

2. a second sorting according to the approximate number of neighbours
3. a third sorting according to the real number of neighbours, because only particles located at a distance smaller than h have a nonzero contribution to the macroscopic quantities calculated at the position of the i th particle.

Steps 1 and 2

To locate the particles we use a 2D grid whose cell size is the maximum diameter $2 * h_{\max}$. In this case the possible neighbours are located in the nine surrounding cells of a given particle (see Fig. 1a). However, since one of the main advantages of this code lies in its variable resolution, the size h of the particles can be very different; one can therefore search for the neighbours in smaller areas such as 3×3 blocks and 5×5 blocks with a block size of $1/2 * h_{\max}$, so that the searches in the 3×3 blocks and in the 5×5 blocks are sufficient in mean density regions, and a search in the 3×3 block only in high density regions (see Fig. 1b). For steep density gradients it can be better to use 7×7 blocks with the appropriate value of the size cell.

After having calculated the location of the j th particle $L(J)$ and $M(J)$, the number of particles per cell $N_1 \text{ CEL}(L, M)$, the particles are sorted in NGROUP groups, according to their values of $N_1 \text{ CEL}(L, M)$. For the understanding of the following it is necessary to detail the way the sorting is done. Let us define NEARM(II) as the maximum number of particles in one cell for the (II-1)th group. Let us define also NINTG(II) as the integrated number of particles over all groups preceding the II group, i.e., $\sum_k \text{Number}(k)$ for $k \leq \text{II}-1$, where $\text{Number}(k)$ is the number of particles in the k th group. Since particles are attributed to new numbers after the group sorting, the label and the rank of any particle in a group are the same. Then we start the search per block:

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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 = NINTG(II) + 1
  N2 = NINTG(II + 1)
C maximum number of neighbours in IIth group
  M2 = NEARM(II + 1)
C loop 2 is over the number of neighbours
DO 2 I = 1, M2
C loop 3 is over the particles
  DO 3 J = N1, N2
    LL = L(J)
    MM = M(J)
    K = NPLOC(J)
C BEGINNING OF THE SEQUENCE

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