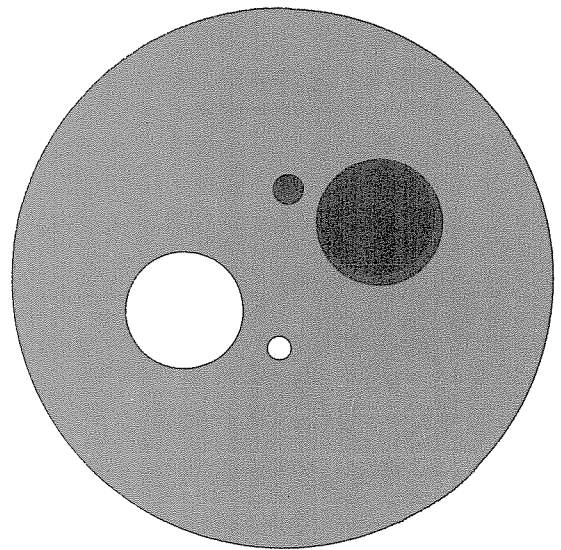


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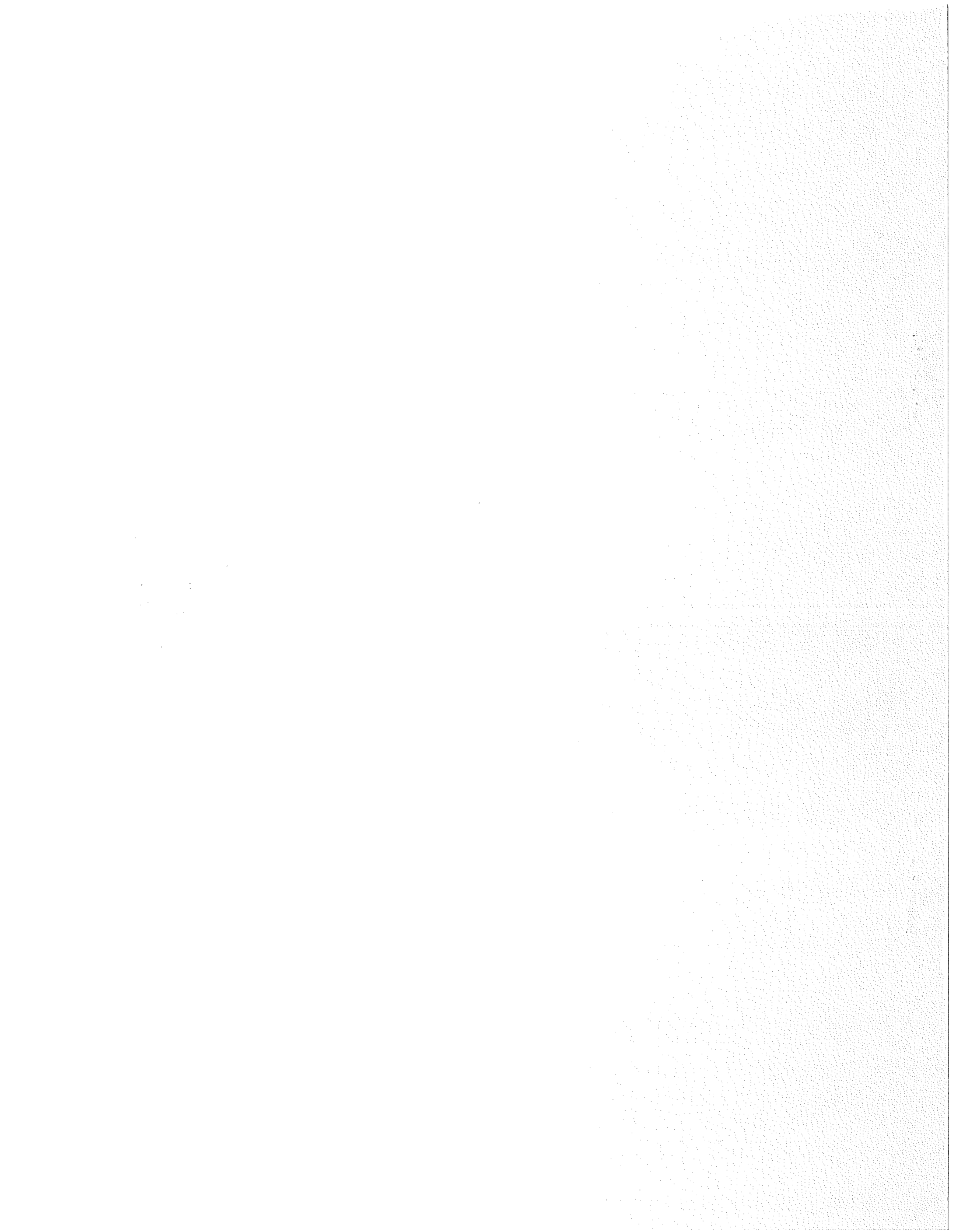
CAVITY FLOW OF A PARTICLE FLUID

by

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Abstract

A new, arithmetic, computer oriented approach to fluid modeling is developed and implemented. Fluids are simulated by finite particle sets which are subjected both to gravity and to molecular type force interactions. A particle liquid is generated on the UNIVAC 1110 and the classical cavity flow problem is studied. The method is economical and applies easily with relatively few particles to phenomena with significant, gross motions.



1. Introduction

Navier-Stokes problems, though now resolvable numerically in many cases, are still not accessible readily, if at all, in both two and three dimensions when the equations of motion are in velocity components and are time dependent (see, e.g., refs. [1-7] and the numerous additional references contained therein). Yet, such equations are often unavoidable in the study of important fluid dynamical problems (see, e.g., [8]). For this reason, we will explore the development of a new numerical approach which uses quasi-molecular models, as recommended by von Neumann in 1944 [9]. In such models, the numbers of molecules are scaled down from their actual values ($\sim 10^{24}$) to much smaller sizes ($\sim 10 \cdot 10^2$), while the intramolecular forces are correspondingly adjusted so as to approximate the correct hydrodynamical situation. The viability of this approach will be illustrated by consideration of the prototype Navier-Stokes cavity flow problem ([10]-[18]), which is formulated as follows.

For $A > 0$, consider a closed square, as shown in Figure 1, with vertices $(\frac{A}{2}, 0)$, $(\frac{A}{2}, A)$, $(-\frac{A}{2}, 0)$, $(-\frac{A}{2}, A)$. Let the base and two lateral sides be fixed, thus representing a cavity. Let the upper side be allowed to move. Thus, if each side of the square is called a wall, only the upper wall is allowed to move. Then the cavity flow problem is that of describing the motion of a fluid contained within the cavity when the upper wall has velocity V .

