

C calculation of the interparticle distance

$$3 \text{ ion is possible only if the } \text{DX} = X(J) - X(KT)$$

$$\text{DY} = Y(J) - Y(KT)$$

$$\text{R2} = \text{DX} * \text{DX} + \text{DY} * \text{DY}$$

$$\text{H2} = H(KT) * H(KT)$$

C if KT is close enough to J then KT is the (NNEIB + 1)th neighbour of J

$$\text{IF } (\text{R2.LT.H2}) \text{ THEN}$$

$$K = \text{NNEIB}(J) + 1$$

$$\text{NNEIB}(J) = K$$

$$\text{ITNEIB}(J, K) = KT$$

ENDIF

C use of the chaining to find the next neighbour

$$KT = \text{ICHAIN}(KT)$$

$$\text{IF } (KT.\text{NE.0}) \text{ GO TO 3}$$

2 CONTINUE

1 CONTINUE

where NC is 1 for the 3×3 block and 2 for the 5×5 one.

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