QUANTITATIVE, QUASIMOLECULAR MODELLING OF THE FALL OF A DROP INTO A BASIN OF WATER

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by

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Abstract

The fall of a drop into a basin of water is simulated by a molecular aggregate approach. The dynamical equations are large systems of nonlinear, ordinary differential equations which are derived using conservation of mass and total energy. These equations have to be solved numerically. Supercomputer examples of backdrop and wave simulations are described and discussed.

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1. **INTRODUCTION.**

The study of fluid drops has long been of interest to mathematicians, scientists and engineers (see, e.g., refs. [1], [2], [5],[8], and the numerous references contained therein). In this paper we explore a quasimolecular, i.e., molecular aggregate, approach to modelling reactions of a basin of water when a drop falls into it. Though related studies have been made which were qualitative [7], we will attempt here to be quantitative through the conservation of both total mass and total energy. Our approach will be distinctly different from continuum, Navier-Stokes simulations, in that we will incorporate molecular type force formulas [3], [4]. Thereby, for example, surface tension will not have to be imposed artificially [1]. The dynamical equations will be large systems of nonlinear, second order, ordinary differential equations which will be solved numerically [4]. CRAY X-MP/24 supercomputer simulations will be described and discussed.

2. **DERIVATION OF THE DYNAMICAL EQUATIONS.**

Consider a cylindrical basin which contains 1896 quasimolecules, that is, molecular aggregates, of water, arranged in a tetrahedral fashion in five layers [7]. Let the distance between any two neighboring quasimolecules be 0.04 cm. The radius of the basin is 0.44 cm, the height of the basin is, approximately, 0.13064 cm, and the resulting fluid volume \( V \) is, approximately, 0.079456 cm\(^3\).

We assume that each quasimolecule is acted upon locally only by those quasimolecules within a distance of 0.06 cm, which is called the distance of local interaction, with a force \( \vec{F} \), in dynes, whose magnitude \( F \) is given by

\[
F = -\frac{G}{R^3} + \frac{H}{R^3},
\]

where \( R \) is in cm. The resulting potential energy \( E \), in ergs, is then

\[
E = -\frac{G}{2R^2} + \frac{H}{4R^4}.
\]
Let the mass of a quasimolecule be $M$. Since 1 cm$^3$ of water has a mass of 1 gram, the total mass of water in the basin is 0.079456 gr. Distributing this mass over the quasimolecules implies $M = (0.079456)/1896 = (4.19)10^{-5}$ gr. In this fashion, mass conservation has been imposed.

In order to determine $G$ and $H$ in (2.1), we impose conservation of energy as follows. For the local interaction of actual water molecules, approximate energy and force formulas [6] are

\begin{equation}
E = (1.9646383)10^{-13} \left[ (2.725)^{12} - (2.725)^{6} \right] \text{erg},
\end{equation}

\begin{equation}
F = (1.9646383)10^{-5} \left[ 12 \frac{(2.725)^{12}}{r^{13}} - 6 \frac{(2.725)^{6}}{r^{7}} \right],
\end{equation}

in which $r$ is measured in angstroms and $F$ is measured in dynes.

Assume first that $F=0$ in (2.4), so that $T = 3.05871 \AA$ implies $F(T) = 0$. One now fills the basin with molecules, in the tetrahedral fashion used for quasimolecules, using $T$ as the distance between neighboring molecules. The number $N$ of molecules which fills the basin is, approximately,

\begin{equation}
N = \pi \left( \frac{0.44}{(3.05871)10^{-8}} \right)^2 (\frac{0.1306392}{(2.4974)10^{-8}}) = (3.4)10^{21}.
\end{equation}

Assuming zero kinetic energy, the total energy $\bar{E}$ of the molecular system is, from (2.3), approximately

\begin{equation}
\bar{E} = 6 \left[-(1.6699)10^{8}\right] \text{erg}.
\end{equation}

Assuming zero kinetic energy for the quasimolecular system and equating the energies of the two systems implies

\begin{equation}
6(1896) \left[ -\frac{G}{2(0.04)^2} + \frac{H}{4(0.04)^4} \right] = 6[-1.6699]10^{8},
\end{equation}

or equivalently,

\begin{equation}
\frac{G}{2(0.04)^2} + \frac{H}{4(0.04)^4} = -(8.807)10^4.
\end{equation}

Finally, assuming zero force between two neighboring quasimolecules implies
The solution of (2.8) − (2.9) is $G=562.58$, $H=0.90014$, so that the local force $\mathbf{F}$ between two quasimolecules has magnitude $F$ given by

$$\mathbf{F} = \frac{562.58}{R^3} + \frac{0.90014}{R^5}.$$

Introducing gravity now, the system of dynamical equations for the quasimolecules becomes

$$M \frac{d^2R_i}{dt^2} = -980M + \alpha \sum \left( \frac{-562.58}{R_{ij}^3} + \frac{0.90014}{R_{ij}^5} \right),$$

in which $i=1, 2, \ldots, 1896$, $R_{ij}$ is the distance from $P_i$ to $P_j$, the summation is taken over all particles $P_j$ whose distance to $P_i$ is smaller than 0.06, and $\alpha$ is a scaling factor which assures that the local force is indeed local relative to gravity. Rewriting (2.11) as

$$\frac{d^2R_i}{dt^2} = -980 + \alpha \sum \left( \frac{-134.27}{R_{ij}^3} + \frac{0.21483}{R_{ij}^5} \right)10^5,$$

and assuming that "local relative to gravity" means

$$\alpha \left| \frac{-134.27}{(0.06)^3} + \frac{0.21483}{(0.06)^5} \right| 10^5 = (1\%) 980$$

yields $\alpha=(2.8)10^{-10}$. Thus, (2.12) reduces to

$$\frac{d^2R_i}{dt^2} = -980 + \sum \left( \frac{-376}{R_{ij}^3} \right)10^5 + \frac{(0.601)}{(R_{ij}^5)} 10^{-5},$$

$i=1, 2, \ldots, 1896$.

