18.X-01 ON THE USE OF MICROPROCESSORS IN CRYSTALLOGRAPHY. By H. Burzlaff, Institut für Angewandte Physik, Lehrstuhl für Kristallographie, Universität Erlangen-Nürnberg, Germany, Fed. Rep.

The paper will give an introductory survey on the use of microprocessors in crystallographic instrumentation and computing facilities. It will consist of:

(i ) a short description of hardware components,

(ii ) a list of direct software support available for microprocessors,

(iii) a discussion of software support by larger computers,

(iv ) a discussion of advantages, handicaps and limitations on the base of practical examples.

18.X-02 CRYSTALLOGRAPHIC COMPUTING ON AN ATTACHED ARRAY PROCESSOR By W. Furey Jr., B. C. Wang and M. Sax, Biocrystallography Laboratory, V. A. Medical Center, Pittsburgh, Pa. and Department of Crystallography, University of Pittsburgh, Pittsburgh, Pa.

The ability of "add on" vector computers called array or parallel processors, to dramatically reduce computation time for certain applications has recently been established. In particular, they have been used successfully for minimization of the conformational energy of proteins, simulation of molecular dynamics, and for Monte Carlo calculations in statistical mechanics. Our initial findings indicate attached array processors can also be used effectively for crystallographic computing. To date, six computationally intense but frequently needed crystallographic applications programs have been adapted to run on an array processor (Floating Point Systems Model AP 190L) attached to a Dec 10. In all of the applications attempted, it was possible to reduce the required processing time to at least an order of magnitude below that required by a large university computer (Dec 10) for the same problem. In fact, the rate determining step in full matrix least squares refinement can be made to run 30 times faster on the attached array processor. For the refinement of proteins, one cycle with a space group general algorithm runs faster on the array processor than a typical small molecule refinement cycle runs on the Dec 10. Details regarding crystallographic computing on an attached array processor will be presented.

18.X-03 THE USE OF VECTOR PROCESSORS IN CRYSTALLOGRAPHY. By D. S. Moss, Department of Crystallography, Birkbeck College, Malet Street, London, WC1E 7HX, UK.

Light travels 30cm in one nanosecond. In order to achieve extremely high processing rates in a computer the physical dimensions of the machine must be small and as many operations as possible must be carried out concurrently.

Two strategies may be adopted to allow operations to occur in parallel. The computer may be provided with an array of processors or the operations may be pipelined.

Machines employing such techniques may either be processors interfaced to a host computer such as the Floating Point FPS-164 which may be interfaced to the VAX-11/780 or they may be fully fledged computers such as the Cray-1.

The Cray-1 has pipelined operations and also single instructions which may accept vector operands. Computing rates of up to 20 times the speed of a CDC 7600 may be obtained when a Fortran program is designed to take maximum advantage of the processor architecture.

The major part of a crystallographer's budget is often spent on structure factor and least squares computations. Fortunately, the time-consuming parts of such calculations are confined by relatively small segments of the Fortran text. These parts of the program are easy to modify so that the object code generated by the Cray-1 Fortran compiler uses the vector instructions in the central processor. Examples of such 'vectorised' code are presented.

Simulations using Monte Carlo methods or molecular dynamics are also being carried out on protein structures and their environments using the Cray-1 and will become increasingly important for modelling the disordered regions of protein structures.

18.X-04 LANGUAGE PREPROCESSORS AND PORTABILITY. By Robert J. Munn and James M. Stewart, Department of Chemistry, University of Maryland, College Park, MD.

The scientist interested in developing large scale, extensively used and long-term programs is faced with a number of conflicting optimizing factors. Two developments in computer science - structured programming and macro processing - have recently emerged as programming tools that allow the scientific programmer to both have his or her favorite cake and eat it. The advantages in using a structured programming language based on FORTRAN will be discussed. These advantages include familiarity, efficiency and portability. The additional advantages that accrue when a macro processor is also available will be emphasized. Included in those advantages are machine dependent efficiency, extendability, operating system interfaces, and input-output definition. The disadvantages of these approaches will also be discussed.

Finally, the relationship of structured FORTRAN to both FORTRAN 77 and other languages such as PASCAL and ADA will be explored.