JOURNAL OF COMPUTATIONAL PHYSICS **13**, 430–432 (1973)

Note

New Method for Searching for Neighbors in Molecular Dynamics Computations

The aim of this note is to propose a technique for saving computer time and required memories in the numerical method called Molecular Dynamics (M.D). This method consists in solving the equations of motion for a microcanonical system of a few hundreds or thousands of molecules, in order to extract some desired equilibrium or dynamical properties. Since in this method a two-body potential is usually adopted, a relatively long time is spent in searching for the "neighbors" of a given molecule; here neighbor means a molecule whose interaction with a reference one is not negligible. Our goal is to reduce the search time and also the necessary storage capacity (memories).

A typical example of a two-body potential is the Lennard–Jones potential

$$U(r_{ij}) = 4\epsilon[(\sigma/r_{ij})^{12} - (\sigma/r_{ij})^{6}]. \tag{1}$$

(Or, for polyatomic molecules, atom–atom combinations of this potential [1]).

The equations of motion for the N molecules of the system are integrated step by step, the step in time being typically $10^{-14}s$. As this integration requires the force (or torque) acting on each molecule, this would necessitate the computation of $N(N-1)/2$ interactions in all, if it were not that, as said above, only a fraction of this number (interaction with "neighbors") need be taken into account.

A known method [2] for doing this consists in associating to each molecule i two concentric spheres of volume V_1 and V_2 and of radius r_1 and r_2, respectively. At a given step the sphere of radius r_1 contains all the molecules whose interaction with molecule i is not neglected (neighbors). The sphere of radius r_2 contains moreover the molecules that have any chance of interacting with i in the p forthcoming steps. For the choice of r_1, using potential (1), 2.5σ is a reasonable value, so that $V_1 = 65\sigma^3$. For dense liquids the mean volume per molecule is about $v = 1.4\sigma^3$, so that the mean number of molecules in V_1 is $N_1 = V_1/v \approx 47$. If one choses $p = 10$, it is sufficient to take $r_2 = 2.75\sigma$ ($V_2 = 87.5\sigma^3$). The mean number of molecules in V_2 is then $N_2 = V_2/v \approx 62$.

A table containing the labels of the N_2 not-too-far molecules is stored for each molecule i. During p steps, the search for identifying the N_1 neighbors of molecule i has to be done only in this table and not among the N molecules. After the p steps, all N tables are reconstructed; this requires the computation of $N(N-1)/2 \approx N^2/2$ distances. Consequently, since p is finite and rather small, an important fraction of the total computing time is proportional to N^2. Also, speaking only of the present problem of the identification of the interacting molecules, the required storage capacity is in this method

$$M = \tfrac{1}{2}NN_2 = \tfrac{1}{2}N(V_2/v). \tag{2}$$

On the other hand, our method takes advantage of the fact that the intermolecular potential is usually extremely repulsive at short distances, so that close proximity of two molecules is highly unlikely. For example, with potential (1), for the situation $r_{ij} = \sigma\sqrt{3}/2$ one has $\exp -U/kT = 2.3 \cdot 10^{-6}$ if $kT = \epsilon$. We subdivide the usual cubic box of edge L containing the N molecules into $\mathcal{N}$ cells of edge l ($\mathcal{N} = L^3/l^3$). If, for example, $l = \sigma/2$, the chance that two molecules be in the same cell is negligible (the probability is of the order of the exponential given above for the configuration which is the most favorable to the two molecules, i.e., when they are at two opposite corners). Consequently, such a situation will not occur in a M.D. run. We now store in the computer a table NT with $\mathcal{N}$ elements labeled $1 \cdots K \cdots \mathcal{N}$. We put $NT(K) = 0$ if cell K contains no molecule, and $NT(K) = i$ if it contains molecule i. The table NT is constructed at the beginning of each integration step (this is simply done by dividing the three coordinates of each molecule by l; the set of the three integer parts of the resulting numbers constitute the index which is summarized by K here). One then orderly scans *the cells, not the molecules*. If a cell is occupied, one computes the distances (and interactions) between the molecule in it and the ones possibly present in the cells within volume V_1. More exactly this computation is done over the ensemble of cells approximating the sphere V_1 or rather over half this ensemble since a distance first computed as r_{ij} need not be recomputed as r_{ji} when the reference molecule has become the jth. Since $V_1/2$ and, hence, the number of cells in it, are constant, and because, for a given density, $\mathcal{N}$ is proportional to N, it is seen that in our method no part of the calculation is proportional to N^2. Consequently, our method supersedes the conventional one when the number of molecules in the system is large. We have tested the proposed method with an M.D. computation of a diatomic liquid (the center of grvaity of each molecule is then the reference point for deciding whether or not a molecule is "contained" in a given sphere or cell). For 500 molecules, we found out that our method is slightly faster in total computer time than the conventional one.

Another, perhaps more timely advantage of our method is the smaller storage capacity required; this is

$$M' = \mathcal{N}. \tag{3}$$

Comparing Eqs. (2) and (3) we have

$$\frac{M'}{M} = \frac{2\mathcal{N}}{NN_2} = \frac{2L^3}{l^3NN_2} = \frac{2v}{l^3N_2}\,.$$

For liquids this ratio is smaller than unity; with the choice of the parameters quoted as examples above, its value is 0.366. As an illustration, consider a cubic box with edge $L = 18\sigma$ containing 4,000 molecules; this yields about, for the mean molecular volume, the value $v \approx 1.4\sigma^3$ as above. We then have, keeping also the same figures for the other parameters: $\mathcal{N} = 36^3 = 46{,}656$. We find $M' = 0.466 \cdot 10^5$, whereas $M = 1.24 \cdot 10^5$.

REFERENCES

1. J. BAROJAS, D. LEVESQUE, AND B. QUENTREC, *Phys. Rev. A* 7 (1973), 1092.
2. L. VERLET, *Phys. Rev.* **159** (1967), 98.

RECEIVED: April 4, 1973

B. QUENTREC

Laboratoire de Physicochimie des Rayonnements[*]
Université Paris XI
Orsay, France

C. BROT

Laboratoire de Physique de la Matière Condensée[†]
Université de Nice
Parc Valrose
06 Nice, France

---

[*] Laboratoire Associé au CNRS no. 75.

[†] Laboratoire Associé au CNRS no. 190.