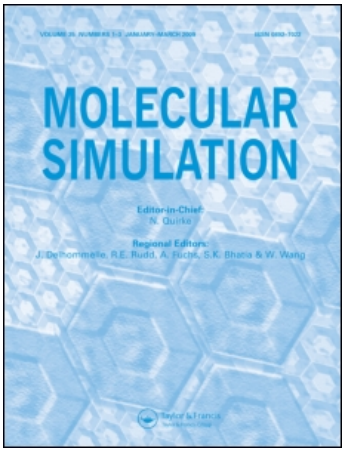

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On the Maximum Displacement Parameter in Monte Carlo Simulations of Mixtures

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Note

ON THE MAXIMUM DISPLACEMENT PARAMETER IN MONTE CARLO SIMULATIONS OF MIXTURES

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When using the Monte Carlo Method in Condensed Matter Physics, the trial configurations of the systems are generated in a Markovian way through configuration space. The particles are moved (conventionally one at a time) an arbitrary distance from their current position to new positions equally distributed on a cube of side 2δ centered on their current positions. This quantity δ, is called the Maximum Displacement Allowed to particles (MDA). Usually this value is adjusted in order to give an average probability of accepting a trial configuration of 0.5 [1]. Chapman and Quirke [2] have studied whether this choice really represents an optimum figure using a Lennard-Jones system. More recently, the influence of the MDA on the mean square displacement for a system in which only one kind of particle moves has been considered [3].

On the other hand, when the system under study has more than one kind of mobile species an assumption about the choice of MDA – or its equivalent: the average probability of accepting a generated configuration – is made: a *single* value for all species is usually selected without any prescription. In this note we report the effect of the MDA on the behavior of mixed systems.

We have carried out calculations in a 108-particle Lennard-Jones system containing 54 A and 54 B particles using a cubic box of side L, with periodic boundary conditions and the Lorentz-Berthelot mixing rules [4].

The cutoffs radii $r_c^{\alpha\beta}$ for different the pair potentials were: $2.5\sigma_{AB}$. Since our interest is in the general behavior of mixed systems, we chose $\varepsilon_{AA} = \varepsilon_{BB} = \varepsilon_{AB} = \varepsilon$ and $\sigma_{AA}/\sigma_{BB} = 2$. Runs were carried out at $\rho^* = .85$ and three temperatures namely $T^* = 1$, 1.2 and 1.4 respectively.

Configurations were generated moving one particle at a time using the following equation:

$$q' = 9 + 2\delta(0.5 - \mathbb{R}) \tag{1}$$

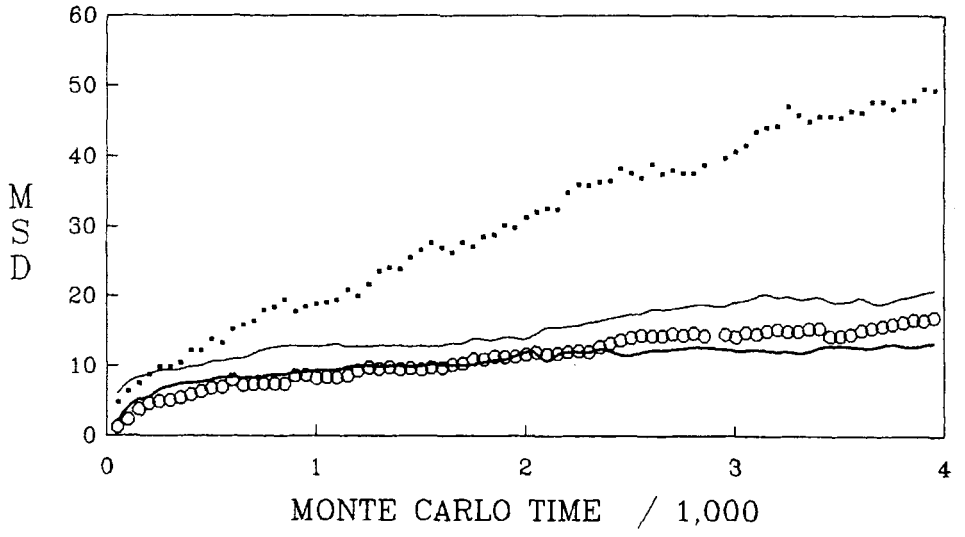

Figure 1 The mean square displacement (in Å^2) vs. the Monte Carlo time at $T^* = 1.4$, for B-particles: ■ $P_W = 0.30$ and ○ $P_W = 0.71$; and for the A-particles: — $P_W = 0.30$ and ··· $P_W = 0.71$.

where q is a coordinate of the particle, $\mathbb{R}$ a random number in the interval [0, 1]. One Monte Carlo time, (t_{mc}) is completed when the coordinates for all the particles were changed.

In order to ensure consistent simulations, the fluctuation of the total energy was tested using the standard deviation over the average value of the energy. This test was carried out during the simulation every 50 Monte Carlo times, and the fluctuations in the energy were 2-3%.

For each single value of δ the whole average probability of accepting a trial configuration during the simulation: P_w, was computed. Simultaneously the same was done for P_A and P_B ie. when the configurations are generated by displacing either A or B respectively. Constant values for P's were reached after approximately 200 Monte Carlo times.

Figure 1 shows the Mean Square Displacement at time t, $\langle R_t^2 \rangle$, which is defined as:

$$\langle R_t^2 \rangle = \langle |r(t) - r(0)|^2 \rangle \tag{2}$$

where $r(t)$ is the position of the particle after time t and $r(0)$ is the initial position of the particle, at time zero. It is plotted against t_{mc} for the particles A and B for two values of P at $T^* = 1.4$. This figure confirms previous results for the α-AgI system [3] where the influence of the MDA was shown for a system with only one kind of moving particle.