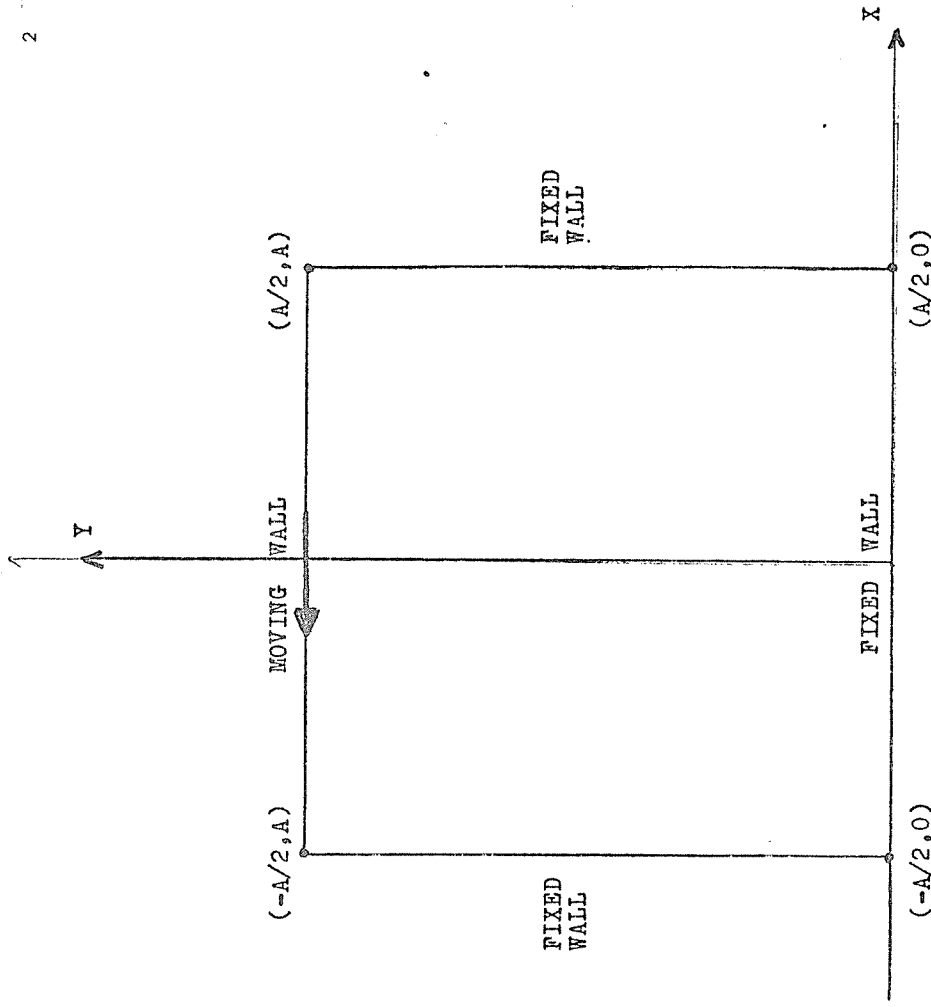


FIGURE 1

2. Dynamical Equations

In our approach to the cavity flow problem, we will let the fluid be represented by the finite particle set P_i , $i = 1, 2, 3, \dots, N$. Each particle P_i will have mass m . At time t_k , we assume P_i is located at $\vec{r}_{i,k} = (x_{i,k}, y_{i,k})$, has velocity $\vec{v}_{i,k} = (v_{i,k,x}, v_{i,k,y})$ and has 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 [19, p. 107]:

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

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

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

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

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

Once an exact structure is given to $\vec{F}_{i,k}$, the motion of each particle will be determined recursively and explicitly by (2.1)-(2.4) 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 (coefficient of attraction), H (coefficient of repulsion), α (exponent of attraction) and β (exponent of repulsion) be constants, subject only to the constraints $G \geq 0$, $H \geq 0$, $\beta > \alpha \geq 2$. Then the force $(\vec{F}_{i,k,x}, \vec{F}_{i,k,y})$ exerted on P_i by P_j is given by

$$(2.5) \quad \vec{F}_{i,k,x} = \left[\frac{-G m^2}{(r_{ij,k} + \xi)^\alpha} + \frac{H m^2}{(r_{ij,k} + \xi)^\beta} \right] \frac{x_{i,k} - x_{j,k}}{r_{ij,k}}$$

$$(2.6) \quad \vec{F}_{i,k,y} = \left[\frac{-G m^2}{(r_{ij,k} + \xi)^\alpha} + \frac{H m^2}{(r_{ij,k} + \xi)^\beta} \right] \frac{y_{i,k} - y_{j,k}}{r_{ij,k}},$$

where ξ 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 $\xi = 0$, 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 $\xi > 0$.

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

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

Finally, we include gravity into the model and have

$$(2.8) \quad F_{i,k,x} = F_{i,k,x}^*, \quad F_{i,k,y} = -980 m + F_{i,k,y}^*$$

The forces (2.5) and (2.6) are of a classical molecular nature [20], 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 stronger force than is attraction.

Note that, in addition to motion determined by (2.1)-(2.8), we must also be sure in the cavity problem to reflect particles when they have collided with a wall, and this will be done in the following simple way. If, at t_k , particle P_i is at $(x_{i,k}, y_{i,k})$, then,

- (a) $x_{i,k} > A \Rightarrow P_i$ reset at $(2A - x_{i,k}, y_{i,k})$
- (b) $x_{i,k} < -A \Rightarrow P_i$ reset at $(-2A - x_{i,k}, y_{i,k})$
- (c) $y_{i,k} < 0 \Rightarrow P_i$ reset at $(x_{i,k}, -y_{i,k})$
- (d) $y_{i,k} > 2A \Rightarrow P_i$ reset at $(x_{i,k}, 4A - y_{i,k})$.

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

- (a) $x_{i,k} > A$ or $x_{i,k} < -A \Rightarrow v_{i,k,x} = -\delta v_{i,k,x}^*, v_{i,k,y} = \delta v_{i,k,y}^*$
- (b) $y_{i,k} < 0 \Rightarrow v_{i,k,x} = \delta v_{i,k,x}^*, v_{i,k,y} = -\delta v_{i,k,y}^*$
- (c) $y_{i,k} > 2A \Rightarrow v_{i,k,x} = \delta v_{i,k,x}^* + v_{i,k,y} = -\delta v_{i,k,y}^*,$

where δ is a damping constant whose value depends entirely

on the nature of the walls and, of course, V is the velocity of the upper wall.

