) = -3.81085, y(202) = 0.03317 \\ x(i+1) &= x(i)+0.03834, y(i+1) = y(1), i = 1, 2, \dots, 200 \\ x(i+1) &= x(i)+0.03834, y(i+1) = y(202), i = 202, 203, \dots, 400 \\ x(i) &= x(i-401), y(i) = 0.06634+y(i-401), i = 402, 403, \dots, 1003. \end{aligned}$$

The resulting slab is 7.668 cm wide, 0.13268 cm high, and is shown in Figure 2. One should note immediately the difference in units between Figures 1 and 2.

Let the force $\vec{F}_2$, in dynes, between two graphite particles R cm apart, have magnitude F_2 given by

$$(2.16) \quad F_2(R) = -\frac{G}{R^3} + \frac{H}{R^5}$$

so that

$$(2.17) \quad \phi_2(R) = -\frac{G}{2R^2} + \frac{H}{4R^4}.$$

Assuming $F_2 = 0$ for two neighbors, (2.16) implies, in analogy with (2.5),

$$(2.18) \quad -(0.03834)^2 G + H = 0$$

Assuming zero kinetic energy, the total energy E_2 of the system is, approximately,

$$(2.19) \quad E_2 = 3(1003) \left(-\frac{G}{2(0.03834)^2} + \frac{H}{4(0.03834)^4} \right)$$

Fig. 2. Initial slab

Fig. 3. Stable fluid

Fig. 4. Stable slab

However, for actual atoms of graphite [5], [9], with r in angstroms,

$$(2.20) \quad \phi(r) = \left(\frac{38591.3}{r^{12}} - \frac{24.3000}{r^6} \right) 10^{-12} \text{ erg}$$

$$(2.21) \quad F(r) = \left(\frac{463095.6}{r^{13}} - \frac{145.8}{r^7} \right) 10^{-4},$$

where $\vec{F}(r)$ is measured in dynes. In (2.20) and (2.21), $\phi(3.41570) = 0$, $F(3.83400) = 0$.

Then, the number N of atoms which fill the slab on a regular triangular mosaic with edge length 3.83400 Å is

$$N = \frac{(7.668)10^8}{3.83400} \cdot \frac{(0.13268)10^8}{3.3203483} = (7.992)10^{14}$$

Assuming zero kinetic energy, the total energy E of the system is, approximately,

$$(2.22) \quad E = 3(7.992)10^{14} \left[\frac{38591.3}{(3.83400)^{12}} - \frac{24.3000}{(3.83400)^6} \right] 10^{-12},$$

so that $E = -9.17149$. Equating E and E_2 implies

$$(2.23) \quad -\frac{G}{2(0.03834)^2} + \frac{H}{4(0.03834)^4} = -(3.04802)10^{-3}$$

The solution of system (2.18), (2.23) is, approximately, $G = (1.792181)10^{-5}$, $H = (2.634426)10^{-8}$. Thus,

$$(2.24) \quad F_2 = -\frac{(1.792181)10^{-5}}{R^3} + \frac{(2.634426)10^{-8}}{R^5}$$

$$(2.25) \quad \phi_2 = -\frac{8.960905}{R^2} 10^{-6} + \frac{(6.586065)10^{-9}}{R^4}$$

Note that $\phi_2(0.0271105) = 0$, so that ϕ_2 can be rewritten as

$$(2.26) \quad \phi_2 = 4\epsilon_2 \left[-\left(\frac{\sigma_2}{R} \right)^2 + \left(\frac{\sigma_2}{R} \right)^4 \right]$$

in which $\sigma_2 = 0.0271105$, $\epsilon_2 = (3.048013)10^{-3}$.

Note that since the mass of a carbon atom is $(1.9938)10^{-23}$ gr, approximately, the total atomic mass of the slab, when distributed over the 1003 graphite particles, yields a particle mass M_2 given by

$$(2.27) \quad M_2 = (1.588679)10^{-11} \text{ gr.}$$

Finally, to determine the force $\vec{F}_3$ between graphite and water particles, we use the empirical bonding law [7]

$$\phi_3 = 4\epsilon_3 \left[\left(\frac{\sigma_3}{R} \right)^4 - \left(\frac{\sigma_3}{R} \right)^2 \right],$$

where $\epsilon_3 = \sqrt{\epsilon_1 \epsilon_2} = 0.0113404$, $\sigma_3 = \frac{1}{2}(\sigma_1 + \sigma_2) = 0.02436945$. Thus,

