The State of Laboratory Automation

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Laboratory automation techniques have evolved over the past several years in parallel with advances in small computer technology. Today costs of both electronic and memory components used to manufacture computers are still decreasing, especially as large scale integrated circuit technology continues advances. The earliest experiments required heavy economic justification which was usually based upon increased throughput and reduced personal requirements as a result of automation. Therefore, only the most expensive instruments, such as X-ray diffractometers and nuclear magnetic resonance and mass spectrometers, or processes that required extensive hand calculations, such as vapor phase chromatography, were automated. Today, however, more processes are being automated, and several instruments are being produced with computers already installed. In this paper we will discuss how the "minicomputer revolution" has allowed new experiments to be designed that would be very difficult or impossible to execute without computer aid.

Scientific experiments in today's research laboratories are being performed with increasingly complex and precise electronic instrumentation. This evolution has been accompanied by a similar advance in computer technology, particularly in the capability for producing low-cost, high performance processors. In the early 1960's chemists began to realize the potential of computer instrument combinations, and since then applications have mushroomed to the point where complete systems for laboratory automation (*i.e.*, nuclear magnetic resonance spectrometry, infrared interferometry, and mass spectrometry, to name a few) are now commercially available. In this paper we will discuss the development of computers for laboratory automation and explore the implications of these developments on the laboratory of the future.

Early approaches to laboratory automation followed one of two different philosophies utilizing on-line computers (Frazer, 1968). Either small computers were dedicated to single instruments or groups of similar low data rate instruments, or large systems were operated in time-shared mode among various types and numbers of instruments. Dedicated systems offer the advantage of operational independence from any other computer user, whereas the larger time-shared systems provided possibilities for cost distribution of the more expensive peripheral devices among all users. Line printers, large memories, card readers, etc., are normally too expensive for use with isolated minicomputers. Moreover, the larger systems can also, if necessary, support certain kinds of administrative computing (Ziegler *et al.*, 1970; Ziegler, 1972). Several examples of implementation of each type of system can be cited; however, rather than argue on either side, we will concentrate here on the system most commonly considered as optimal today. It is termed "hierarchical," since small and large computers are combined to provide the best elements of each approach, while minimizing cost and duplication in manpower efforts.

Hierarchical computer networks have been defined in a number of ways. For the purpose of this paper, any system that distributes computer tasks among a network of devices will be considered hierarchical. At one extreme, special purpose hardware which can punch numbers on paper tape, dedicated to controlling and acquiring data from a single experiment, might be considered as a data collection device for a distributed computer network. The data collected from such interfaces are transferred to some larger computer system for processing. At the more complex extreme, experiments can be controlled by a very large computer through a series of interfaces and smaller computers which communicate directly with the laboratory devices.

The advantage afforded by distributing computer functions among machines of varying size and capability through a hierarchical network is that very expensive bulk memory and sophisticated hardcopy input-output devices (line printer, card reader-punch, etc.) are centralized and are managed in such a way that their usage is available to anyone who might be connected into the network. The use of a high-speed line printer which may cost as much as $25,000–$30,000 is made available to any user. Furthermore, a computer center can better afford to hire relatively sophisticated systems programmers and highly qualified computer operators to maintain the system than it can supply laboratory scientists with singular needs. Where computer facilities have been developed for use in chemistry laboratories, in general, chemists have been left with the task of implementation and operation of the system. Although chemists can become sophisticated computer programmers, it is usually difficult for them to justify the time that must be taken from research to be devoted to these activities. In fact, at all successful installations, at least some of the chemists involved never return to chemical research, but instead make computer technology their career.

The obvious advantage offered by combined operating systems is that the best of both worlds in computer power is provided. That is, great flexibility is afforded to the individual scientists in his laboratory through the use of dedicated computer hardware for control of and data acquisition from the experiment, and large computer power in high level languages is available in the central system. Implementation of major software tools such as cross assemblers, compilers, and simulators increases the power of these systems tremendously. With them scientists and students can develop, debug, and modify programs without requiring access to the dedicated computer. Only final on-line testing requires the current experiment to be suspended, and therefore experiment throughput of over 90% can be maintained. A particular advantage for instructional installations is that the number of students that can simultaneously be developing programs is limited only by the number of jobs that can be logged into the time share system, and is in no way dependent upon the number of available minicomputers.

