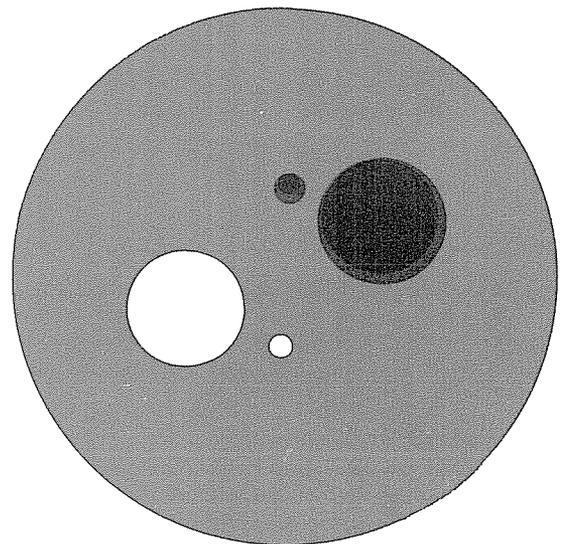


COMPUTER SCIENCES
DEPARTMENT

University of Wisconsin-
Madison



Computer Studies of a von Neumann Type Fluid

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Donald Greenspan

Computer Sciences Technical Report #261

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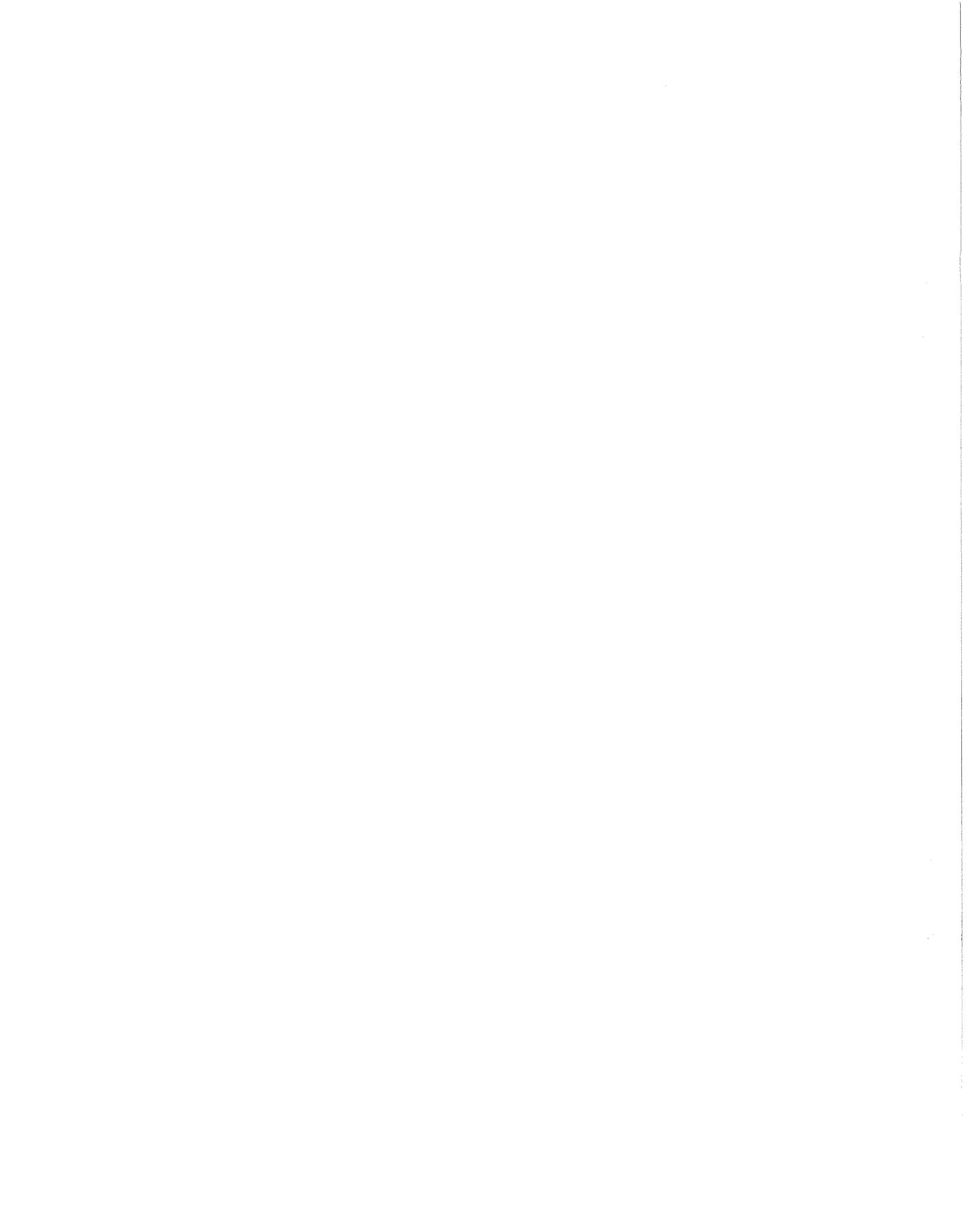
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Abstract

A particle fluid model, first recommended by von Neumann for the study of shock waves, is reformulated and implemented. A particular fluid is constructed by the computer and is shown to have such basic physical properties as buoyancy and expansion due to heating. Examples of convective motion, free surface flow, and wave generation are given.

