

Minimum Image Calculations on IBM-3090 VF

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Keeping the computing requirements of minimum image calculations low can be important in order to keep the overall CPU requirements of molecular dynamics and Monte Carlo simulations low. In this regard, the review paper of Fincham and Heyes (Adv. Chem. Phys., **63**, 493, (1985)) discusses some of the minimum image methods applicable to different vector processing computers. In the past (Comp. Phys. Comm., **48**, 197, (1988)), we have tested one of these methods (developed by Fincham and Ralston),

$$\underline{t} = \underline{t}(i) - \underline{t}(j)$$

$$\underline{r} = (L/2.) * (\underline{t} - 2. * INT(\underline{t}))$$

on an IBM-3090 E series computer with vector facility using the IBM VS-FORTRAN 2 vectorizing compiler. Here \underline{t} represents coordinates of molecular centers in the (-1,1) system, L is the side length of the cubic box, and \underline{r} is the distance between the centers of molecules i and j. This method was shown to work quite well with vectorization.

Recently, it was suggested to us by the IBM Kingston (New York) specialists to use the AINT function instead of the INT function in the above calculations. Our test Monte Carlo simulations of 108 LJ sphere systems show further savings of nearly 8% using the VS-FORTRAN 2 compiler on IBM-3090 with VF after switching on the vectorization option (savings were not observed during the scalar-only runs) when the AINT function was used. We believe that such savings can also be obtained in molecular dynamics simulations.

We are grateful to the staff of IBM Kingston Laboratory for their suggestions. We point out that this discussion is limited only to the use of the particular software and hardware discussed here.