The motion of P_1, P_2, \dots, P_N from given initial positions and velocities is, now, well defined.

TABLE I

| X | Y | V _X | V _Y | X | Y | V _X | V _Y | X | Y | V _X | V _Y |
|---------|--------|----------------|----------------|---------|--------|----------------|----------------|---|---|----------------|----------------|
| -0.9999 | 0.0003 | 0.0175 | 0.0335 | -0.4567 | 1.3441 | 2.5831 | 0.6271 | | | | |
| -1.0000 | 0.1845 | 0.0859 | -0.0114 | -0.3937 | 1.5563 | 1.0731 | 0.3656 | | | | |
| -0.9999 | 0.3867 | 0.1239 | 0.0078 | -0.2128 | 1.7752 | 0.0944 | -1.7890 | | | | |
| -0.9999 | 0.5944 | 0.0723 | -0.0277 | 0.1315 | 1.5529 | -1.081 | -1.5496 | | | | |
| -1.0000 | 0.8137 | 0.0483 | -0.2877 | -0.3206 | 1.9386 | -0.8910 | -1.6213 | | | | |
| -0.9999 | 1.0325 | 0.1209 | -0.0000 | -0.3405 | 0.4599 | -0.0453 | -1.1775 | | | | |
| -0.9999 | 1.2825 | 0.0694 | 0.0091 | 0.0244 | 0.2139 | 1.7261 | -1.3293 | | | | |
| -0.9999 | 1.5001 | -0.8568 | -0.2245 | -0.1811 | 0.6648 | 1.6068 | -0.7887 | | | | |
| -1.0000 | 1.7501 | 0.0437 | 0.0296 | -0.2442 | 0.9068 | 0.9783 | 0.6773 | | | | |
| -1.0000 | 2.0000 | -0.1151 | -0.0338 | -0.2152 | 1.3342 | 0.1230 | 0.1032 | | | | |
| -0.9999 | 0.0000 | 0.0272 | 0.1290 | -0.0325 | 1.5513 | -0.7573 | 0.0457 | | | | |
| -0.9999 | 0.0001 | -0.0077 | 0.1350 | 0.1376 | 1.0625 | 0.6070 | 0.4360 | | | | |
| -0.9999 | 0.0001 | -0.0060 | 0.1291 | 0.2821 | 1.3542 | 2.2278 | 0.5130 | | | | |
| -0.9999 | 0.0000 | -0.1270 | -0.0872 | -0.0699 | 1.9988 | -0.3522 | -1.1087 | | | | |
| -0.9999 | 0.0000 | -0.0036 | 0.1192 | 0.3931 | 0.8346 | -1.6579 | 1.7787 | | | | |
| -0.9999 | 0.0001 | 0.0025 | -0.1513 | 0.4250 | 1.0508 | 0.4508 | -0.7200 | | | | |
| -0.9999 | 0.0000 | 0.0127 | 0.0832 | 0.1394 | 0.054 | -0.4357 | 0.7226 | | | | |
| -0.9999 | 0.0001 | -0.0005 | 0.1090 | -0.5688 | 0.6275 | -0.6868 | 1.4256 | | | | |
| -0.9999 | 0.0001 | -0.0138 | 0.0163 | 0.1917 | 0.8171 | -0.0559 | 1.4256 | | | | |
| -0.9999 | 0.0000 | -0.0584 | -0.0200 | 0.0355 | 1.3221 | -0.2693 | 0.3993 | | | | |
| -0.9999 | 0.0000 | 0.0363 | -0.0344 | 0.2427 | 1.1581 | 0.0031 | -2.0824 | | | | |
| -0.9999 | 0.0000 | -0.1126 | 0.0124 | 0.0157 | 1.7772 | 0.4132 | -0.9811 | | | | |
| -0.9999 | 0.0000 | -0.0441 | -0.0486 | 0.1315 | 1.9068 | 0.1817 | 1.5274 | | | | |
| -0.9999 | 0.0000 | -0.0467 | -0.0393 | 0.2639 | 0.2086 | -1.4256 | 0.4770 | | | | |
| -0.9999 | 0.0000 | -0.0466 | 0.0124 | 0.5003 | 2.0090 | -0.2020 | 2.2657 | | | | |
| -0.9999 | 0.0000 | -0.0898 | 0.0191 | -0.1013 | 1.1119 | -0.5624 | 1.6809 | | | | |
| -0.9999 | 0.0000 | 0.0493 | -0.2175 | -0.0341 | 0.8706 | 1.7872 | 2.8150 | | | | |
| -0.9999 | 0.0000 | -0.0120 | -0.0254 | 0.0276 | 0.6284 | 2.1045 | -1.4934 | | | | |
| -0.9999 | 0.0000 | 0.0729 | -0.3234 | 0.5669 | 1.0593 | -1.0637 | -1.4934 | | | | |
| -0.9999 | 0.0000 | -0.0210 | 0.8505 | 0.585 | 1.5600 | -0.1227 | 0.2401 | | | | |
| -0.9999 | 0.0000 | 0.0533 | -0.9045 | 0.2450 | 1.7757 | 1.3980 | -0.0265 | | | | |
| -0.9999 | 0.0000 | 0.4746 | -0.3865 | 0.3586 | 1.9094 | -0.2872 | 1.4295 | | | | |
| -0.9999 | 0.0000 | -4.2230 | -1.4585 | 0.772 | 0.9326 | -0.8326 | 2.5661 | | | | |
| -0.9999 | 0.0000 | -0.0693 | -0.2694 | 0.2447 | 0.5766 | -0.8637 | 1.3988 | | | | |
| -0.9999 | 0.0000 | 0.013 | 0.0549 | 0.668 | 0.6872 | 0.0479 | -1.1698 | | | | |
| -0.9999 | 0.0000 | -0.0202 | 1.5579 | 0.3601 | 0.9337 | -2.1234 | -0.6271 | | | | |
| -0.9999 | 0.0000 | -0.6034 | -0.513 | 0.8201 | 1.6018 | -0.7921 | 0.9254 | | | | |
| -0.9999 | 0.0000 | -0.2962 | 1.8336 | 0.5780 | 0.8232 | -1.2877 | 1.2614 | | | | |
| -0.9999 | 0.0000 | -1.9836 | -1.1985 | 0.528 | 1.3197 | -0.0095 | 1.7249 | | | | |
| -0.9999 | 0.0000 | -2.1179 | 0.9059 | 0.582 | 2.0000 | 0.129 | -0.0474 | | | | |
| -0.9999 | 0.0000 | 0.5192 | 0.343 | 0.8004 | 0.4433 | -1.6429 | 0.010 | | | | |
| -0.9999 | 0.0000 | 0.4317 | 0.1422 | 0.582 | 0.5745 | -0.6328 | 0.2669 | | | | |
| -0.9999 | 0.0000 | -0.0175 | -0.0969 | 0.7780 | 1.1512 | 0.2753 | 0.1740 | | | | |
| -0.9999 | 0.0000 | -1.4564 | -0.2460 | 0.6086 | 0.3661 | 2.0795 | -0.5032 | | | | |
| -0.9999 | 0.0000 | -0.2817 | -1.4574 | 0.7745 | 1.3844 | -1.3298 | 0.9979 | | | | |
| -0.9999 | 0.0000 | -1.8021 | -1.6609 | 0.7138 | 1.7834 | -0.3144 | 0.6698 | | | | |
| -0.9999 | 0.0000 | 0.4377 | 0.0257 | 0.4909 | 1.7800 | -0.2975 | 1.0410 | | | | |
| -0.9999 | 0.0000 | 0.4377 | 0.0257 | 0.3709 | 1.5591 | -0.2739 | 0.6564 | | | | |
| -0.9999 | 0.0000 | 0.4377 | 0.0257 | 0.5029 | 1.9999 | -0.002 | -0.0564 | | | | |