1. Introduction

In 1944, von Neumann [1] recommended the study of complex hydrodynamical problems by returning from the continuum theory to a kinetic theory by using a quasi-molecular model. In this model the number of molecules is scaled down from its actual value ($\sim 10^{24}$) to much smaller sizes ($\sim 10-10^2$), while the intramolecular forces are correspondingly adjusted so as to approximate the correct hydrodynamical situation. In this paper we will explore the computer generation of such a fluid and various computer experiments with it.

2. Computer Generation of a von Neumann Fluid

In the spirit described above, let us first model a fluid which is held within a circular, cylindrical container which is open at the top. We will proceed in two dimensions and use metric units. The fluid will be simulated by a finite set of circular particles P_1, P_2, \dots, P_N . The basic forces between the particles will be of a classical molecular nature [2], in that when two particles are "far apart" they will attract each other, when they are "close" they will repel, and repulsion will be a much stronger force than is attraction. Viscosity will be viewed as the loss of kinetic energy and will receive special attention only when a particle collides with a wall of the container.

Specifically, we proceed as follows. For positive time step Δt , let $t_k = k\Delta t$, $k = 0, 1, 2, \dots$. For $i = 1, 2, \dots, N$, let particle

P_i have mass m_i and at time t_k let P_i be located at $\vec{r}_{i,k} = (x_{i,k}, y_{i,k})$, have velocity $\vec{v}_{i,k} = (v_{i,k,x}, v_{i,k,y})$, and have acceleration $\vec{a}_{i,k} = (a_{i,k,x}, a_{i,k,y})$. Let position, velocity and acceleration be related by the "leap-frog" formulas [3, p 107]:

$$(2.1) \quad \vec{v}_{i, \frac{1}{2}} = \vec{v}_{i,0} + \frac{\Delta t}{2} \vec{a}_{i,0}$$

$$(2.2) \quad \vec{v}_{i, k+\frac{1}{2}} = \vec{v}_{i, k-\frac{1}{2}} + (\Delta t) \vec{a}_{i,k}, \quad k = 1, 2, 3, \dots$$

$$(2.3) \quad \vec{r}_{i, k+1} = \vec{r}_{i,k} + (\Delta t) \vec{v}_{i, k+\frac{1}{2}}, \quad k = 0, 1, 2, \dots$$

If $\vec{F}_{i,k}$ is the force acting on P_i at time t_k , where $\vec{F}_{i,k} = (F_{i,k,x}, F_{i,k,y})$, then we assume force and acceleration are related by

$$(2.4) \quad \vec{F}_{i,k} = m_i \vec{a}_{i,k}.$$

Once an exact structure is given to $\vec{F}_{i,k}$, the motion of each particle will be determined recursively and explicitly by (3.1)-(3.4) from prescribed initial data. The special structure to be used is described as follows.

At time t_k , let $r_{ij,k}$ be the distance between P_i and P_j . Let G_{ij} (constant coefficient of attraction), H_{ij} (constant coefficient of repulsion), α_{ij} (constant exponent of attraction) and β_{ij} (constant exponent of repulsion) be determined

by P_i and P_j subject to the constraints $G_{ij} \geq 0$, $H_{ij} \geq 0$, $\beta_{ij} \geq \alpha_{ij} \geq 2$ (see [4]). Then the force $(\bar{F}_{i,k,x}, \bar{F}_{i,k,y})$ exerted on P_i by P_j is given by

$$(2.5) \quad \bar{F}_{i,k,x} = \left[\frac{-G_{ij}^{m,m}}{(r_{ij,k} + \xi_{ij})^{\alpha_{ij}}} + \frac{H_{ij}^{m,m}}{(r_{ij,k} + \xi_{ij})^{\beta_{ij}}} \right] \frac{x_{i,k} - x_{j,k}}{r_{ij,k}}$$

$$(2.6) \quad \bar{F}_{i,k,y} = \left[\frac{-G_{ij}^{m,m}}{(r_{ij,k} + \xi_{ij})^{\alpha_{ij}}} + \frac{H_{ij}^{m,m}}{(r_{ij,k} + \xi_{ij})^{\beta_{ij}}} \right] \frac{y_{i,k} - y_{j,k}}{r_{ij,k}},$$

where ξ_{ij} is a nonnegative measure of how close one will allow the centers of P_i and P_j to come. For small Δt , one can choose $\xi_{ij} = 0$, since repulsion will then prevent the physical impossibility that $r_{ij,k} = 0$. For computational economy, however, one may have to choose a relatively large Δt , in which case it may be necessary to choose $\xi_{ij} > 0$.