For computational convenience, we now make the changes of variables $R=\alpha \bar{R}$, $t=\beta \bar{t}$, with $\alpha=0.02$, $\beta^2=0.002$, so that (2.13) reduces to

$$\frac{d^2\bar{R}_i}{dt^2} = -98.0 + \sum \left( \frac{-47.0}{\bar{R}_{ij}^3} + \frac{187.8}{\bar{R}_{ij}^5} \right),$$

(2.14)
for which the equilibrium distance is \( R = 2.0 \) and the distance of local interaction is \( D = 3.0 \).

3. **EXAMPLES.**

Let us first construct a relatively stable liquid basin. All 1896 particles are assigned initial velocities at random with speeds less than \( 8 \times 10^{-5} \). They are then allowed to interact in accordance with dynamical equation (2.14). The numerical solution is generated with \( \Delta t = 0.0001 \). Those particles colliding with a wall or with the bottom of the basin are reflected with the damping factor 0.9. The system was allowed to interact through \( t = 80000 \), at which time the fluid reached the relatively steady basin shape shown in Figure 1. Removal of the wall and the resulting flow outward of the particles verified their fluid state. The height of the fluid is approximately \( R = 1.3 \).

In order to study the reaction of the basin to a falling drop, we consider next two cases. In each, the counter was reset to zero.

**Example 1.** Nine particles, \( P_{1897}, P_{1898}, \ldots, P_{1905} \) were introduced at the points \((0, 0, 1.45), (1, 1, 3.18), (-1, 1, 3.18), (1, -1, 3.18), (-1, 1, 3.18), (-1, 1, 5.18), (-1, -1, 5.18), (1, -1, 3.18), (1, -1, 5.18)\) as shown in Figure 2. These particles, called the drop, are each assigned twice the mass of a basin particle and the velocity \((0, 0, -100)\). Figure 3 shows at \( t = 300 \) the drop penetration into the basin. Figure 4 at \( t = 450 \) shows a rapid backdrop reaction which consists of a single particle rising to the height \( R = 3.6 \). In Figure 5 at \( t = 750 \), the isolated particle has risen to \( R = 6.9 \), while a more substantial backdrop has now appeared and has risen to \( R = 3.3 \). In Figure 6 at \( t = 900 \) the isolated particle has risen to \( R = 7.9 \) while the large backdrop has begun to fall and also exhibits the phenomenon of pinching. The production of the isolated particle is a molecular type phenomenon. The pinch off of the large backdrop is a phenomenon which is reproducible in the large and has been exhibited.
FIGURE 1. BASIN EQUILIBRIUM

FIGURE 2. NINE PARTICLE DROP

FIGURE 3. DROP ENTRY INTO THE BASIN
FIGURE 4. BASIN REACTION
AT T_{450}

FIGURE 5. BASIN REACTION
AT T_{750}

FIGURE 6. BASIN REACTION
AT T_{900}
FIGURE 7. OUTGOING WAVE AT T\(_{900}\)

FIGURE 8. OUTGOING WAVE AT T\(_{1050}\)
by means of high-speed photography [9].

We did not notice outgoing waves in the above reaction. This may have been due to any of several factors, including the speed of the reaction, the relatively small number of quasimolecules, and a relatively unnoticeable wave amplitude. To generate outgoing waves we proceeded as follows.

Example 2. Example 1 was repeated with a single modification. The drop velocities were reduced to $(0, 0, -75)$. Wave motion was defined in terms of particle heights being greater than the average surface height [7]. Figures 7-8 then show a small amplitude, outgoing wave at the respective times $t_{900}$ and $t_{1050}$. The simulation was continued beyond $t_{1050}$ and the wave did reach the wall. However, the associated backdrop did not pinch.

4. REMARKS

With regard to the large number of other examples run, the results are summarized as follows.

For wave velocities smaller than those of Example 2, that is, for $(0, 0, -50)$, $(0, 0, -25)$, $(0, 0, -10)$, $(0, 0, -5)$, backdrop and wave formations became decreasingly less evident. For four particle and eight particle drops with initial velocity $(0, 0, -100)$, the results were similar to those of Example 1, but with lower backdrop heights. A rearrangement of the basin so that it had a smaller radius and a greater height yielded less clear results too often.

In terms of improvement, we would like to study a basin with many more particles than 1896. Unfortunately, the memory requirements for simulating even a 10000 particle basin exceeded the computer’s capacity. Such a system can be simulated in two dimensions, but we felt a full three dimensional simulation was essential. Also, the inclusion of temperature in the model would be of great interest.
REFERENCES


