A Computer Approach Toward Automation of a Chemical Services Laboratory: I. Instrument Support[1]

E.L. SCHNEIDER and **A.W. MUNSON,**
Ralston Purina Company, St. Louis, Missouri 63199

ABSTRACT

The use of a medium scale computer for instrument support results in several distinct advantages. Instruments of differing data rates and calculation requirements may be supported on the same system at the same time. There is no interference between any of the instruments since each is assigned its own block of time for scanning and its own set of programs for data support. The use of both the on-line and off-line modes permits the easy development of programs and their subsequent incorporation into the program library. It becomes advantageous to look at data supporting instruments that require only small computer support since the off-line mode can be used for this purpose. Instruments previously considered too low in volume to support can enjoy the benefits of off-line computer support at little additional cost. The use of high level languages such as are supported on the medium scale computers make it possible to train laboratory personnel to write and modify their own programs. Their involvement in the programming effort can result in a greater acceptance of the computer as a useful tool in the laboratory, instead of the attitude that sometimes prevails that the computer is a hindrance rather than a help. The ease with which program changes can be made makes the program modification task easier for the programming staff of the computer installation, if laboratory personnel do not perform this function. The medium scale computer provides computational power far exceeding that available on a series of small dedicated computers. The "pooling" of resources results in having available a larger scale computer for those programs and instruments that require it. The degree of sophistication of software available on the medium scale computers is far above that available on the smaller units.

INTRODUCTION

The rapid growth of instrumental methods of analysis over the last decade has changed the character of work done in many clinical and industrial laboratories. Today, instruments such as the Technicon AutoAnalyzer can perform routine colorimetric analyses at a rate far in excess of their manual counterparts. Fully automatic gas chromatographs and atomic absorption units are commercially available. Other automatic and semiautomatic instruments are becoming available to relieve the analyst of routine and repetitive work.

In implementing these new techniques into the laboratory, however, a new problem arises. Instead of being free to perform other tasks, the analyst is deluged with recorder charts or integrator printouts which must be interpreted to arrive at a result. In addition, he must monitor the performance of the instrument to insure that the data from the instrument is valid. Depending on the data rate, the analyst may find that his daily production of work with the instrument may fall far short of the capacity of the unit. He may have to operate the instrument at a greatly reduced rate in order to keep up with the data. In order to utilize the instrument to its full capacity, some means of rapidly handling the vast amount of data produced by the automated instrument had to be found.

In recent years there has been a trend toward coupling a small dedicated computer to the instrument to handle the data acquisition and calculation task. This has been an interesting and successful approach to the problem, but in many laboratories the expenditure of $10,000 to $15,000 to data support an instrument costing only $5000 is not justifiable. Some efforts have been made at using the same computer for several instruments with varying success. While it is possible to data support different types of instruments on the same small dedicated computer system, the small computer will not support different instrument types at the same time. To change from one type of instrument to another required the changing of the computer program for the new instrument and abandoning the old instrument support function. Thus, the small scale dedicated computer can be made to data support different types of instruments only if the instruments are used one at a time. This usually required careful scheduling of analyses on a basis of available computer time. This type of support does not represent a realistic approach to the problem of data handling in a full service laboratory such as we operate.

To support several different types of instruments simultaneously requires the installation of a larger and more sophisticated computer system. Such a system should allow the scheduling of the execution of computer programs on a priority basis. Programs shoud be executed in response to some stimulus such as the closing of a switch on an instrument or the expiration of a computer resident clock. Unfortunately, the cost of such a system equals and often exceeds the cost of separate dedicated computers for each instrument. Typical costs for such a system start at $100,000 and go up depending on the complexity. Such an expenditure is seldom justifiable unless the laboratory is very large or has sufficient work to justify the instrument support.

This was the problem we faced at Ralston. We had need of computer support for the many new instruments we were installing, but the justification for full computer support was not there. As the instrument list swelled to include more Technicon AutoAnalyzers, atomic absorption units, gas chromatographs, an automated amino acid analyzer and a neutron activation unit, the problem became more acute. Because of the variable nature of the workload in the laboratory, we found that when one technique became busy, they all seemed to become busy. Faced with the problem of a growing need for instrument support, but having insufficient instrument work to fully justify the computer, we began to look for other functions that the computer could perform for us. We felt that by sharing the justification between several functions all being carried on at the same time on the computer system, we could justify the installation of the computer. In this and the companion paper that follows, my colleague Dr. Munson and I will

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describe the resulting approach to the problem of data handling employed at the Ralston Purina Laboratories in St. Louis. We feel that this approach can make it possible for many medium size laboratories to afford the benefits of computer support and to derive many other benefits as well.

