18.X-1   CRYSTALLOGRAPHIC MICROCOMPUTING.
By H. Schenk, Laboratory for Crystallography, University
of Amsterdam, Nieuwe Achtergracht 166, 1018WV Amsterdam,
The Netherlands.
In the past computing has contributed a lot to the
improvements in the field of Crystallography and will
certainly continue to do so in the next future. However,
it will change its character due to micro-computers and
local area networks. As a result it will also be easier to
access for scientists from developing countries and it
will change the teaching of crystallography as well.
Traditionally crystallographic methods are implemented on
mainframes or mini's, the latter generally controlling
apparatus at the same time. Multi-user systems enable many
users to run their jobs in competition, so that when the
computer is too busy, every user is equally discontented.
Modern computer hardware technology, however, will make it
possible to get a remarkable powerful computer on the desk
for the price of a video terminal. As a result many of
present mainframe jobs then will rather be done by local
desk-top computers and future mainframes will be used for
special purposes only. The desk-top will also be useful in
teaching and in countries where mainframes are scarce.
However, the bottleneck may well be the software to be
developed by the crystallographic community itself. Only
when great efforts are invested, the intrinsic power of
the micros will be fully exploitable in our field.
Part of the future development can be and is realised
already now, because the IBM PC's, Atari 1040's and others
comprise impressing computing power, not to talk about the
coming 32-bit microcomputer generation. Certainly within a
few years crystallographic computing may have been changed
completely!
The Computing Lab at this conference will not give a
complete overview of microcomputer programs for teaching
and research in crystallography, but will certainly be
useful and impressive. This paper intends to give an
introduction to the intrinsic power of microcomputing and
to the options of the Congress Computing Lab.

18.X-2   DESKTOP CRYSTALLOGRAPHY - THE NEXT
GENERATION OF COMPUTERS. By P.E. Bourne, Howard Hughes
Medical Institute, Department of Biochemistry & Molecular
Biophysics, Columbia University, New York, USA.

The continued decrease in the price:performance ratios of computer
systems may change the way in which even the most complex
crystallographic calculations are performed. The current trend is
away from the central institutional mainframe computers and
departmental minicomputers and toward individual and multi-user
processors (workstations).

The potential benefits of the latest workstation technology, including
system architecture, performance comparisons, graphics capability,
mass storage and software design will be discussed. Likewise, the
negative implications of such distributed processing, including the
additional care required for data and program management, as well
as the need to understand computer networks and system
management, will also be addressed.

18.X-3   THE   MACROMOLECULAR   WORKBENCH.
Robert Langridge, Computer Graphics Laboratory, University of Cali-
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A schematic view of the Macromolecular Workbench system being
developed at UCSF is shown below. The graphics is a high
bandwidth window for interaction with the computations at all levels.
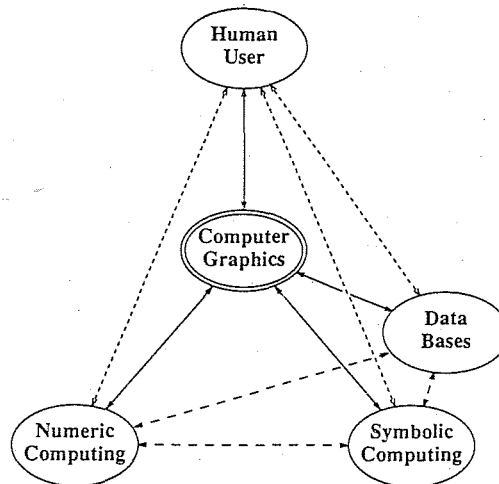
I describe the realization of this concept in silicon, copper and code,
with applications to protein engineering and drug design.

18.X-4   COMPUTER GRAPHICS TECHNIQUES FOR
EXPLORING   MOLECULAR   STRUCTURES   AND
PROPERTIES. Jane M Burridge. IBM UK Scientific Centre,
Athelstan House. St Clement Street, Winchester, Hampshire
SO23 9DR, England.

The molecular scientist is faced with the fundamental problem
of comprehending and visualising the large masses of data which
arise as a result of the increasing use of computers in theoretical
and experimental research. This data might take the form of
atomic coordinates and thermal parameters; be the results of a
molecular dynamics or mechanics simulation; or come from
rapidly expanding databases, such as the nucleic acid data bank.
A molecular graphics system should be flexible enough both in
data handling and available graphical representation, to allow
the distilling of such data into a picture which the researcher can
assimilate, and thus aid the exploration and visualisation of
known structures and properties.

Despite great progress, the determination of molecular
structures by protein crystallography remains a time-consuming
process; nmr techniques are not yet developed to the point of
providing unambiguous structural information for the larger
molecules. Thus we require educated guesses about unknown
structures (or modifications to known structures): guesses based
upon our current knowledge. A molecular graphics system
should allow the addition and modification of basic
assumptions, inclusion of expertise and hypothesis, and the
handling of uncertainties to allow reasoning about unknown
structures and their interactions.

The Winchester Graphics System (WGS), developed at the IBM
UK Scientific Centre, incorporates various methods for
representing molecular structures and properties.   These
representations utilise both calligraphic and raster display
devices, and include dynamic as well as static images.
Applications of the system will be discussed and illustrated.