Computer Assistance in the Chemical Pathology Laboratory

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Current clerical procedures in the clinical chemistry laboratory not only create a bottleneck in laboratory operations, but can be shown to be wasteful of the time of technically skilled personnel, prone to error and liable to produce records that leave much to be desired in terms of presentation, retrievability and even legibility. These problems have been tackled at University College Hospital by making use of a computer to aid the necessary manipulation of data.

Operating in an off-line mode with the hospital's Elliott 803 computer and with equipment that automatically or semi-automatically captures the significant part of the analogue output from Auto-Analyzers in machine-readable form, substantial benefits have been demonstrated. The amount of clerical work for the technical and scientific staff has been cut, the frequency and magnitude of laboratory errors have been decreased, results have been produced more rapidly, the interpretation and presentation of results have been improved, quality control has been made more sophisticated and results have been analysed for research purposes in a way and on a scale that was not possible previously.

A comprehensive automatic data-processing system is now being implemented with an Elliott 903 computer that is sited within the laboratory. The configuration includes a special data-acquisition unit that enables 24 AutoAnalyzer channels to be connected on-line to the computer. With this system the task of monitoring analytical performance has been transferred to the computer, which samples and digitizes all the analogue signals at 2s intervals and validates the peaks by software. Analytical errors due to such faults as incorrect calibration standards or abnormal degrees of instrumental drift are consequently promptly brought to light. With this system the scheduling of analyses in a manner that gives priority to urgent specimens and to those that must be repeated after dilution has been made automatic. Final results become available at short intervals during the run of analyses and are promptly entered into the appropriate patient's laboratory record, which is held on magnetic tape. After the input of results of the manually performed tests via paper tape, the system will link all the current results on a patient with past results and print cumulative reports with appropriate flagging of unusual findings.

Small versus Big Computers for Data Processing

By S. P. SPRAGG. (*Department of Chemistry, University of Birmingham, Birmingham 15, U.K.*)

The question that first arises in discussing the subject of small versus large computers is what the terms 'small' and 'big' mean in this context. Obviously they could describe the physical dimensions of the machine, but since technological developments have considerably diminished the size of computer components this definition would mean that the most powerful modern computers are small relative to the early machines. Common-sense shows that as far as their capabilities are concerned this is not true, and so a more realistic definition of 'small' and 'big' is required. For the present purposes it is assumed that these terms describe the relative size of the computer word of a machine having a reasonable size of core; it may also happen that economic factors limit the total extent of the computer complex in terms of extra peripheral devices, but this is incidental to the definition. In principle, however, it is possible to expand a small computer by the addition of peripheral devices until it measures up to the size of a large computer as far as physical dimensions are concerned, but the unit would still be regarded as a small computer within the definition of the word size. The effect of this rigid constraint on the computer is to limit both the precision of the integer arithmetic and the range of programming languages that can be usefully employed in programming the computer.

The arithmetic precision is defined by the rounding error of the machine and for a small computer this can be appreciable. A common word length for small computers is 12 binary bits (equivalent to between three and four decimal digits), and it is normal when using these machines to use three words for a floating point variable within a program. Of these three words one holds the characteristic while the other two are used as one unit to hold the mantissa, so increasing the precision to 23 binary bits (approximately equivalent to six decimal digits). This may seem sufficient for all normal computations, but experience shows that unless the algorithms for many numerical exercises are correctly formulated the result is prone to considerable errors (see, for instance, the example quoted by Sapega, 1967). This extension of the word size is necessary, but it can only be made possible by decreasing the usable number of core words, and this in turn means that the programming and variable space is corresponding less than expected from the total core size. The effect of this is that both the programming language and the algorithms must be chosen with care in order to use the available

space efficiently. Higher-level languages are extravagant in storage space and hence generally excluded, making it necessary to use low-level language to program small computers.

Sapega, A. E. (1967). *Decuscope*, 6, 2.

Molecular Modelling and Computer Graphics

By C. D. BARRY and A. C. T. NORTH. (*Laboratory of Molecular Biophysics, Department of Zoology, University of Oxford, South Parks Road, Oxford OX1 3PS, U.K.*)

Computer graphics is a new and rapidly growing branch of computer technology. Its bearing on problems involving molecular structure seems obvious. This communication seeks to examine the field of molecular graphics and aims to outline the achievements and the hardware cost involved.

Specific uses of an interactive graphics system considered include: the display and manipulation of a computer-generated protein model and its application to the crystallographic determination of protein structure; the production of animated sequences and graphs illustrating chemical reactions and mechanisms for teaching purposes; and the use of programs capable of generating trial conformations for small molecular structures starting from input in the form of chemical formulae.

These examples indicate some current applications. There are many fields in which a graphical form of output is more readily comprehended than a digital one, and the true potential of the technique is likely to be limited only by the ingenuity of the user.

On-Line Applications in X-Ray Crystallography

By O. S. MILLS. (*Department of Chemistry, University of Manchester, Manchester M13 9PL, U.K.*)

The relative merits of consoles, terminals, computing terminals and graphical units are discussed in the context of application to crystallographic computation. In all these, there is a play-off between effectiveness, convenience, priority and intrinsic cost. The use to which terminal consoles, whether simple computing or allied with graphical facilities, will be put is discussed.

Computer Control of Mechanical Experiments on Muscle

By R. H. ABBOTT. (*Agricultural Research Council Unit of Muscle Mechanism, Department of Zoology, University of Oxford, Parks Road, Oxford OX1 3PS, U.K.*)

The special property of insect fibrillar flight muscle which enables it to contract rhythmically without synchronous nervous stimulation is the delayed component of the tension that results from an imposed length change. We have been investigating this phenomenon by using small bundles of glycerol-treated fibres of giant tropical water bugs. They are glued between a fixed-tension transducer and a moving-coil vibrator, and are bathed in a solution containing ATP and inorganic ions. The vibrator is mounted on a micro-manipulator to allow changes of mean fibre length, and is itself used to impose only periodic changes of length on the muscle fibres. If sinusoidal length changes are imposed, the delay appears as a phase lag between length and tension changes. Analysis of the change of this phase relationship with frequency shows that the delay is exponential, and its magnitude and time constant can be evaluated.

Information about the contractile mechanism may be obtained by measuring these characteristics under different mechanical and chemical conditions. To obtain a useful amount of information from a single preparation, the manipulation of the apparatus and logging of results must be done as fast as possible, and a human operator is unequal to the task. We have interfaced a PDP8/I computer to all the necessary devices, namely (i) a Solatron JM 1600 oscillator and resolved-component indicator to provide the sinusoidal drive and measure the phase and amplitude of the tension changes, (ii) a stepping motor drive attached to the micro-manipulator that adjusts mean muscle length, and (iii) a mechanism for changing the solution in which the fibres are immersed. The software allows the machine to be controlled by typing individual commands on the on-line teletype. These are single letters followed in some cases by a number. More usually, however, the commands are stored in the computer memory for automatic sequential execution. In this way the computer may be programmed with great simplicity to run an experiment lasting several hours without any manual intervention. A record of the experiment is printed on the on-line teletype, and a codified form of the results may be produced on paper tape.

It is known from other experiments that both Ca^{2+} and an increase of mean fibre length will activate the fibres in the sense of increasing their oscillatory work output. Closer analysis of their effects, by using the apparatus described, has revealed that, although both increase the magnitude