18.X-01   ON THE USE OF MICROPROCESSORS IN
CRYSTALLOGRAPHY. By H. Burzlaff, Institut für
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many, 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 compo-
      nents,

(ii) a list of direct software support avail-
      able for microprocessors,

(iii) a discussion of software support by lar-
      ger 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,
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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 confor-
mational energy of proteins, simulation of molecular
dynamics, and for Monte Carlo calculations in statis-
tical mechanics. Our initial findings indicate
attached array processors can also be used effectively
for crystallographic computing. To date, six computa-
tionally 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 pro-
cessing 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 pro-
cessor will be presented.

18.X-03   THE USE OF VECTOR PROCESSORS IN CRYSTAL-
LOGRAPHY. 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 phys-
ical 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 proces-
sors 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 in-
structions 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 maxi-
mum 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 com-
piler uses the vector instructions in the central proces-
sor. Examples of such 'vectorised' code are presented.

Simulations using Monte Carlo methods or molecular dynam-
ics are also being carried out on protein structures and
their environments using the Cray-1 and will become in-
creasingly 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, ex-
tensively used and long-term programs is faced with a
number of conflicting optimizing factors. Two develop-
ments 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 addi-
tional advantages that accrue when a macro processor
is also available will be emphasized. Included in those
advantages are machine dependent efficiency, extenda-
bility, 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.