3. A Particle Fluid

A major problem which confronts us next is that of assigning initial positions and velocities to P_1, P_2, \dots, P_N so that the set of particles possesses basic hydrodynamical properties, like buoyancy. This problem is entirely intractable analytically, but is resolved computationally as follows [21].

First, let us assign a set of parameter values. Let $N=100$, $A=2$, $G=\xi=0$, $H=100$, $\alpha=1$, $\beta=3$, $m=1$, $\delta=0.1$, $\Delta t=10^{-4}$, $V=0$. Thus, only gravity and inter-particle repulsion are considered significant, strong damping occurs at the walls, and the exponent of repulsion, β , is approximately one fourth of its magnitude for actual molecular interactions [22]. Further, since short range repulsive forces are of relatively greater significance than are those at long range, we will introduce the computationally economical assumption that only those particles whose centers are within a radius of 0.25 from each particle P_i will be considered when computing (2.7) for P_i .

Next, the particles are distributed uniformly throughout the interior of the cavity and are assigned random velocity components not exceeding 10 in absolute value. From these initial data, the particles are allowed to interact according to (2.1)-(2.8) until they reach their own state of equilibrium. The resulting particle configuration at t_{100000} , that is, after ten seconds of physical time, is recorded in Table I. (The FORTRAN program for this and all further examples is given in the Appendix

of [23].) It is, perhaps, of interest to note that the initial mean particle speed was 5.3, that the mean speed has decreased to 1.2 at t_{100000} , and that the mean speed from t_{60000} to t_{100000} deviated from 1.2 by at most ± 0.2 .

4. Cavity Flow

We are now ready to consider the cavity problem for various nonzero values of V . In each of the examples which follows, the initial positions and velocities are those of Table I.

For convenience in describing the various motions, we will first refine the concept of velocity in the following way. The velocity given by (2.1) and (2.2) will be called the particles' molecular velocity. Within any "short" period of time, molecular velocity can change very rapidly because the forces are qualitatively similar to molecular forces. However, over a "long" period of time, we will require a second type of velocity which will more accurately describe the net motions of the particles. For this purpose, let $\vec{v}_{i,k,s}$, called P_i 's average velocity at t_k , be the arithmetic mean of P_i 's molecular velocities over s time steps previous to t_k . The respective speeds of these velocities will be called the molecular speed and the average speed.

Consider now a relatively slow motion of the upper wall by setting $V = -1$. It was observed almost at once that the mean molecular speed increases very rapidly at first, reaches a plateau, and thereafter increases at an exceptionally slow rate. (This qualitative effect is valid for all examples in this section and corresponds to the physical property that the fluid reaches a "steady state" very quickly, usually in less than 5 seconds [14].) Precisely, the increase was from an initial value of

1.2 to 2.1 by t_{2200} , while, at t_{18000} , it had increased to only 2.3. Incidentally, this process of increasing is not exactly monotonic.

Next, let $s = 5000$, that is, let average velocity be defined as the mean molecular velocity over 5000 time steps. Then Figure 2 shows the particle distribution at time t_{5000} . The velocity direction field has been given, however, only for those particles with average speed greater than 0.1 in order to show the development of the flow pattern. Figure 3 is restricted similarly and shows the flow at t_{25000} . Finally, Figure 4 shows the full direction field at t_{49000} , without restrictions. The flow pattern in Figure 4 is in good agreement with both experimental and numerical studies ([10]-[15],[18]).

Next, consider $V = -5$. In this case, the mean molecular speed increased to 9.3 by t_{6000} and to only 9.6 by t_{34000} . Since the gross motion will be more extensive than in the previous case, let $s = 1600$. Figures 5-8 show the particle distributions at t_{1600} , t_{7600} , t_{21600} , and t_{35600} , respectively. The velocity direction fields, however, are given only for particles whose average speed is greater than 0.5, and the vortex development is especially clear in Figure 7. However, the restriction of attention to average speeds greater than 0.5 is no longer only to show the flow development. The differential between the minimum and maximum average speeds is now large enough so that no single value of s provides an adequate description for both the faster