During the fall and winter of 1968 studies were conducted on the various phases of laboratory operation. We soon learned that the record keeping function in our laboratory represented a sizable job that was possible on the computer system. As the study progressed we felt confident that many benefits could be derived by sharing the computer between instrument support and the record keeping function. Completing our study in the winter of 1968, management was convinced that definite advantages could be obtained by installing a medium scale computer for the combined functions of instrument support and record keeping.

DATA SUPPORT

During the summer of 1969 an IBM 1800 computer was installed in the laboratory. This computer is a medium scale, third generation unit capable of data acquisition and calculation of data arising from analogue and digital scanning of instruments. The computer has connected to it a communications adapter with 10 communications terminals and 3 random access magnetic disks. The computer mainframe has 24,576 words of core storage with a cycle time of 4 μsec. The card reader and punch operates at 120 cards per minute and provides input of program and some data in the system. The line printer has a print speed of 150 lines per minute and provides "hard copy." The disks have a combined capacity of 1.5 million words and provide bulk storage for both programs and data files. The communications terminals are buffered IBM type 2740s and communicate with the computer over two telephone lines. Their transmission speed is 4500 characters per minute while their typing speed is 900 characters per minute. The system is capable of supporting up to five different instrument types of the analogue variety and one digital instrument in the on-line mode in its present configuration. In addition, it can support a wide variety of instruments in the off-line mode on a one at a time basis. Both the on-line and off-line support functions can be done simultaneously under the IBM TSX operating system employed.

Computer core memory is divided into two sections. The skeleton or permanently resident area has 16,576 words of core. This area includes all of the routines for handling the input and output devices on the system such as the disks, the card reader, the line printer and the communications adapter. A portion of the skeleton controls the scheduling of programs and handles any errors that may arise during operation. The analogue and digital scanning routines are in the skeleton area as well as data buffer areas for the digital instrument, the analogue instruments and the communications terminals. The remaining 8000 words of computer core, called the variable core area, are used to execute the data manipulation and calculation programs. These programs are brought from a program library on the disk when they are required.

In its simplest form, instrument support involves data acquisition from an instrument, digitizing and interpreting the data and placing it in a peak parameter table. An appropriate computer program then operates on this data and outputs a report by means of one or more of the output devices on the system. In the off-line mode, the data is acquired from the instrument by means of a recorder or integrator. The chart, or integrator printout, is interpreted by the analyst to identify salient features such as peak time, peak area or peak height as required by the analysis. These peak parameters are entered into the computer by means of one of the input devices, usually the card reader, whereupon the appropriate computer program is called into the variable core area to manipulate the data and output a report.

In the on-line mode the instrument is physically connected to the computer. A piece of computer hardware, called an analogue to digital converter, is used to convert the analogue data into digital data suitable for input to the computer. The data is stored in a temporary holding area in the computer skeleton. Since the analogue to digital converter is used for only a very short period of time during the scanning of an instrument, it is possible to share this device between many instruments by means of a device called a multiplexer. This device is nothing more than a high speed switch that connects a selected instrument to the analague to digital converter. As many as 1000 instruments may be selectively connected to the computer in this manner. When sufficient data points from a given instrument have been accumulated a program interprets these points to do digital smoothing to remove noise and then determines the salient features of the smoothed data such as peak time, peak height, peak area, etc. These detected features are entered into a peak parameter table on the disk. Each on line instrument has a separate peak parameter table on the disk, preventing the scrambling of data from instruments. When the analyst signals that the run has been completed, the disk stored peak parameter table is brought into the variable core area and the appropriate calculation program operates on it. This program need not destroy or alter the peak parameter table on the disk. As a result, it is possible to have several different programs operate on any given peak parameter table to determine the effect of program changes on the type of finished data that emerges. This is especially useful in program development. Selected peak parameter tables may be stored in a disk file indefinitely. The programs that operate on the peak parameter table need not distinguish between tables read in from the off-line mode or those built as a result of on-line operation. This allows for the easy development of programs while in the off-line mode.

The on-line mode of operation provides a means of instrument support requiring a minimum of analyst attention. Having started his run, he is free to pursue other activities, returning only when the run is complete to review the data and to start the next run. In the fully automatic mode even the function of signalling the computer that the last run has been completed can be done for the analyst. The unit waits a few minutes for the computer to generate the report and then picks up another sample and starts a new run without operation intervention.