$$\phi_3 = -\frac{2.6938}{R^2}10^{-5} + \frac{1.5998}{R^4}10^{-8}.$$

Hence,

$$(2.28) \quad F_3 = -\frac{5.3877}{R^3}10^{-5} + \frac{6.3992}{R^5}10^{-8}.$$

In summary, the water-water interparticle force $\vec{F}_1$, graphite-graphite interparticle force $\vec{F}_2$, and water-graphite interparticle force $\vec{F}_3$ yield, to four significant figures,

$$(2.29) \quad F_1(R) = -\frac{1.579}{R^3}10^{-4} + \frac{1.477}{R^5}10^{-7}$$

$$(2.30) \quad F_2(R) = -\frac{1.792}{R^3}10^{-5} + \frac{2.634}{R^5}10^{-8}$$

$$(2.31) \quad F_3(R) = -\frac{5.388}{R^3}10^{-5} + \frac{6.399}{R^5}10^{-8},$$

while

$$(2.32) \quad F_1(0.03059) = F_2(0.03834) = F_3(0.03446) = 0.$$

The distances $R_1 = 0.03059$, $R_2 = 0.03834$, $R_3 = 0.03446$ are called equilibria radii.

3. Dynamical Equations

In order to derive dynamical equations for particle motions, let us begin with the motion of a water particle P_i as it interacts with other water particles. The motion of P_i , in general, is given by

$$(3.1) \quad M_1 \frac{d^2 R_i}{dt^2} = -980M_1 + \alpha_1 \sum_j \left(-\frac{1.579}{(R_{ij})^3} 10^{-4} + \frac{1.477}{(R_{ij})^5} 10^{-7} \right),$$

in which the summation is taken over particles P_j which are within a prescribed distance D_1 to P_i , R_{ij} is the distance between P_i and P_j , α_1 is a scaling factor which assures that the particle interaction is local relative to gravity, and M_1 is the mass of a water particle, given by (2.15). Division by M_1 yields

$$(3.2) \quad \frac{d^2 R_i}{dt^2} = -980 + \alpha_1 \sum_j \left(-\frac{0.61060}{(R_{ij})^3} 10^7 + \frac{0.57115}{(R_{ij})^5} 10^4 \right).$$

We now assume, as in common in molecular mechanics, that P_i is acted upon only by particles P_j which are within five equilibria radii of P_i , so that $D_1 = 5(0.03059) = 0.15295$. By "local relative to gravity," we assume the usual 5% experimental error allowance, so that

$$\alpha_1 \left| -\frac{(0.61060)}{(0.15295)^3} 10^7 + \frac{(0.57115)}{(0.15295)^5} 10^4 \right| = 5\%(980),$$

which yields $\alpha_1 = (2.99095)10^{-8}$. Thus, (3.2) reduces to

$$(3.3) \quad \frac{d^2 R_i}{dt^2} = -980 + \sum_j \left(-\frac{(1.82627)}{R_{ij}^3} 10^{-1} + \frac{(1.70828)10^{-4}}{R_{ij}^5} \right)$$

Finally, making the changes of variables

$$(3.4) \quad \bar{R} = 10R, \quad T = 10t,$$

(3.3) reduces to

$$(3.5) \quad \frac{d^2 \bar{R}_i}{dT^2} = -98.0 + \sum_j \left(-\frac{18.2627}{(\bar{R}_{ij})^3} + \frac{1.70828}{(\bar{R}_{ij})^5} \right)$$

Using the same line of reasoning, the dynamical equation for the interaction of a graphite

particle with other graphite particles is

$$(3.6) \quad \frac{d^2 R_i}{dt^2} = -980 + \sum_j \left(-\frac{0.359575}{(R_{ij})^3} + \frac{5.285275}{(R_{ij})^5} 10^{-4} \right)$$

and the distance of local interaction is $D_2 = 0.1917$. Under transformations (3.4), the equation becomes

$$(3.7) \quad \frac{d^2 \bar{R}_i}{dT^2} = -98.0 + \sum_j \left(-\frac{35.9575}{(\bar{R}_{ij})^3} + \frac{5.285275}{(\bar{R}_{ij})^5} \right).$$

The interaction of a water particle P_i with graphite particles P_j is governed by the equation

$$(3.8) \quad \frac{d^2 R_i}{dt^2} = -980 + \sum_j \left(-\frac{0.261085}{(R_{ij})^3} + \frac{(3.10075)}{(R_{ij})^5} 10^{-4} \right)$$

with the local interaction distance $D_3 = 0.1723$. Under transformations (3.4), the equation becomes

$$(3.9) \quad \frac{d^2 \bar{R}_i}{dT^2} = -98.0 + \sum_j \left(-\frac{26.1085}{(\bar{R}_{ij})^3} + \frac{3.10075}{(\bar{R}_{ij})^5} \right).$$

Note, incidentally, that the first transformation in (3.4) has the effect of multiplying all coordinates in Figures 1 and 2 by the factor 10. Hereafter, all discussion is in the $\bar{R}$, T variables. However, the random initial velocities prescribed for particles $P_1 - P_{823}$ will be retained.

