

# DL\_POLY : Progress report

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## **DL\_POLY Progress report**

In issue 35 (September 92) of this publication the inauguration of work on a package DL\_POLY was announced. The purpose of this package is to apply parallel molecular dynamics methods devised by participants in the CCP5 (the Collaborative Computational Project for the computer simulation of condensed phases) project into a sophisticated package capable of accurate modeling of complex systems. It is hoped that the final product will be a world-beating package available *free* to academic groups. The target machines for the package is the Intel iPSC/860 parallel computer and workstations. We emphasize that DL\_POLY is designed as a *package* not as a program. It is thus highly modular in nature and relatively easy to tailor to modelling specific systems.

DL\_POLY is being developed at Daresbury Laboratory under the auspices of CCP5 and the Advanced Research Computing Group (ARCG) at Daresbury Laboratory. The package is the property of the United Kingdom Science and Engineering Research Council (SERC).

The special emphasis of the package is on macromolecules but the package is designed to be flexible enough to incorporate a wide range of systems including ionic melts, liquid mixtures, polymers, crystals etc.

Currently DL\_POLY has the following features :

The parallel strategy is that of *Replicated data*. The integration algorithms include; Verlet leapfrog (NVE); Nose - Hoover with Verlet (NVT); Evans thermostat with Verlet leapfrog (NVT); multiple timestep; and Shake. All common periodic boundary conditions are available including: none, cubic, rectangular; parallelepiped; truncated octahedral; and rhombic dodecahedral.

The default force field is that of GROMOS but all common force fields for macromolecules (e.g. AMBER, Universal force field) will be accommodated. At present the force field contains terms for: all common short-range atom-atom potentials; the Coulombic potential; a truncated coulombic potential (non-periodic systems); valence angle potentials; dihedral angle potentials; and improper dihedral angle potentials. In periodic systems the Coulombic potential is handled by the Ewald sum for point charges.

It is anticipated that a first general release of the package will be available in time for the CCP5 annual general meeting in september 1993. At present work is being carried out to thoroughly test and refine the existing package before the first public release.