The total force $(\bar{F}_{i,k,x}^{\#}, \bar{F}_{i,k,y}^{\#})$ on P_i due to all the other $N-1$ particles is given by

$$(2.7) \quad \bar{F}_{i,k,x}^{\#} = \sum_{\substack{j=1 \\ j \neq i}}^N \bar{F}_{i,k,x}^{\#}, \quad \bar{F}_{i,k,y}^{\#} = \sum_{\substack{j=1 \\ j \neq i}}^N \bar{F}_{i,k,y}^{\#}.$$

Finally, we include gravity into the model and have

$$(2.8) \quad \bar{F}_{i,k,x}^{\#} = \bar{F}_{i,k,x}^{\#}, \quad \bar{F}_{i,k,y}^{\#} = -980 m_i + \bar{F}_{i,k,y}^{\#}$$

Particles which have collided with the walls of the container will be reflected and damped in the following simple fashion. Let the radius of the cylinder be A and let the ends of the cylinder base be located at $(-A, 0)$ and $(A, 0)$ in the XY -plane. If at t_k particle P_i is at $(x_{i,k}, y_{i,k})$, then

$$(a) \quad x_{i,k} > A \Rightarrow P_i \text{ reset at } (2A - x_{i,k}, y_{i,k})$$

$$(b) \quad x_{i,k} < -A \Rightarrow P_i \text{ reset at } (-2A - x_{i,k}, y_{i,k})$$

$$(c) \quad y_{i,k} < 0 \Rightarrow P_i \text{ reset at } (x_{i,k}, -y_{i,k}).$$

If $\bar{v}_{i,k}^{\#}$ is taken as the velocity of P_i at t_k and $\bar{v}_{i,k}$ is to be the reset velocity, then

$$(a) \quad x_{i,k} > A \text{ or } x_{i,k} < -A \Rightarrow \bar{v}_{i,k,x}^{\#} = -\delta v_{i,k,x}^{\#}, \quad \bar{v}_{i,k,y}^{\#} = \delta v_{i,k,y}^{\#}$$

$$(b) \quad y_{i,k} < 0 \Rightarrow \bar{v}_{i,k,x}^{\#} = \delta v_{i,k,x}^{\#}, \quad \bar{v}_{i,k,y}^{\#} = -\delta v_{i,k,y}^{\#},$$

where $0 \leq \delta \leq 1$. Of course, the value of the damping constant δ will depend entirely on the nature of the wall.

In particular, let us now consider the parameter choices

$N = 50$, $A = 1$, $G_{ij} \equiv \xi_{ij} \equiv 0$, $H_{ij} \equiv 1$, $\alpha_{ij} \equiv 1$, $\beta_{ij} \equiv 6$, $m_i \equiv 2.5$, $\delta = 0.1$, and $\Delta t = 10^{-4}$. (The FORTRAN program used for the discussion which follows is available in the Appendix of [5].) The major problem which confronts us immediately is that of determining all initial positions and velocities so that the fluid is physically stable. Mathematically, this problem is entirely intractable.

For this reason, we fix the particles' initial data in some approximate fashion and then let the particles interact in accordance with (2.1)-(2.4) and (2.8) until physical stability results. This was done on the UNIVAC 1110 in the following way. First, the particles were distributed uniformly and in rows so that the height of the top row was k . For each of $k = 0.5, 1.0, 1.5, 2.0, 2.5, 3.0, 3.5$ and 4 , the particles were allowed to interact with $\vec{0}$ initial velocities. Only the top row was observed. For $k = .5, 1.0, 1.5$, and 2.0 , the top row exhibited upward motions only. For $k = 3.0, 3.5$ and 4.0 , the top row showed downward motions only. So, $k = 2.5$ was selected as a first approximation for the height of the fluid. With this height fixed, the particles were then reset in a more physical way by having their density increase with the depth, but with no particle set on a wall of the container. Initial velocities were determined at random in the range

$$(2.9) \quad \begin{aligned} -200 \leq v_{i,0,x} \leq 200 \\ -200 \leq v_{i,0,y} \leq 200 . \end{aligned}$$

After 40 hours of computer run time, or 14.4 seconds of physical

time, the particle arrangement which resulted is shown in Figure 1. Particles without direction arrows showed no significant motion. The exact positions and velocities of all 50 particles are given in Table I.