4. Drop and Slab Stabilization

If, for example, one proceeds numerically with $\Delta T = 0.00005$ and one allows the water particles to interact in accordance with (3.5), the system exhibits large expansion and contraction modes. The reason is that the initial potential energy is large. To overcome this situation, $P_1 - P_{823}$ were allowed to interact in accordance with (3.5), but every 1000 time steps all velocities were damped by the factor 0.9. At the end of 37000 time steps, the damping was removed and the particles were allowed to interact for 9000 more time steps to t_{46000} . The large oscillating modes were no longer present. The resulting stable configuration is shown in Figure 3, where, most importantly, the outermost particles show a lower density than the inner particles, which is characteristic of liquid surface tension. The average diameter in Figure 3 is approximately $\frac{2}{3}$ that of Figure 1.

The slab was stabilized in accordance with (3.7), but in the following fashion in order to

Fig. 5. $T = 0.0$.

Fig. 6. $T = 0.28$, $KE = 4500$.

Fig. 7. $T = 0.50$, $KE = 1200$.

Fig. 8. $T = 0.92$, $KE = 340$.

Fig. 9. $T = 1.40$, $KE = 35$.

Fig. 10. Contact angle fit.

maintain its solid state. Again, we chose $\Delta T = 0.00005$. Whenever the total system kinetic energy exceeded 100, all velocities were damped by the factor 0.25. The system was allowed to run to t_{25000} , at which time the slab had contracted vertically primarily to the relatively stable configuration shown in Figure 4. More extensive time calculations led to crumbling, which was considered to be physically unreasonable. The result in Figure 4 has a height which is approximately $\frac{2}{3}$ of that shown in Figure 2.

5. Sessile Drop Formation

The drop shown in Figure 3 is now translated vertically upward 4.5 units so that it sits immediately above the slab shown in Figure 4. This arrangement is shown in Figure 5, with only the central slab particles being plotted. The mode of presentation in this and the next graphs distinguishes between the water and carbon particles so that the interaction can be discerned easily.

The slab particles were allowed no further motion, but P_1 - P_{823} were allowed to interact with themselves and with the graphite particles in accordance with (3.5) and (3.9). For the first 200000 steps of the computer simulation, we used $\Delta T = 1(10^{-6})$. Thereafter, we used $\Delta T = 2(10^{-6})$. To account for the energy increase due to the effect of gravity, all velocities were damped 0.9 every 2000 time steps all through the calculations. This was not considered to be significant since our interest was only in a relatively steady state configuration.

The results are summarized in Figures 6-9 at the respective times $T = 0.28, 0.60, 0.92, 1.40$. The kinetic energy KE is also recorded in each caption, since it reflects the temperature of the system. The figures show an interlocking of particles below the central fluid mass and a relative steady state at $T = 1.40$. Using linear least square approximations with the four lowest boundary particles on the left and right sides of the system, as shown in Figure 10, we found a left contact angle of 64° and a right contact angle of 68° , the average being 66° . An experimentally determined contact angle measurement reported [1] is 60° .

6. Remarks

Improvement in the results reported here should follow as the numbers of water and graphite particles are increased and the interaction parameters are made more precise.

The problem of determining the temperature through the kinetic energy remains, since no precise connecting relationship is available for quasimolecular systems, as is for molecular systems.

