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.

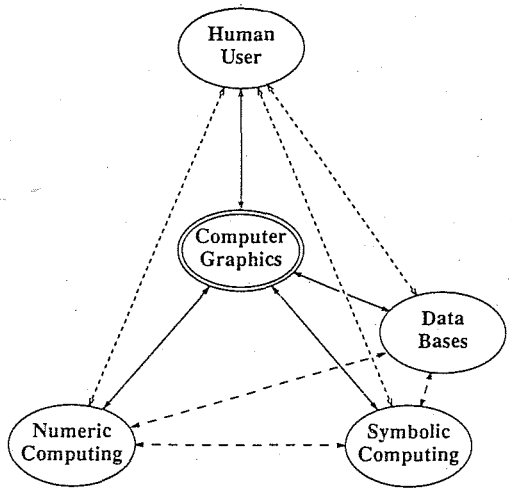
18.X-2 DESKTOP CRYSTALLOGRAPHY - THE NEXT GENERATION OF COMPUTERS. By P.E. Bourne, Howard Hughes Medical Institute, Department of Biochemistry & Molecular Biophysics, Columbia University, New York, USA.

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 California, San Francisco, CA 94143-0446

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.