We calculated the total average energy using:

$$E = \left\langle \sum_{i<j} V_{\alpha\beta(r_{ij})} \right\rangle \tag{3}$$

and the variation of E, for P_w between 0.20 and 0.71, was of the order of 2-3% ie. the same value on the calculated energy fluctuations.

Table 1 The ratio between the average probability of accepting a configuration when it is generated moving particle B or A respectively: P_B/P_A; and the average probability of accepting a configuration: P_W, P_A and P_B.

	P_B/P_A			T^*								
	T^*			1.4			1.2			1		
δ/L	1.4	1.2	1	P_W	P_B	P_A	P_W	P_B	P_A	P_W	P_B	P_A
0.02	1.09	1.10	1.11	.81	.84	.77	.80	.84	.76	.78	.82	.74
0.03	1.15	1.15	1.16	.73	.78	.68	.71	.76	.66	.69	.74	.64
0.04	1.21	1.21	1.24	.64	.70	.58	.62	.68	.56	.60	.67	.54
0.05	1.26	1.27	1.33	.57	.63	.50	.54	.61	.48	.52	.60	.45
0.06	1.32	1.37	1.39	.50	.57	.43	.47	.55	.40	.45	.53	.38
0.07	1.44	1.44	1.52	.44	.52	.36	.41	.49	.34	.39	.47	.31
0.08	1.52	1.61	1.64	.39	.47	.31	.37	.45	.28	.33	.41	.25
0.09	1.68	1.74	1.76	.34	.42	.25	.32	.40	.23	.29	.37	.21
0.10	1.76	1.89	2.12	.29	.37	.21	.28	.36	.19	.25	.34	.16
0.11	1.89	2.00	2.00	.26	.34	.18	.24	.32	.16	.21	.28	.14
0.12	1.94	2.31	2.36	.23	.31	.16	.22	.30	.13	.19	.26	.11

Table 1 shows of the dependence of the ratio P_B/P_A on δ. It is clear that this ratio depends strongly on the MDA and the value of P_B is higher when the MDA is increased.

As was pointed out for the single component system, a measure of the efficiency ($\mathbb{E}$) with which the simulation explores the configuration space should have the form [2]:

$$\mathbb{E} = \delta \cdot P \tag{4}$$

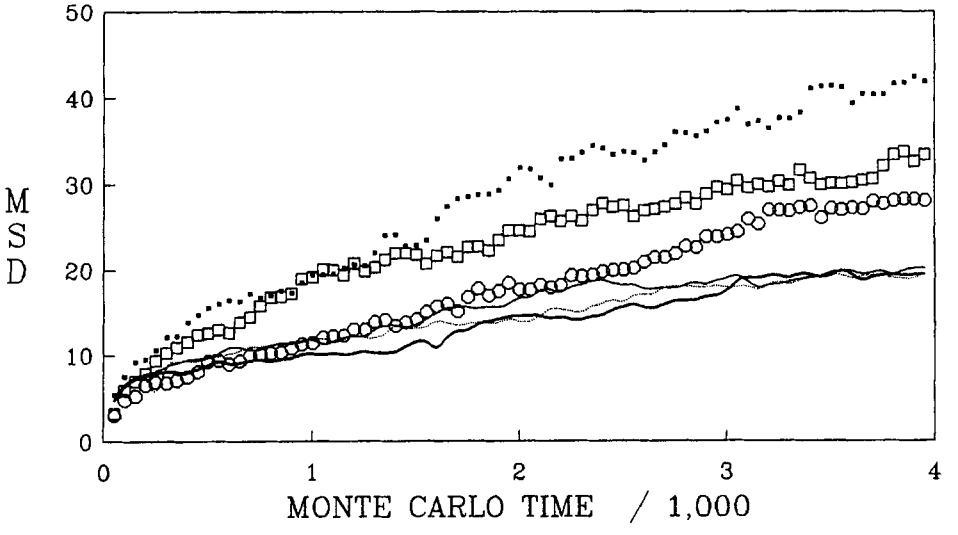

Figure 2 The mean square displacement (in Å^2) vs. the Monte Carlo time at $T^* = 1.4$: for B-particles at: ■ $P_{AB} = .37$; □ $P_W = .37$ and ○ $P_W = .50$ and for A-particles at: — $P_{AB} = .37$; ··· $P_W = .37$ and — $P_W = .50$

Now, if we assume that P has an exponential form (Table 1):

$$P = \exp(-\mathbb{C}\delta) \tag{5}$$

- were $\mathbb{C}$ is a constant -, by introducing eq. (5) into eq. (4) it is seen that the function $\mathbb{E}$ has a maximum for $\delta_{max} = 1/\mathbb{C}$, and the corresponding maximum value for P is 0.37.

On the other hand, for the present kind of systems, it is clear that the probability of accepting a trial configuration will depend on the nature and properties of the particle which generate the configuration. Thus, in Figure 2 we have plotted the curve labeled $P_{A,B}$ for which the values of the whole average probability and the values of the average of partial probabilities are the same - $P_{A,B} = P_W = P_A = P_B = 0.37$ - , due to the choise of a particular value for the δ *for each kind* of particle.

It is also evident from these plots that the importance of the adequate value of δ for each particle becomes stronger for the particle with the lower Lennard-Jones radius.

To sum up it is clear that a careful choice of the MDA is necessary when studying a system with more than one mobile kind of particle: a) due to the influence of δ on the MSD and b) to prevent certain configurations from being forbidden and the ergodicity from became a problem.

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