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APPENDIX

hx12.for

c The water particles are numbered 1-823 and are allowed to
 c interact between themselves and with the carbon particles.
 c The carbon particles are numbered 824-1826 and are kept
 c fixed throughout.
 c The force formulas between the particles are as follows.
 c H-H: $-98 + \text{sum}(-18.2627/R^{**3} + 1.70828/r^{**5})$
 c H-C: $-98 + \text{sum}(-26.1085/R^{**3} + 3.10075/r^{**5})$

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    DIMENSION XO(1826),YO(1826),VXO(1826),VYO(1826),
    1X(1826,3),Y(1826,3),VX(1826,2),VY(1826,2),
    1ACX(1826),ACY(1826),rr(1826),FX(1826),FY(1826),F(1826)
    1,r(1826),ffx(1826),ffg(1826),ff(1826)
    OPEN (UNIT=21)
    OPEN (UNIT=31)
    OPEN (UNIT=41)
    K=1
    kdamp=2000
    kprint=40000
    DO 4 I=1,1826
      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
      READ (21,10) (XO(I),YO(I),VXO(I),VYO(I),I=1,1826)
10      FORMAT (4F16,10)
265     FORMAT (I12,F25,10)
      DO 30 I=1,1826
        X(I,1)=XO(I)
        Y(I,1)=YO(I)
        VX(I,1)=VXO(I)
        VY(I,1)=VYO(I)
30      CONTINUE
        do 31 i=824,1826
          x(i,2)=x(i,1)
          y(i,2)=y(i,1)
          vx(i,2)=vx(i,1)
          vy(i,2)=vy(i,1)
31      continue
        GO TO 3454
65      DO 70 I=1,823
        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=1,823
        ACX(I)=0.
        ACY(I)=0.
        F(I)=0.

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      ffw(i)=0.0
      ffx(i)=0.0
701      CONTINUE
c we first calculate the force between h2o molecules
c and the between h2o and C molecules.
3456      DO 78 I=1,822
      ACXI=ACX(I)
      ACYI=ACY(I)
      XI=X(I,1)
      YI=Y(I,1)
      IP1=I+1
      DO 77 J=IP1,823
      F(J)=0.
      rr(J)=(XI-X(J,1))**2+(YI-Y(J,1))**2
      IF (rr(J).gt.2.339) go to 77
      F(J)=(-18.2627+1.70828/(rr(J)))
1      /(rr(J)*rr(J))
      ACX(J)=ACX(J)-F(J)*(XI-X(J,1))
      ACY(J)=ACY(J)-F(J)*(YI-Y(J,1))
      ACXI=ACXI+F(J)*(XI-X(J,1))
      ACYI=ACYI+F(J)*(YI-Y(J,1))
77      CONTINUE
      ACX(I)=ACXI
      ACY(I)=ACYI
78      CONTINUE
3457      DO 788 I=1,823
      ffxi=ffx(I)
      ffyi=ffY(I)
      XI=X(I,1)
      YI=Y(I,1)
      DO 777 J=824,1826
      ff(J)=0.
      rr(J)=(XI-X(J,1))**2+(YI-Y(J,1))**2
      IF (rr(J).gt.2.969) go to 777
      ff(J)=(-26.1085+3.10075/(rr(J)))
1      /(rr(J)*rr(J))
      ffx(J)=ffx(J)-ff(J)*(XI-X(J,1))
      ffY(J)=ffY(J)-ff(J)*(YI-Y(J,1))
      ffxi=ffxi+ff(J)*(XI-X(J,1))
      ffyi=ffyi+ff(J)*(YI-Y(J,1))
777      CONTINUE
      ffx(I)=ffxi
      ffY(I)=ffyi
788      CONTINUE
C NOW INSERT GRAVITY and combine forces.
      DO 8406 I=1,823
      acx(i)=acx(i)+ffx(i)
      acy(i)=acy(i)+ffY(i)-98.0
8406      CONTINUE
C FORCES HAVE JUST BEEN ACCUMULATED. BUT F=A SINCE MASS=1.
      DO 7123 I=1,823
      VX(I,2)=VX(I,1)+0.000002*ACX(I)
      VY(I,2)=VY(I,1)+0.000002*ACY(I)
      X(I,2)=X(I,1)+0.000002*VX(I,2)
      Y(I,2)=Y(I,1)+0.000002*VY(I,2)
7123      CONTINUE
      K=K+1
      IF (MOD(K,kdame).GT.0) GO TO 1883
      do 9900 i=1,823
      vx(i,2)=0.9*vx(i,2)
      vy(i,2)=0.9*vy(i,2)
9900      continue
      XKE=0.0
      DO 6555 I=1,823
      XKE=XKE+.5*(UX(T,2)*UX(T,2)+UY(T,2)*UY(T,2))

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```

0000  CONTINUE
      WRITE (41,265) K,XKE
1883      if (mod(k*kerint),41,0) go to 32
2014      WRITE (31,10) (X(I,2),Y(I,2),UX(I,2),UY(I,2),I=1,1826)
82      IF (K.LE.80001) GO TO 65
      STOP
      END
$

```