With regard to Figure 1 and Table I, it is worth noting that the wall particles achieved a relatively stable formation first, due to the strong damping, that the particles below $y = 1$ did so next, and that the particles above $y = 1$ did so last. The central particles do exhibit strong, but stable, motion with the entire range of particle velocities having been reduced from (2.9) to

$$(2.10) \quad \begin{aligned} -19.0 \leq v_{i,x} \leq 22.5 \\ -19.5 \leq v_{i,y} \leq 17.5 . \end{aligned}$$

However, and most importantly, the number of particles per unit area, or density, does increase appropriately with the depth.

The relatively small time step $\Delta t = 10^{-4}$ was necessary because of the large forces which result from (2.9) when $\xi_{ij} \equiv 0$. Larger values of Δt did yield physical instability. The choice $\xi_{ij} \equiv 0$ was made because it approximates more closely than does $\xi_{ij} > 0$ the actual physical situation. Moreover, related studies with $\xi_{ij} > 0$ had been made at least once already [3, pp 87-93].

3. Buoyancy

We will now demonstrate that the fluid generated in Section 2, and shown in Figure 1, possesses the very fundamental property

TABLE I

i	x_i	y_i	$v_{i,x}$	$v_{i,y}$
1	-1.00000	1.95036	.00302	-.00403
2	-.99999	1.52836	.01837	.01689
3	-.99999	1.22001	.01787	.00175
4	-.99997	.92618	.04950	-.00226
5	-.99998	.63421	.03329	-.02091
6	-.99998	.31279	.03246	-.01149
7	-.99996	.00002	.00858	.00405
8	-.73971	.00012	-.02802	.22592
9	-.46429	.00004	.01048	.07245
10	-.17672	.00008	.01832	.08513
11	.20491	.00005	-.01359	.08998
12	.47061	.00011	-.14877	.24262
13	.74116	.00017	.15559	.30062
14	.99996	.00004	-.00882	.00883
15	.99997	.26371	-.04457	-.01092
16	.99997	.53491	-.04382	.00282
17	.99998	.80376	-.02515	-.00468
18	.99998	1.08184	-.03357	.01520
19	1.00000	1.36799	-.00306	.00925
20	1.00000	1.67576	-.00294	.01645
21	1.00000	2.08237	-.00187	-.00349
22	-.44996	.70198	-.459188	1.59317
23	-.72648	.49708	-.125516	4.52656
24	-.65549	1.23696	-3.07382	-3.91355
25	-.72187	.89006	-7.64629	2.03463
26	-.66118	.23382	-2.21826	1.36702
27	-.32188	.24609	-2.94630	-2.30909
28	-.48689	.44677	.19605	.29515
29	-.25090	.85715	20.52295	17.33698
30	-.52670	1.90130	1.85109	.82166
31	-.66589	1.57306	2.55064	1.73466
32	-.31608	1.39533	-8.26716	9.40706
33	-.04120	1.25491	10.21712	4.12646
34	-.41568	1.09505	1.55708	16.96256
35	-.00103	2.00753	-.48555	-1.20311
36	.10493	1.57983	-2.94540	2.32423
37	.02533	.18456	-3.79583	6.31884
38	-.17786	.49087	-8.89438	-.54457
39	.06249	.68675	1.11961	12.81914
40	.34696	1.31034	13.05481	2.29751
41	.36724	.64143	-18.87114	-19.08997
42	.12091	1.02842	22.49168	2.02820
43	.30053	.30162	1.02449	2.99422
44	.54960	1.91040	-.23773	.24322
45	.72549	.97424	4.79892	8.45447
46	.74085	.40231	12.84907	-4.15402
47	.52366	1.54075	7.73409	1.76992
48	.64446	.63925	-6.13839	-5.82199
49	.61433	.19184	4.01968	.67543
50	.44979	.94777	-15.73143	8.05649

