

MORE ON NEIGHBOURHOOD TABLES

David Adams

Like everybody else, so it seems, I have used coordinates scaled from -1 to +1 in the periodic cell. This is not necessary in order to use the INT or AINT functions for the calculation of the nearest image, and I find it more convenient now to use coordinates from -1/2 to +1/2 so that the cell volume is one. Then the nearest image transformation becomes:

```
DX = X(I) - X(J)
DX = DX - AINT(DX + DX)
```

on the CRAY. On other machines the $DX + DX$ may be written as $2.0 * DX$ equally well¹.

In the calculation of a neighbourhood table only the distance to the nearest image is needed and there is a more elaborate but considerably faster method for that. It will work for any cell length, but the -1 to +1 version goes as follows:

In the outer loop:

```
XI = X(I)
IF(XI.GT.0.0) XI = XI - 2.0
XI = XI + 1.0
```

and similarly for Y and Z.

In the inner loop:

```
R2 = ((1.0 - ABS(X(J) - XI))**2 +
1| ((1.0 - ABS(Y(J) - YI))**2 +
2| ((1.0 - ABS(Z(J) - ZI))**2
```

where R2 is the square of the smallest distance between particles I and J. Should the coordinates used go from 0 to 1 then the code is slightly different:

In the outer loop:

```
XI = XI + 0.5
```

```
IF(XI.GT.1.0) XI = XI - 1.0
```

and similarly for Y and Z

In the inner loop:

```
R2 = ((0.5 - ABS(X(I) - A))**2 + (0.5 - ABS(Y(I) - B))**2  
1    + ((0.5 - ABS(Z(I) - C))**2
```

Obviously the method can be very useful in Monte Carlo also. I have found that for hard sphere potential Monte Carlo on the 7600 it is roughly twice as fast as any other method.

David Heyes in his article suggested Verlet's method³ of calculating the neighbourhood tables very tenth step. For the cautious there is a safer method which has been around for a long time but has only recently appeared in print¹. When the neighbourhood table is constructed a copy is kept of the particle coordinates at that time. Then at every step the displacement of every particle is checked. When any one has moved more than $1/2(r_2 - r_c)$, where r_c is the cut off radius and r_2 the maximum distance at which a pair of particles goes into the neighbourhood table, then the table is reconstructed. There is a slight variation of this which makes the reconstruction slightly less frequent. The two largest displacements are found instead of just the largest. Only when the sum of these two is greater than $r_2 - r_c$ does the table need recalculating.

¹ D. Fincham and B.J. Ralston, *Comp. Phys. Comm.* 23, 127 (1981).

² D.M. Heyes, *CCP5 Newsletter* 2 (1981).

³ L. Verlet, *Phys. Rev.* 159, 98 (1967).