

THE EWALD SUM PROGRAM "MDIONS"

Nicholas Anastasiou and David Fincham

This note gives a brief description of the program MDIONS in the CCP5 program library. Copies of the program source and full documentation can be obtained from the program librarian, Dr. Bill Smith.

The program performs dynamic simulations (MD) on charged particles. The non-Coulomb part of the interaction is specified by means of rigid ion potentials of the Born-Mayer-Huggins form. A mixture of several different species of ion may be simulated. The Coulombic part of the interaction is handled by means of the Ewald sum technique. The routine performing the reciprocal space part of the Ewald sum is very easily adaptable to an ortho-rhombic computational box, which would be useful in the study of non-cubic crystals. The leapfrog algorithm is used to integrate the equations of motion of the ions.

As well as the usual thermodynamic averages the program calculates the mean square displacement of the ions (diffusion) and the partial r.d.f.'s. The partial structure factors are found by two methods. At low k values they are calculated by direct evaluation of the sums $\sum \exp(i\mathbf{k}\cdot\mathbf{r})$. This method involves negligible extra work as these sums are required in the reciprocal space sum, and it complements the second calculation which works by Fourier transform of the r.d.f.'s. (the latter method can lead to spurious oscillations at low k -values because of the cut-off).

There are three versions of the program. The first version is written in conventional Fortran to be suitable for any computer. This has been submitted for publication in the Computer Physics Communications program library, and users of any version of the program are requested to make reference to this publication where appropriate. This version allows both the use of look-up tables and direct evaluation for the real space force calculation. A second version involves the minimal changes necessary to vectorise the force calculation on the Cray. Look-up tables are not included in this version as they would inhibit vectorisation. A third version has been optimised by Bill Smith for the Cray, partly by means of assembly language routines.

Typical execution time for the vectorised version on the Cray is 115 ms per step for 216 ions, with the r.d.f. calculation switched off. The optimised version reduces this to 100 ms.