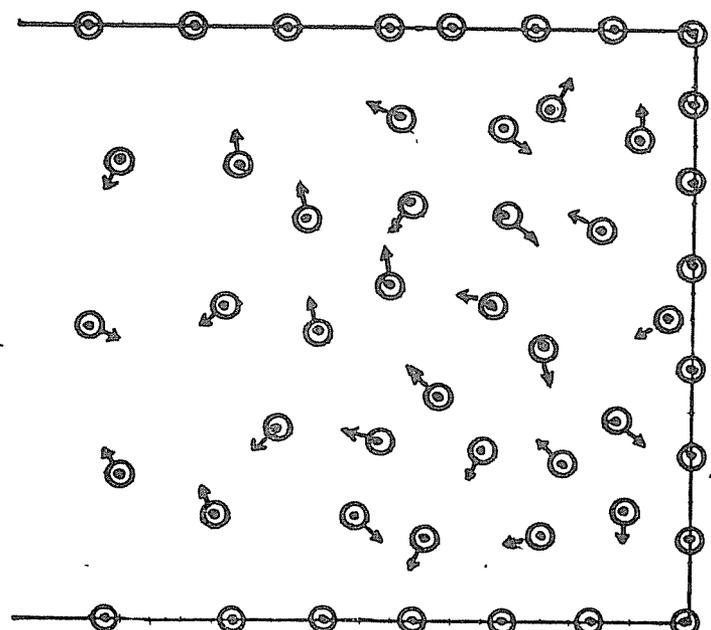


Figure 1

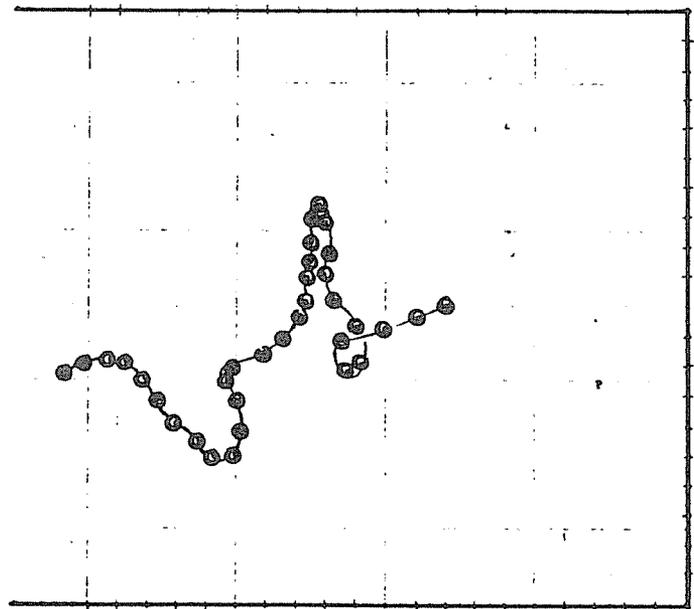


Figure 2

of buoyancy. For this purpose a new particle, P_{51} , whose mass of 0.25 is one tenth that of each fluid particle, is inserted into the fluid at (0,0.6) and is assigned an initial velocity of $\vec{0}$. Again, with $t = 10^{-4}$, the resulting motion of P_{51} at every tenth time step, for a total of 330 time steps, is shown in Figure 2. The very rapid ejection of P_{51} is seen to include relatively large lateral motions in the center of the fluid, due, of course, to the fact that the fluid particles in this region still exhibit such motions. Heuristically, the lighter particle is "carried with the currents" in this central area. The final ejection of P_{51} is to a position above the fluid, from which it descends very slowly.

Varying the mass of P_{51} reveals, as was to be expected, that increasing m_{51} decreases its rate of rise, while decreasing m_{51} increases its rate of rise. However, for $m_{51} = 0.04$, for example, the particle is ejected in a single time step, indicating that $\Delta t = 10^{-4}$ is not sufficiently small for an adequate description of the motion. It is interesting, nevertheless, that even in this case the particle is ejected to a position directly above the fluid.

4. Heating

We will show now that, in general, heating the fluid generated in Section 2 results in fluid expansion, while "judicious" heating can yield convective currents.

By heating the fluid we will mean increasing the velocity, and hence the kinetic energy, of various fluid particles. First,

let us do this in the following way. Every time a particle is found in the region bounded by $0.5 \leq x \leq 1.0$ and $0 \leq y \leq .2$, let its component of velocity $v_{i,y}$ be increased by 100. The resulting effect is to have the particles in this special region move out vertically and very rapidly, and to have the resulting partial vacuum filled by particles directly to the left of the region. This follows since the particles directly to the left are most densely arrayed and hence balance greater repulsive forces than do particles in other portions of the fluid. Again with $\Delta t = 10^{-4}$, computation for 600 time steps yields the fluid expansion shown in Figure 3. It is interesting to note that, as in Section 2, the first particles to achieve physical stability are those along the walls of the cylinder, as is especially apparent along the left wall.

Suppose next that we decrease the amount of heat and the size of the heating area in the above example. This time let each particle which collides with the base of the cylinder in that portion where $0.7 \leq x \leq 1$ be reflected with its component of velocity $v_{i,y}$ increased by 25. The resulting particle motions are now much slower and less erratic than those shown in Figure 3. Indeed, Figure 4 shows the resulting motion after 900 time steps, where the appearance of a counterclockwise convective current appears to be present and is so indicated, while Figure 5 shows the development of a larger motion of this type after 1600 time steps.