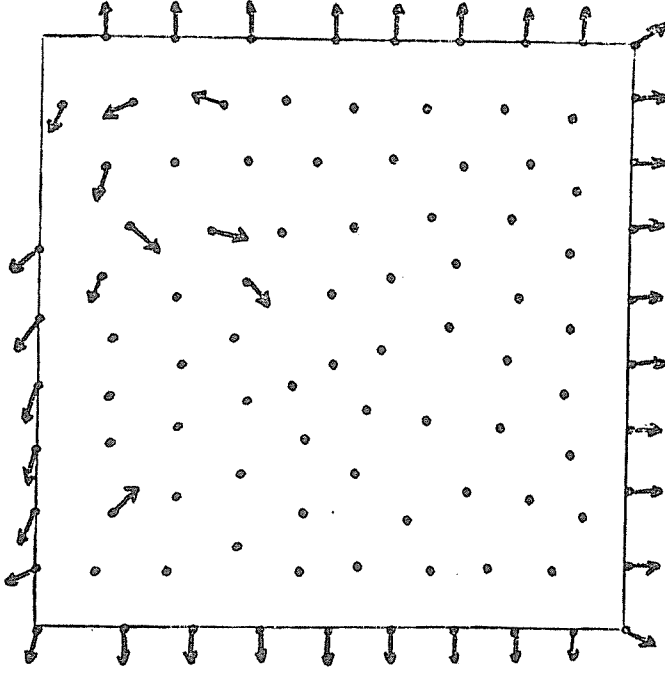


FIGURE 2

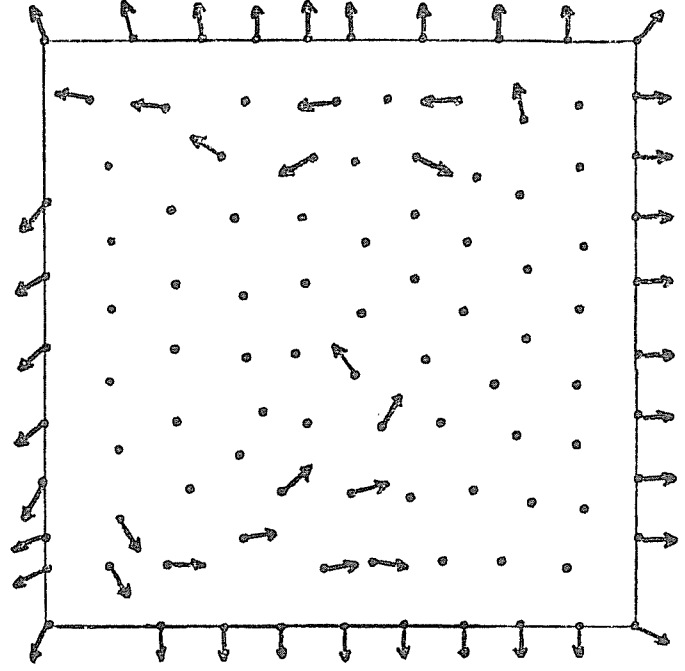


FIGURE 3

moving and the slower moving particles. Thus, the choice $s = 1600$ is adequate to show the primary vortex development, but is not adequate to show either the development of secondary vortices in the lower corners or the "acorn" shaped flow in the upper corners [11, p. 225]. Hence, other possible approaches must be discussed, and these will be explored in the next example.

Now, let $V = -20$. In this case the mean molecular speed increased to 20.3 by t_{4000} but was only 23.5 at t_{40000} . With $s = 500$ and the direction field restricted to particles with average speed greater than 5.0, Figure 9 shows little more than general counter-clockwise motion and a primary vortex around the point $(-0.25, 1.05)$. As a first alternative to considering average particle speeds, an Eulerian type analysis was then formulated so that the motion at fixed interior points could be studied. For this purpose, the grid points $(\pm 0.2 k, \pm 0.2 j)$, $k = 0, 1, 2, 3, 4$, $j = 1, 2, 3, 4, 5, 6, 7, 8, 9$ are considered to be the fixed points. As shown in Figure 10, each such point is the center of a subsquare whose sides are parallel to the respective cavity sides and whose edge has length 0.2. At each time step t_{500p} , $p = 1, 2, 3, 4, 5, 6, 7, 8$, the particles' positions and average velocities with $s = 500$ are recorded. Each particle's average velocity is then assigned to the grid point of the subsquare in which the particle is located. (Of course, a few particles will not lie within any subsquare). Finally, at each grid point, the mean of the recorded average velocities is calculated and is defined to be the fluid velocity at that point.