Obviously, all of these features are not without some disadvantages. We have mentioned the matter of instrument and computer costs. There is also the matter of computer programming. There are some programs available to support many types of instruments, but it has been our experience that the user will usually modify the programs to meet his particular situation. Those programs resident in the skeleton are usually written in machine language because of the efficient use of core that such a language affords the programmer. The modification of machine language programs such as Assembler requires the assistance of an experienced programmer. Programs to be executed in the variable core are are usually written in one of the higher languages, characteristically Fortran. While the higher languages are not as efficient in their use of computer core, they are easy to modify. Laboratory personnel with no prior experience in computer programming can be trained to write and modify programs and soon acquire a proficiency in programming. The ease with which these programs can be modified easily overcomes their disadvantages of higher core requirements. During the development phases of programming, programs should be written in a high level language such as Fortran.

In the on-line analogue acquisition programs developed for our system, the instruments are scanned in response to an interrupt generated at specific timed intervals by a computer resident clock. The scanning program identifies which instrument is next to be scanned and calculates the addresses of the instrument and the data buffer. The multiplexer and analogue to digital converter are given these two parameters and proceeds to scan the instrument whose multiplexer address is given and to store the data in the buffer addressed. The scanning operation is carried on by the multiplexer and analogue to digital converter without any computer interaction. Thus, while the scanning is being carried out, the computer is free to proceed with other calculations. These calculations include the identification of the next instrument to be scanned, the time interval to delay the calling of the scanning program and the updating of the scanning clock. Each instrument on the system has its own assigned time slot for scanning, preventing a shift in scan time when instruments are put on-line or taken off. When no instruments are on-line, the scan clock is stopped. The entire scanning function requires 500 μsec per data point scanned. To scan five instruments at one data point per instrument per second requires only 0.25% of the available computer time. The interpretation and calculation programs require considerable longer to execute, but since they are called very infrequently, the total CPU usage will seldom exceed 15% of the available CPU time, even with five instruments on-line.

Digital instruments are scanned by a routine that responds to an external interrupt. Each digital instrument connected to the system is required to generate an interrupt when it has data to transfer to the computer. The digital scan program identifies the instrument to be scanned, calculates the input address and the data address and scans the instrument. The computer transfers digital data at a rate of 250,000 words per second. This transfer rate is sufficiently fast that unless huge amounts of digital area are to be transferred, the CPU usage is too low to calculate.

On recognizing an interrupt from either the analogue scanning clock or the external interrupt from a digital instrument, the program being executed in the variable core area is temporarily suspended and the analogue or digital input routine executed. Since the analogue and digital input routines are in the skeleton, no time is lost in getting the data in from the instrument, and upon completion, the suspended program may be resumed. This mode of operation allows the interleaving of computer operations without losing any of the data in either program string.

Instruments are placed on-line or removed from an on-line status by means of control boxes connected to each instrument. Program selection and calculation parameters are entered from any of the communications terminals on the system. The analyst has full control over the type of program that will be called upon to handle his data, giving a flexibility to the system that the small dedicated computer is hard pressed to match. Programs are available or under development for digital smoothing, peak detection, peak area integration, peak height selection and for the identification of detected peaks by means of their time of occurrence on a given type of technique. Support is available or planned for atomic absorption units, Technicon AutoAnalyzers, amino acid analyzers as well as the new neutron activation technique. Due to the variable nature of the gas chromatographic work performed in our laboratory, only off-line support is available for the gas chromatography laboratory.

Program development proceeds by first supporting an instrument in the off-line mode. This permits changes to be made to the programs without affecting any of the programs for the on-line mode instruments already on the system. The off-line mode permits the programmer to study the effect of different programs on the data from the instrument and to tailor the program to what the chemist in the laboratory needs and wants. When a program has been fully tested and has been shown to meet the needs of the laboratory, it is incorporated into the program library and is then ready to support instruments in the on-line mode. Under the Time Sharing Executive System used on the 1800, it is possible to do this entire function from the "background" or nonprocess users mode with no interference to any other on-line programs in use at the time. Even when one of the on-line programs must be deleted from the library and replaced with a new version, the entire process can be done in about 5 min without taking the system away from the users. Only those users who have called for the deleted program are effected for the approximately 5 min it take to make the change.

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