

## MANY PARTICLE MOLECULAR DYNAMICS METHODS

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In a Molecular Dynamics, MD, program the number of distinct pair separations is  $N(N-1)/2$  for a MD cell containing  $N$  molecules. Usually the range of the interaction potential is limited to several molecular diameters so that a spherical truncation can be applied when evaluating the interactions. However, in a conventional program the nearest-image transformation must be applied to each pair in the system, and their separation determined, before the "cut-off" is applied. Thus the computer time contains a component which increases quadratically with  $N$ . Consequently, an upper limit of approximately 1000 molecules is usual. Further, on a vector processor the spherical truncation would inhibit vectorisation<sup>(1)</sup> so that the energy and forces as well must be evaluated for each pair in the system, even though when  $N$  is large most of them will be out of range.

Two methods which enable a large number of molecules in the MD cell to be simulated are discussed below. In these schemes the computer time increases approximately linearly with time because they use ways of pre-eliminating the more distant, non-contributing, interactions before the inter-particle separations are calculated.

The first method establishes a table of neighbours for each particle at time steps of roughly equal interval (typically every 10)<sup>(1)</sup>. This table is used at intervening time steps to determine those molecules with a chance of being within the truncation radius of each particle. Unfortunately this method has considerable memory requirements. The table of neighbours needs  $\sim 45 N$  words on using a truncation radius of  $2.5\sigma$  and  $r_2 = 2.94\sigma$  [see ref.(1)] on a Lennard-Jones liquid near the triple point.

In the second method the molecules are assigned to  $N_L$  smaller sub-cells or link cells which completely fill the original MD cell<sup>(2,3)</sup>. The minimum side length of a link cell equals the truncation range of the interactions. Particles within a link cell only then need to interact with those in the first shell of link cells about it. The contents of each link cell are efficiently obtained through an array, LINK, of dimension  $N$ , which contains a consecutive series of closed chains of particle indices,

each chain being associated with a particular link cell. Each element in LINK contains the index of the next particle in the chain. The periodic boundary conditions are applied to the co-ordinates of each link cell and then automatically to their contents. The computer memory requirements of this method are rather modest. A part from array LINK(N), two more arrays of dimension NL are the only others needed to incorporate this method.

Using the Lennard-Jones MD program MDATOM<sup>(4)</sup> on the state point  $\rho^* = 0.8552 = N \sigma^3/V$  and  $kT/\epsilon = 0.7053$  the speeds of the three methods are as follows.

Average c.p.u. time on the ULCC CDC 7600 to perform a time-step

Method	N:	108	256	864	2048	6912
Conventional method		0.036	0.163	1.573	8.460	94.173
Neighbourhood tables		-	0.093	0.310	*	*
(r <sub>2</sub> = 1.001 nm, see ref.(1))						
Link cells		-	-	0.834	2.321	6.666
(NL)				(64)	(125)	(512)
- untried, * l.c.m. memory exceeded						

The conventional method is too time consuming for N larger than approximately 1000. Although the neighbourhood lists method is much faster than the conventional method, it too is not practicable for N greater than 1000 because of the considerable memory requirements. Even if this is overcome, the approximately one-in-ten time steps at which all interactions must be considered in order to create the neighbour lists, would be a prohibitive factor in its implementation. Timings for the conventional method indicate the long time required for this albeit infrequent operation.

The link cell method provides rather unspectacular gains in speed for moderately large samples of N ~ 1000 to 2000, but becomes a progressively more attractive method when the very large N values of ~ 7000 are considered.

## REFERENCES

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