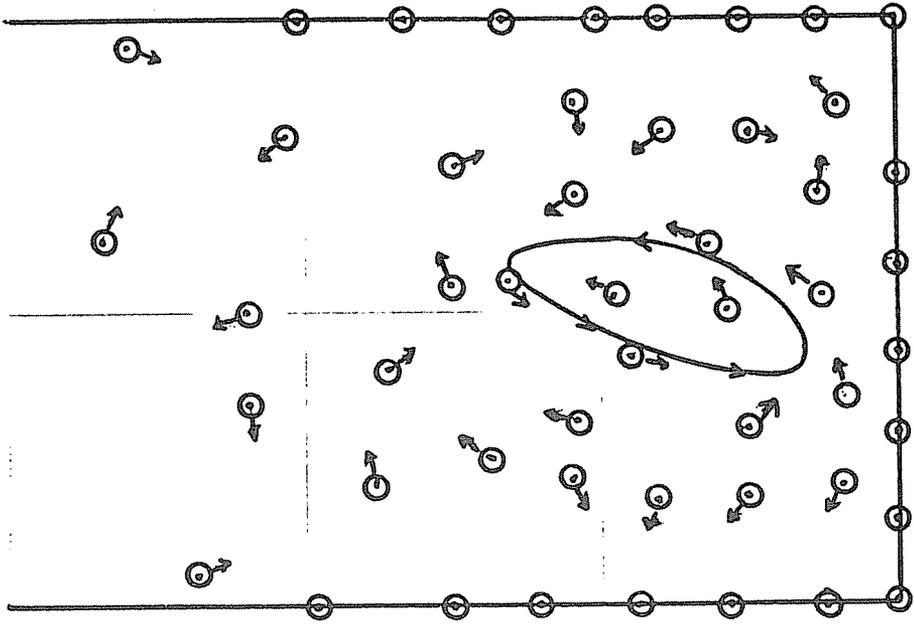


Figure 4

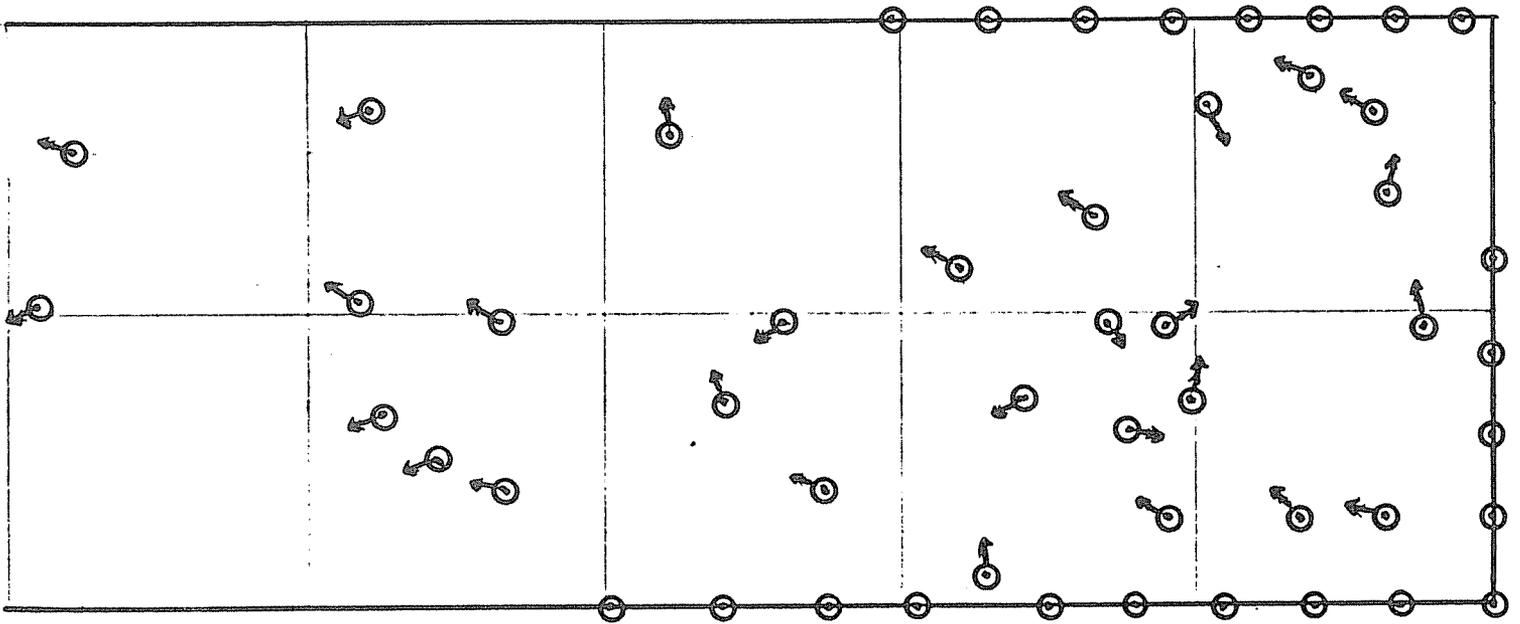


Figure 3

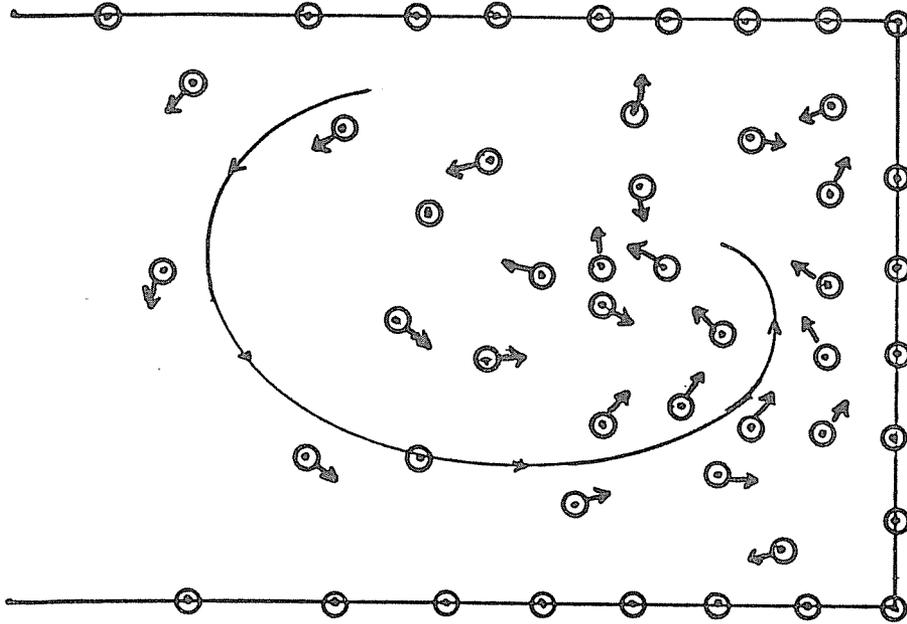


Figure 5

5. Free Surface Dam Break

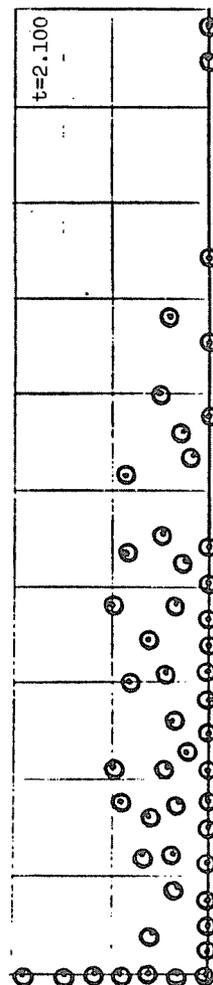
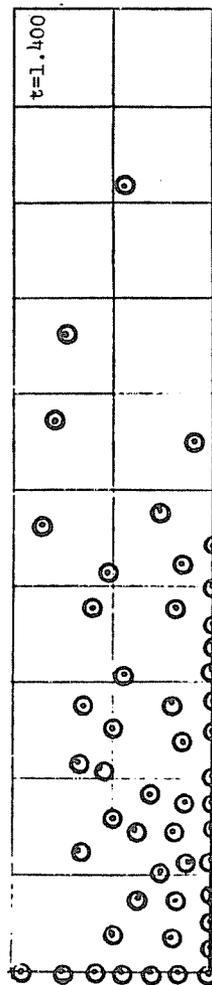
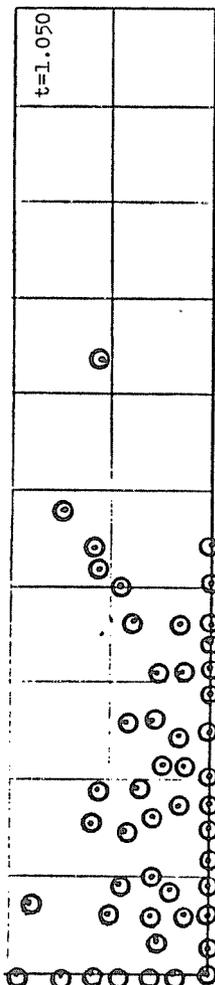
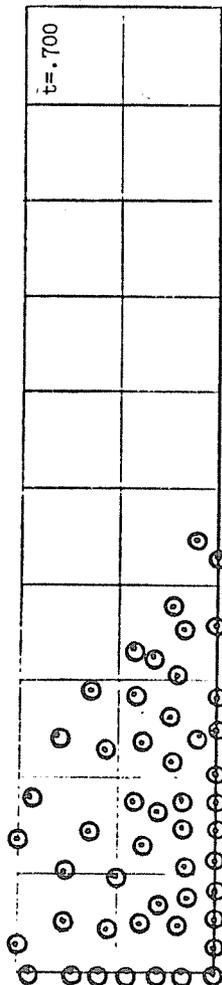
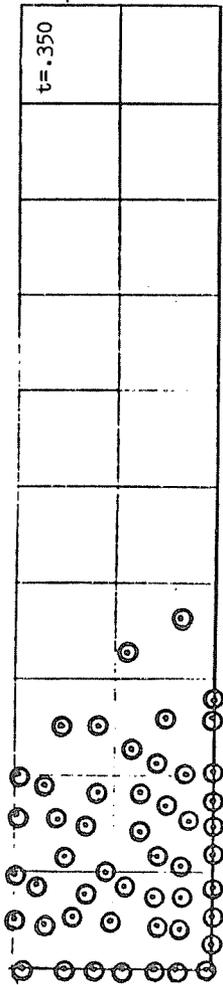
As a final example, we consider the consequences of removing the right wall of the cylinder in Figure 2. Such a model is a rough simulation of the free surface flow from a reservoir behind a breaking dam. The choice of damping factor $\delta = 0.1$ is especially appropriate in such an example.