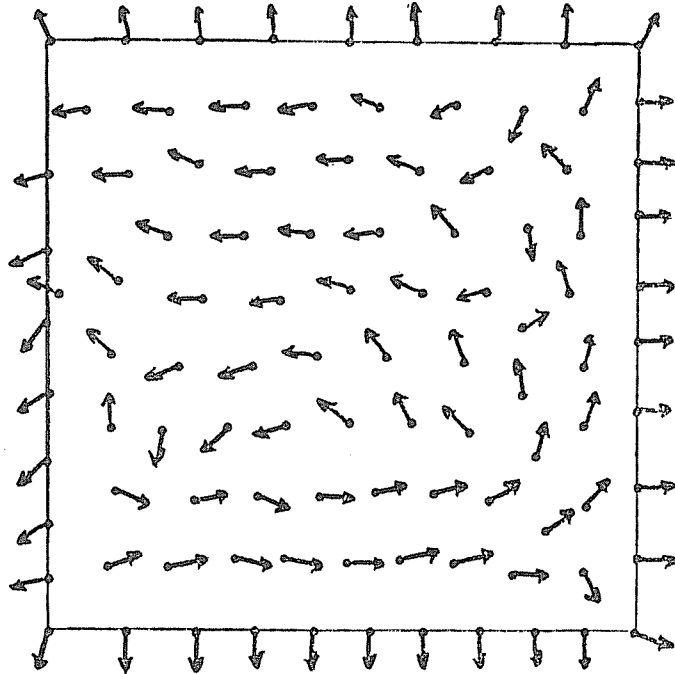


FIGURE 4

FIGURE 7

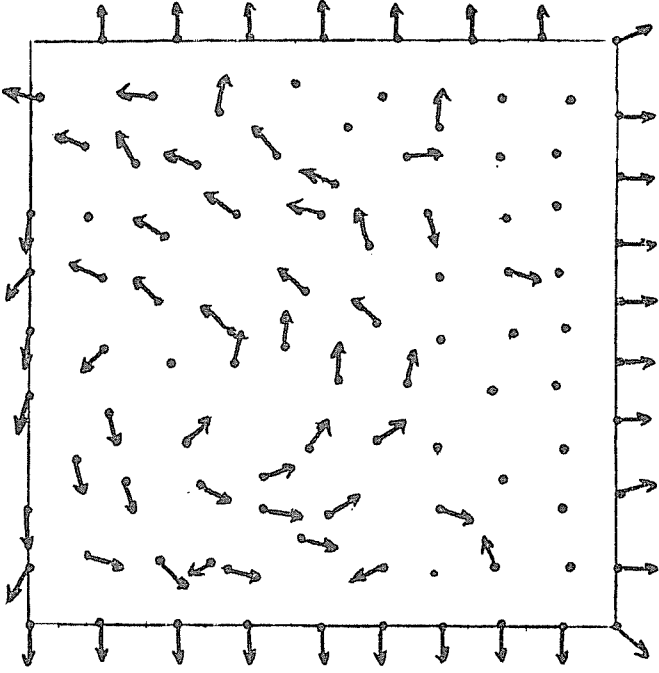


FIGURE 8

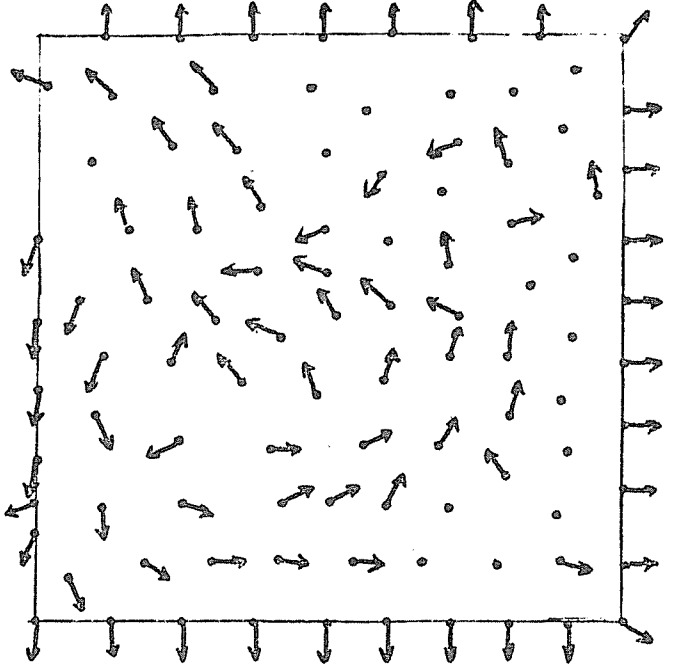


FIGURE 5

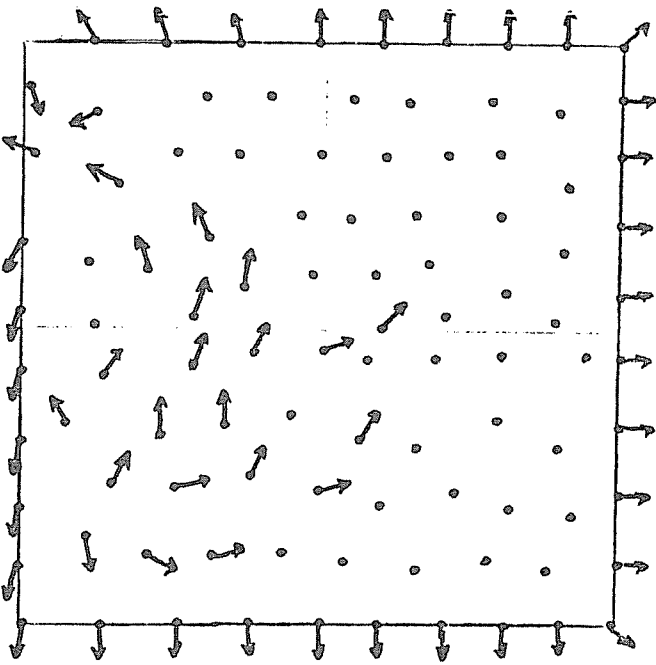
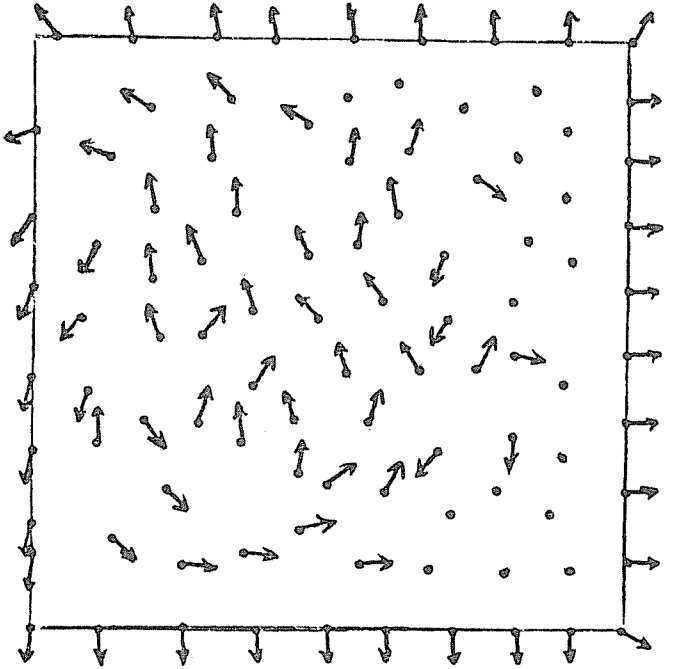


FIGURE 6



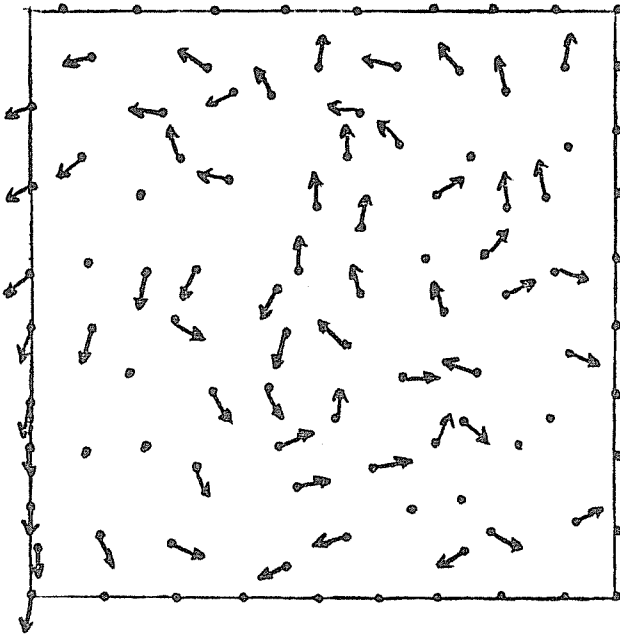


FIGURE 9

Figure 10 shows the direction field of all such velocities with magnitude greater than 1.0. The other velocities had random directions and seemed to be physically meaningless, so that the final result, again, does not reveal the more sensitive, relatively smaller motions. Other choices of s also yielded no improvement.

