

C study of the cell $LL - 1, MM - 1$

C if there is a I th particle (KT) in the cell, it is the $(k + 1)$ th potential
 C neighbours of J

```

KT = ITPCEL(LL - 1, MM - 1, I)
IF (KT.NE.0) THEN
K = K + 1
ITBLOC(J, K) = KT
ENDIF

```

C END OF THE SEQUENCE

C new value of the number of particles in group J

```
NPBLOC(J) = K
```

```
3 CONTINUE
```

```
2 CONTINUE
```

```
1 CONTINUE
```

$NPBLOC(J)$ and $ITBLOC(J, K)$ are respectively the number of particles and the K th particle number in the J th particle block, and $ITPCEL(L, M, K)$ the number of the K th particle in (L, M) cell. The sequence shows the principle of the search for the cell $(LL - 1, MM - 1)$, and it will be enough to repeat it over all the cells to unroll the loop. The inner loop is also longer and is completely vectorised.

The number of particles per block depends on the density distribution. To give an idea we fix the number of particles at $N \approx 3000$. For a constant density NBLOC lies between 7 and 50 with a mean value of 29, and for a density decreasing exponentially from the center, NBLOC lies between 2 and 200 with a mean value of 80.

The particles are then arranged in 9 or 10 groups according to the numbers of neighbours in the blocks, with 300 to 1000 particles per group.

Step 3

After having found the possible neighbours we have to search more exactly for the true neighbours, by carrying out the inter-particle distance $R(I, J)$ calculations inside each group. The second sorting groups have the same order as the first sorting ones and use the NINTG2 and NEARM2 arrays, but NEARM2 here is the maximum number of particles in the blocks occupied by the particles of the $(II - 1)$ th group:

C loop 1 is over the group number

```
DO 1 II = 1, NGROUP
```

C definition of the first and last particles in group II

```
N1 = NINTG2(II) + 1
```

```
N2 = NINTG2(II + 1)
```