```
C  maximum number of neighbours in group II
                M2 = NEARM2(II + 1)
C  loop 2 is over the number of neighbours
                DO 2I = 1, M2
C  loop 3 is over the particles
                        DO 3J = N1, N2
C  if the Ith particle in the bloc of J is close enough to J then it is the
C  (NNEIB + 1)th true neighbour
                                KT = ITBLOC(J, I)
                                IF (R(J, I).LT.H(KT)) THEN
                                NNEIB(J) = NNEIB(J) + 1
                                K = NNEIB(J)
                                ITNEIB(J, K) = KT
                                ENDIF
    3                   CONTINUE
    2               CONTINUE
    1           CONTINUE
```

NNEIB(J) is the number of neighbours of particle J, and ITNEIB(J, K) is the label of the Kth neighbour of particle J.

The particles are then sorted into new groups according to the real number of neighbours. After this the number of particles per group lies between 6 and 40 with a mean value of 21 for the two density distributions.

Discussion

The three sorting steps are necessary but play different roles. Without the first ordering the external loop in the blocks calculation would be performed over the maximum number of particles in a cell. Both other sortings are used because the calculations of the inter-particle distances and the comparison with the particle size can be penalizing if the calculations are carried out over too many particles. The second sorting also reduces the number of particles used to carry out the third ordering. The third sorting groups have the same order as the first sorting ones and use the NINTG3 and NEARM3 arrays, but NEARM3 here is the maximum number of neighbours in the (II − 1)th group. The structure of a vectorisable and optimized loop for the density calculation is then:

```
C  loop 10 is over the group number
   DO 10II = 1, NGROUP
C  definition of the first and last particles in the group
                N1 = NINTG3(II) + 1
                N2 = NINTG3(II + 1)
C  maximum number of real neighbours in the group
                M2 = NEARM3(II + 1)
C  loop 20 is over the number of real neighbours
                DO 20I = 1, M2, 2
```