For $\Delta t = 10^{-4}$, Figure 6 shows the resulting motion at $t = .350$, $.700$, 1.050 , 1.400 , and 2.100 . Initially, the particles which are densely arranged near the bottom, and balance relatively large forces of the repulsion, move to the right at relatively high speeds. The particles above these move more slowly, while viscosity prevents the bottommost particles from exhibiting any significant motion. These results are shown at $t = .350$ and $t = .700$. Most interestingly, at $t = 1.050$ the fluid seems to have developed a "wave" which appears to be "breaking" at $t = 1.400$. Finally, at $t = 2.100$ is shown one stage of the final phase of the flow, as all the particles above the X-axis move to the right to seek a position on this axis.

Phenomena similar to those described above are also present when considering the flow of fluid near and on beaches, an area of wide current interest [6]-[8].

6. Remark

It has been our primary intention, in this first of a series of papers, to establish the viability of a new method of computer



fluid modeling. It is believed that the qualitative results achieved, through the computer examples given, do exactly this. A variety of quantitative studies are now under way when the fluid is specified to be water. It is expected, however, that results will be obtained slowly, because of the large number of parameter choices and combinations which must be tested in order to get quantitative agreement with the very accurate experimental data available. Nevertheless, the absence of viable numerical methodology for three dimensional Navier-Stokes problems, for free surface problems, and for gaseous motion problems to which Boltzmann's equation cannot be applied (as in the outer atmosphere) would seem to make further endeavor most worthwhile.

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C ACCEL CALCULATES FORCES BETWEEN PARTICLES AND RESULTING ACCELERATIONS

```

CALL DIST
DO 6000 I=1,NM1
  IP1=I+1
  DO 5999 J=IP1,N
    C CONSTANTS OF INTERACTION
    G=0.0
    H=1.0
    IALPHA=1
    IBETA=6
    XI=0.0
    C FORCE CALCULATIONS
    FX(I,I)=0.0
    FY(I,I)=0.0
    FX(N,N)=0.0
    FY(N,N)=0.0
    ATTREP=(-G*PMASS(I)*PMASS(J)/(R(I,J)+XI)**IALPHA)
    + (H*PMASS(I)*PMASS(J)/(R(I,J)+XI)**IBETA)
    1 FX(I,J)=ATTREP*(X(I,I)-X(J,I))/R(I,J)
    FX(J,I)=-FX(I,J)
    FY(I,J)=ATTREP*(Y(I,I)-Y(J,I))/R(I,J)
    FY(J,I)=-FY(I,J)
    C CONTINUE
  5999
6000
C ACCELERATION IS NOW CALCULATED. GAMMA IS A CONSTANT WHICH REFLECTS
HOW MUCH FORCE WORKS FROM BELOW AGAINST GRAVITY.
DO 6200 I=1,N
  ACX(I)=0.0
  ACY(I)=0.0
  DO 6100 J=1,N
    ACX(I)=FX(I,J)+ACX(I)
    ACY(I)=FY(I,J)+ACY(I)
    C CONTINUE
  6100
  GAMMA=1.0
  ACY(I)=ACY(I)-980.0*PMASS(I)*GAMMA
  ACX(I)=ACX(I)/PMASS(I)
  ACY(I)=ACY(I)/PMASS(I)
6200
  RETURN
C
C SUBROUTINE WALCOL
C WALCOL REFLECTS PARTICLES FROM THE WALLS
DO 9999 I=1,N
  IF (X(I,2).GT.0.AMINUS) GO TO 9002
  EPS=AMINUS-X(I,2)
  X(I,2)=X(I,2)+2.0*EPS
  VX(I,2)=-ZETA*VX(I,2)
  VY(I,2)=ZETA*VY(I,2)
  IF (X(I,2).LT.0.A) GO TO 9003
  EPS=X(I,2)-A
  X(I,2)=X(I,2)-2.0*EPS
  VX(I,2)=-ZOOM*VX(I,2)
  VY(I,2)=ZOOM*VY(I,2)
  IF (Y(I,2).GT.ZERO) GO TO 9999
  Y(I,2)=-Y(I,2)

```

```

VX(I,2)=ZETA*VX(I,2)
VY(I,2)=-ZETA*VY(I,2)
CONTINUE
RETURN
END
9999
C

```