As a second alternative and, indeed, one which should be explored in any case, the actual motions of the particles was followed. In Figure 11, the continuous, piecewise linear path shows the motion of P_{39} from t_{4000} to t_{8000} at intervals of 0.02, beginning at the point $(.32, .40)$. The dotted, piecewise linear path shows the motion of P_{46} from t_{4000} to t_{9600} at intervals of 0.02, beginning at the point $(-.70, 2.0)$. It is quite remarkable that both motions are essentially counterclockwise and the trajectories are almost closed paths. Indeed, approximately 50% of the non-wall particles showed analogous type motions for some time period between t_{4000} and t_{10000} . Of the remaining particles, 20% showed either very slow motion, or relative stagnation, and were at some time adjacent to the bottom wall, while the remaining 30% showed gross counterclockwise motions that were difficult to categorize.

The reason why trajectories like those of Figure 11 can correspond only crudely to actual physical trajectories is simply that the model has too few particles. Indeed, with only one hundred particles, so much motion can result at each time step that particles

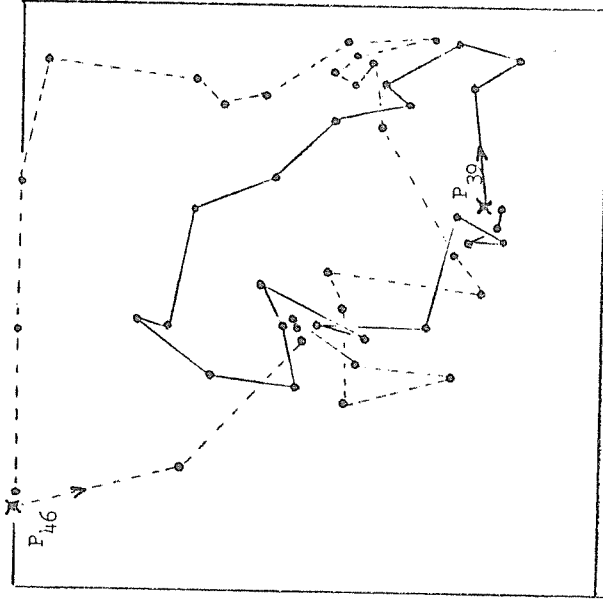


FIGURE 11

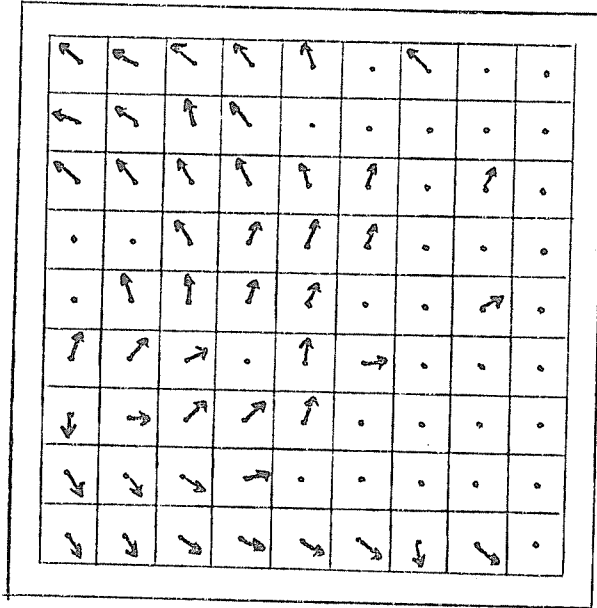


FIGURE 10

drift easily from one streamline to another, which results in the nonsmooth type of motion shown in Figure 11. The addition of more particles would result in a tighter packing and a reduction of motion per time step due to molecular interaction, and should yield more acceptable trajectories. Such results would simplify the selection of the parameter s and should even yield a more accurate Eulerian analysis.

With regard to the computations of this section, note that a variety of other parameter choices were studied, but were abandoned in favor of the ones used. For example, $V = -40$ showed such large molecular velocities that a smaller time step would have been required; $H = 50$ resulted in a particle fluid which settled with almost no contact with the upper wall; and changing δ from 0.1 to 0.01 seemed to make no difference at all. Also, note that the introduction of impulsive motion by decreasing V from -5 to -10 at t_{35000} led to instability, while the application of elementary two and three point velocity formulas, using particle positions at times t_{k-s} , t_k , and t_{k+s} , led, essentially, to the same results as those obtained using the concept of average velocity.

5. Liquid or Gas?

It is of interest to ask, now, whether the fluid generated in Section 3, and perturbed in Section 4, is a liquid or a gas. This question is a difficult one to answer since the fluid consists of only one-hundred particles and the techniques of statistical mechanics do not apply. Let us then reason in a heuristic, ad hoc, fashion from the following "principles" of fluid dynamics [24]. For a liquid, pressure p increases linearly with depth and density d is constant throughout. For a gas, $\ln p$ increases linearly with depth while d increases with depth accordingly.

Consider now the fluid given in Table I. To avoid boundary effects, let us first eliminate from consideration all particles whose distance to any wall is smaller than 0.01. Of the remaining particles, let us consider their vertical distribution from $y = 0.2$ to $y = 1.8$. As shown in Table II, one then finds a relatively uniform distribution throughout. Thus, the fluid seems to be a liquid.

TABLE II

| <u>Range of y</u> | <u>Number of Particles in the Range</u> |
|-------------------|---|
| 0.2-0.4 | 8 |
| 0.4-0.6 | 9 |
| 0.6-0.8 | 7 |
| 0.8-1.0 | 8 |
| 1.0-1.2 | 8 |
| 1.2-1.4 | 7 |
| 1.4-1.6 | 7 |
| 1.6-1.8 | 8 |

To check on this conclusion, other subdivisions were tried, more sophisticated mass distribution formulas were tried, and the analysis was repeated several times after the fluid had been set into motion. The upper wall was even removed, the fluid was allowed to reorganize itself, and the resulting distribution was studied. In all cases, the indications were, as above, that the fluid is a liquid.

6. Concluding Remarks*

The method of this paper extends readily dimensionwise and is economical for $N = 100$. With relatively few particles it can be used to analyze large fluid motions. With the addition of more particles, it should even yield refined, more sensitive fluid motions. Also, since it allows each particle to move freely, subject only to force law (2.8), the method has the additional advantage of applying directly to free boundary problems [21].

