## HADDAD, CLAUSSET, AND COMBES

where NNEIB(J) is the number of neighbours of the particle J. Then our second goal is to reverse the loops in order that the inner loop be longer, because only the inner one is vectorised. We have to replace the natural scheme 1 by scheme 2, since N is much greater than NEIB, the maximal number of neighbours:

DO 20 KT = 1, NEIB DO 10J = 1, N

## 10 CONTINUE

b

## 20 CONTINUE

But this scheme involves unnecessary calculations and a loss of CPU time of a factor  $\approx 10$ . In the following we describe a method to circumvent the problem.

The solution is to put the particles in groups, each group being characterized by an approximate number of neighbours. We can also distinguish three steps:

1. the determination of the particles locations, a first sorting according to the number of particles per cell, and the search for the closest particles for a given one.





FIG. 1. (a) In case the cell size is  $2h_{\max} = \Sigma$  the possible neighbours are located in the nine surrounding cells. (b) In case the search is performed per block the cell size is  $\frac{1}{2}h_{\max} = \frac{1}{4}\Sigma$ . For the given particle (size  $\sigma$ ) the search in the 3 × 3 block is sufficient.

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