

## NEAREST-IMAGE TRANSFORMATION ON CDC COMPUTERS

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The nearest-image transformation, inside the force loop, is one of the most time-consuming parts of a molecular dynamics program. Many people use the following technique to look for the nearest-image vector between a pair of particles (the co-ordinates are scaled to lie between -1 and +1)

```
RX = X(I)-X(J)
RX = RX-2*INT(RX)
```

with similar expressions for y and z components. This works well on many computers. However, for CDC machines there is a faster method which requires minimal program changes. We start the force evaluation by defining a set of integer co-ordinates

```
IX(I) = INT(X(I)*TWOTW)
```

where  $TWOTW = 1048576.0 = 2^{20}$ . This power of two is chosen so that the truncation introduces negligible errors, but integer overflows are avoided. The n.i. transformation can then be programmed using shift operations

```
IRX = IX(I)-IX(J)
IRX = IRX-SHIFT(SHIFT(IRX,-20),21)
```

Then  $RX = IRX/TWOTW$  is the correctly transformed component of the particle-particle vector. In practice we work with IRX until the cut-off has been applied, to take advantage of the greater speed of integer arithmetic.

For 108 argon atoms this method reduced the CPU time per step of the simulation from 36 ms to 29 ms.