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APPENDIX

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C CAVITY FLOW WITH VON NEUMANN FLUID - LEAP FROG FORMULAS - INPUT
C IS AT HALF STEPS SO SPECIAL STARTING FORMULAS ARE NOT NEEDED - TIME STEP
C IS .0001 - H=1, G=0, M=100 (OR, EQUIVALENTLY, H=100, G=0, M=1) - EXPONENT
C OF REPULSION IS 3 AND APPEARS AS 4 BECAUSE OF COMPONENT FACTORS X/R, Y/R
C DAMPING FACTOR IS 0.1 AND APPEARS IN VELOCITY REFLECTIONS OF WALLCOL
C ONLY NEAR PARTICLES (R.LT.0.25) ARE COUNTED IN FORCE CALCULATIONS
    PARAMETER N=100
    NM1=N-1
    ZFRQ=0.0
    WALLV=1.
    TWO=2.
    A=1.0
    AMINUS=-A
    K=1
    KPRINT=500
C DIMENSION STATEMENT
    DIMENSION PMASS(N),X0(N),Y0(N),VX0(N),VY0(N),X(N,2),Y(N,2),
    1VX(N,2),VY(N,2),ACX(N),ACY(N),VBARX(N),VBARY(N),SPDBAR(N)
C INITIALIZATION SET TO ZERO AUTOMATICALLY ON 1110
C INITIAL DATA INPUT
    READ 10, (PMASS(I),X0(I),Y0(I),VX0(I),VY0(I),
    1VBARX(I),VBARY(I),I=1,N)
10    FORMAT (7F10.4)
C PRINT INITIAL DATA
    DO 20 I=1,N
    PRINT 15,I,PMASS(I),X0(I),Y0(I),VX0(I),VY0(I),VBARX(I),VBARY(I)
15    FORMAT (5X,I5,7F11.5)
20    CONTINUE
C UPDATE. X(I,1) IS X COORDINATE AT PREVIOUS TIME STEP. X(I,2) IS X
C COORDINATE AT PRESENT TIME STEP. SIMILARLY FOR OTHER VARIABLES.
    DO 30 I=1,N
    X(I,1)=X0(I)
    Y(I,1)=Y0(I)
    VX(I,1)=VX0(I)
    VY(I,1)=VY0(I)
30    CONTINUE
    GO TO 71
65    DO 70 I=1,N
    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
C CALCULATION OF ACCELERATIONS IS DONE THROUGH STEP 770
    DO 701 I=1,N
    ACX(I)=0.
    ACY(I)=0.
701    CONTINUE
71    DO 77 I=1,NM1
    IP1=I+1
    DO 76 J=IP1,N
    R=SQRT((X(I,1)-X(J,1))**2+(Y(I,1)-Y(J,1))**2)
    IF (R.GT.0.25) GO TO 73
    FX=PMASS(I)*PMASS(J)*(X(I,1)-X(J,1))/R**4

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      FY=PMASS(I)*PMASS(J)*(Y(I,1)-Y(J,1))/R**4
      GO TO 75
73      FX=0.
      FY=0.
C ACCUMULATION OF FORCES ON PARTICLE I DUE TO ALL OTHER PARTICLES IS DONE
C IN NEXT FOUR FORMULAS
75      ACX(I)=ACX(I)+FX
      ACX(J)=ACX(J)-FX
      ACY(I)=ACY(I)+FY
      ACY(J)=ACY(J)-FY
76      CONTINUE
77      CONTINUE
C NOTE THAT WE HAVE JUST ACCUMULATED FORCES, NOT ACCELERATIONS - THE ABOVE
C NOTATION, THOUGH MISLEADING, ENABLES US TO SAVE MEMORY LOCATIONS. WE
C NOW CALCULATE THE ACCELERATIONS
      DO 770 I=1,N
      ACX(I)=ACX(I)/PMASS(I)
      ACY(I)=(ACY(I)/PMASS(I))-980.
770     CONTINUE
79      DO 80 I=1,N
      VX(I,2)=VX(I,1)+.0001*ACX(I)
      VY(I,2)=VY(I,1)+.0001*ACY(I)
C VBARX AND VBARY ARE AVERAGE VELOCITY VECTORS OVER ALL PREVIOUS VELOCITIES
      VBARX(I)=(K*VBARX(I)+VX(I,2))/(K+1)
      VBARY(I)=(K*VBARY(I)+VY(I,2))/(K+1)
      X(I,2)=X(I,1)+.0001*VX(I,2)
      Y(I,2)=Y(I,1)+.0001*VY(I,2)
      SPDBAR(I)=SQRT(VBARX(I)**2+VBARY(I)**2)
80      CONTINUE
      CALL WALCOL
      K=K+1
C PRINT ONLY EVERY KPRINT STEPS
      IF (MOD(K,KPRINT).GT.0) GO TO 82
      IF (MOD(K,KPRINT).LT.0) GO TO 82
      DO 810 I=1,N
      PRINT 81,K,I,X(I,2),Y(I,2),VX(I,2),VY(I,2),VBARX(I),VBARY(I) ,
1SPDBAR(I)
81      FORMAT (5X,2I5,7F12.6)
810     CONTINUE
C CALCULATE MEAN SPEED
      SPEFD=0.0
      DO 8100 I=1,N
      SPEFD=SPEFD+SQRT(VX(I,2)*VX(I,2)+VY(I,2)*VY(I,2))
8100    CONTINUE
      SPEED=.01*SPEFD
      PRINT 8101,SPEED
8101    FORMAT (5X,F20.10)
C TERMINATION AFTER A FIXED NUMBER OF STEPS
82      IF (K.LT.10000) GO TO 65
C PUNCH OUTPUT FOR RESTART
      PUNCH 10, (PMASS(I),X(I,2),Y(I,2),VX(I,2),VY(I,2),
1VBARX(I),VBARY(I),I=1,N)
      STOP
C SUBROUTINE WALCOL FOLLOWS - REFLECTS PARTICLES AFTER WALL COLLISION
      SUBROUTINE WALCOL
      DO 9999 I=1,N

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      IF (X(I,2).GT.AMINUS) GO TO 9002
      X(I,2)=X(I,2)+2.*(AMINUS-X(I,2))
      VX(I,2)=-.1*VX(I,2)
      VY(I,2)=.1*VY(I,2)
9002      IF (X(I,2).LT.A) GO TO 9003
      X(I,2)=X(I,2)-2.*(X(I,2)-A)
      VX(I,2)=-.1*VX(I,2)
      VY(I,2)=.1*VY(I,2)
9003      IF (Y(I,2).GT.ZERO) GO TO 9004
      Y(I,2)=-Y(I,2)
      VX(I,2)=.1*VX(I,2)
      VY(I,2)=-.1*VY(I,2)
9004      IF (Y(I,2).LT.TWO) GO TO 9999
      Y(I,2)=TWO-(Y(I,2)-2.)
      C WALLV IS THE WALL VELOCITY
      VX(I,2)=.1*VX(I,2)-WALLV
      VY(I,2)=-.1*VY(I,2)
9999      CONTINUE
      RETURN
      END
```

