

THE WORK OF THE ATLAS COMPUTER LABORATORY 1974/75

by
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COMPUTER SERVICES

Computing services are continuing to be made available on a guaranteed basis to SRC Committee approved users. In addition, a number of ancillary services based on the microdensitometer scanning equipment, the FR80 microfilm recorder, and the PDP15 interactive graphics system are used by other supported groups. The Laboratory continues to recognise the importance of software both in systems and applications and original work in both these areas was a feature of the last year's activities.

ICL 1906A

The computer was scheduled for service for 6,054 hours and was available to users for 93% of the time during the financial year 1974/75.

Hardware faults were responsible for over 70% of the down-time. In common with other university 1906A installations, ICL have put in a special effort to improve the hardware performance and more recent figures show some improvement. For the period March 1975 to September 1975, 3,062 hours were available to users for 94% of the time. 37% of the computing time went to users guaranteed by the Science Board, and Astronomy and Engineering accounted for 8% and 13% respectively.

Work for the Natural Environmental Research Council (NERC) accounted for 120 hours, and the activities of State House in connection with research grant accounting used 64 hours. Over 50% of the background jobs were submitted via remote workstations, and over 80% of the users input their work via remote interactive terminals.

Improved versions of the GEORGE 4 operating system have been installed during the year, and the complex operating system together with its generalised filestore is operating at a very high level of availability. Very few software faults now remain in the system.

IBM 360/195 service to Atlas users

The Atlas users accounted for 1,475 hours of CPU time during the financial year 1974/75 and 108,426 jobs were processed. The demand for time on the 360/195 provided by the Atlas Laboratory to the non-nuclear physics disciplines is under considerable pressure (April 1975 - September 1975. 733 hours and 66,565 jobs) and the guaranteed time is now fully committed for the next 15 months. The use is still dominated by the demand from the Chemistry Committee of the Science Board (with 710 hours) but both Physics (282 hours) and Astronomy (208 hours) are now demanding increasing amounts of time to be made available. The Natural Environmental Research Council (NERC) with 44 hours, continue to increase their demands, and special classes of work in connection with the Institute of Geological Sciences have had to be accommodated; the analysis of data from North Sea oilfields has been carried out with great effect using software developed at the Atlas Laboratory and the powerful facilities available from the 360/195.

FR80 Microfilm Recorder

This has been commissioned and a service has been offered since June 1975. The use of microfiche is proving to be heavy and the prospects of producing good quality colour frames has been realised. The associated software development is not yet complete but an operational system is now available. Copies of the software have been made available to Reading and Oxford universities so that prepared data tapes can be processed.

SCIENTIFIC ACTIVITIES

The 5th symposium in a series of symposia on major applications of computing took place in Oxford 14-16 April 1975 on "Computational Physics of Liquids and Solids". A great deal of progress has been made in the understanding of the liquid state through computer studies of model systems. Since a sizeable proportion of ACL's computer resources is used in this way, a symposium in this area was organised with a number of eminent practitioners both from the UK and abroad. To paraphrase one of the invited speakers "Computer simulation techniques, which it was once thought might replace theory, have made a theory of liquids possible". Some exploratory discussions within this general topic are currently being held with ILL, Grenoble, to consider some possible collaboration.

The Atlas Laboratory Meeting House in Computational Physics and Chemistry commenced practical operation in October 1974, with the recruitment of the first Meeting House Fellow. Work has commenced on the first project, "Correlated Wavefunctions". This is a subject in which progress is essential as a precursor to success in other fields of theoretical physics and chemistry, and is of considerable importance and interest in its own right. The work up to the present has resulted in the production of a large computer program for performing highly accurate calculations of correlated wavefunctions, and has required the collaboration of workers from the Universities of York, Manchester, Cambridge and Sussex, and from the Max-Planck Institute in Munich. The recruitment of a second Meeting House Fellow is being actively considered.

Microdensitometer

The past year has seen the first full year of the crystallographic film-scanning service. A total of 43 sets of structural data were collected for crystallographers in the United Kingdom. The use of the service is widespread since these films came from 22 different Universities and Polytechnics. The accuracy of the measured data is exceeding expectations: for the first 8 structures which have been solved, the conventional crystallographic agreement factor is in the range 5-7% which is almost as good as is achieved with more expensive counter techniques. The instrument has been very reliable, allowing over 200 films from miscellaneous sources to be digitised as an auxiliary service to non-crystallographers. At the request of the SRC Data Compilation Committee, we have been implementing the system CSSR written by Feldman of NIH, Maryland, to access interactively and display the crystallographic database developed by Dr Olga Kennard at Cambridge. The retrieval program has been implemented on the PDP10 in the Oxford Nuclear Physics department; we are now investigating the problems of implementing various ancillary programs (in particular the file inversion program) on our 1906A.

STAFF

The number of staff in post at 1 October 1975 is 136. The latest statement on complement is that a total of 135 is planned for 31 March 1976.

Dr J Howlett, founder Director of the Atlas Computer Laboratory, retired on 31 August 1975 after occupying this post from 1961 with great distinction.

Two Fellows have been appointed during the past year: Dr W R Rodwell of Sussex, and Dr P J Hunter of St Catherine's, Oxford.

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