

THE COMPUTER PHYSICS COMMUNICATIONS PROGRAM LIBRARY

David Fincham (D.Fincham @ keele.ac.uk)

Many readers will be familiar with the North-Holland journal "Computer Physics Communications" which has published many papers relevant to the CCP5 fields of interest. Papers are usually computational in nature, discussing such issues as integration algorithms, neighbour search methods, efficient evaluation of long-range interactions, optimisation and vectorisation. For example the papers of Smith and Forester expounding the fundamental parallel algorithms of the DLPOLY project have recently appeared.

As a Specialist Editor of the journal I would like to encourage readers of the CCP5 Newsletter to submit more such papers, which may be sent directly to me. However, my main purpose in writing is to describe a unique feature of the "Computer Physics Communications", its associated program library. As well as papers on computational methods, the journal includes program descriptions, and the programs themselves are made available through a program library. An important point about this library, which distinguishes it from others such as the CCP5 program library, is that the programs themselves are refereed before being accepted into the library. The CPC library is therefore playing an important role in raising the standards of scientific software. Personally I attach great importance to this. Developments in computational methods will only receive the use they deserve if they are incorporated in robust, efficient and easy-to-use software.

At the moment the library is particularly weak in the area of molecular simulation. There is my very old Ewald sum program, Laaksonen's aqueous solution program, and a series of programs from Rycerz and Jacobs which primarily illustrate neighbour search algorithms, plus a few other rather specialised programs. We would really appreciate more programs from the CCP5 community. How about some rigid molecule programs, some Monte-Carlo and Gibbs ensemble programs, some multipolar and polarisable models, some stochastic dynamics? In the solid-state area there are some specialised lattice dynamics programs, but room for more, as well as for m.d programs in this area.

If you are writing simulation programs, please consider submitting them to Computer Physics Communications as well as to the CCP5 library. I know that bringing programs up to the required standards to get through the refereeing process, as well as producing documentation, is a very time-consuming process, but it is also a very useful service to the community which will be appreciated. And it will count as a refereed publication!