
DL_POLY: A Macromolecular Simulation Package

W. Smith Daresbury Laboratory
C. Dean

D. Fincham Keele University and Daresbury Laboratory

D. Tildesley University of Southampton

The Collaborative Computational Project CCP5, dealing with computer simulation of molecular systems, has recently been awarded a grant by the Computational Science Initiative for postdoctoral assistance to develop a *Macromolecular Simulation Package* on the Daresbury Laboratory Intel iPSC/860 parallel computer. The project is expected to become fully active in late 1992, though much preliminary work has already been done.

The purpose of this package, named DL_POLY, will be to apply the parallel molecular dynamics methods devised by participants in the CCP5 project [1-8] in a sophisticated package capable of accurate dynamical modelling of complex systems, with a special emphasis on macromolecules, but with capabilities in most other areas of molecular simulation. It is hoped that the wide range of expertise available through CCP5 will permit the development of a world-beating package that will be *free* to academic groups. The open nature of the project is intended to encourage wider utilisation of the best techniques of simulation, provide proven and adaptable source code essential to the new projects and reduce the dependency of the community on commercial 'black box' codes, which are incompatible with free academic exchange.

The initial objective is the development of a *Replicated Data* (RD) [1] program which will

be suitable for both the Intel iPSC/860 and serial workstations. The program will incorporate traditional simulation models, including atomic and molecular ions, rigid and flexible (macro-)molecules, multicomponent systems and a variety of ensembles and boundary conditions. Bond forces (including valence and dihedral angles) will also be incorporated. Nonbonded forces will be handled by the Replicated Data method. The long ranged forces will optionally be handled via direct summation or the Ewald method [4,7].

In the longer term, domain decomposition algorithms (i.e. Link Cells) will be incorporated, based on existing parallel methods [6,8]. The *Fast Multipole Method* (FMM) [10] will be developed for long range forces, with the PPPM [9] method as an option for periodic systems.

It is intended that the code development take place in conjunction with a study of polymeric species in solution.

In the initial phases the project will be assisted by the Parallel Applications Team at Daresbury.

References

- [1] W. Smith, *Comp. Phys. Comm.* (1991) **62** 229.
- [2] D. Fincham, *Molecular Simulation* (1987) **1** 1.
- [3] A.C. Raine, D. Fincham and W. Smith, *Comp. Phys. Comm.* (1989) **55** 13.
- [4] W. Smith, *Comp. Phys. Comm.* (1992) **67** 392
- [5] D. Fincham and P.J. Mitchell, *Molecular Simulation* (1991) **7** 135.
- [6] D. Rapaport, *Comp. Phys. Comm.* (1991) **62** 217.
- [7] D. Fincham, R.A. Jackson, S. Miller and P.J. Mitchell, "Applications of Transputers 2", D.J. Pritchard and C.J. Scott (Eds.), Amsterdam: IOS Press, (1990).
- [8] M.R.S. Pinches, D.J. Tildesley and W. Smith, *Molecular Simulation* (1991) **6** 51
- [9] R.W. Hockney and J.W. Eastwood, "Computer Simulation Using Particles" McGraw-Hill, New York 1981.
- [10] J. Ambrosiano, L. Greengard and V. Rokhlin, *Comp. Phys. Comm.* (1988) **48** 117.