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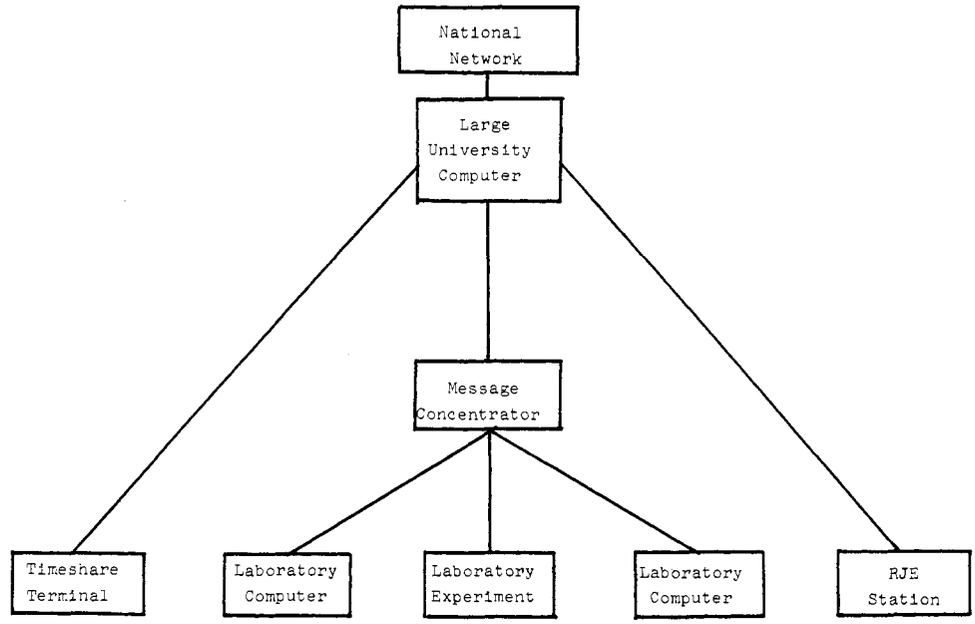

Figure 1. Hierarchical computer system.

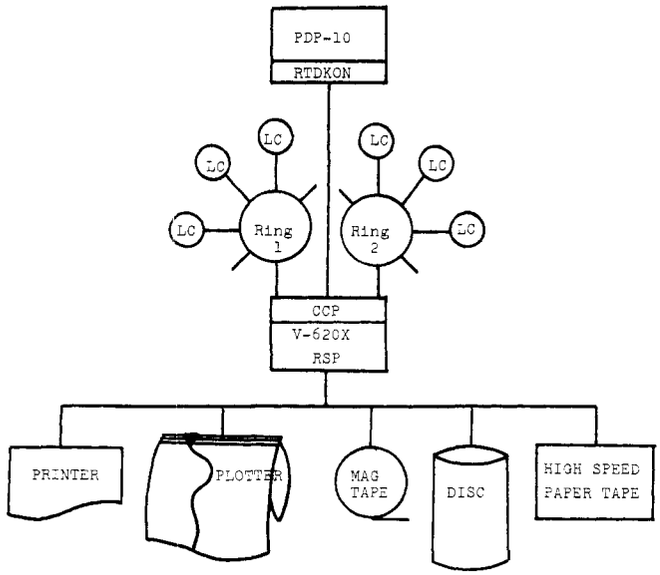

Figure 2. Message concentrator system.

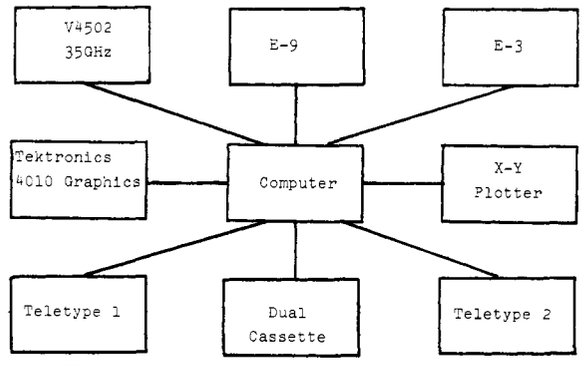

Figure 3. Electron spin resonance laboratory.

IMPLEMENTATION OF THE HIERARCHICAL SYSTEM

To achieve the system described above requires a combination of events to occur in succession.

In order to illustrate one possible approach to implementation of a hierarchical system, the procedure used at the University of Oregon, which divided the process into three steps, will be discussed here.

In the first stage three identical portable minicomputers were acquired with a complement of shared peripheral devices such that most of our urgent requirements could be met immediately. The systems operated standing alone in nuclear magnetic resonance, electron spin resonance, lasar Raman, and other laboratories for whatever time span was necessary to complete an experiment.

In stage 2 the University acquired a large computer which was capable of supporting time-share and real-time computing. Currently, stage 3 is implementing a communications network and an expansion of stage 1 capabilities. A schematic block diagram of the resulting system is given in Figure 1.

This tri-level approach was adopted to allow near transparent usage of the system on a 24-hr basis by laboratory scientists. As described above, the large time-sharing computer is University owned and operated, with the Chemistry Department being treated the same as any other user with the exception that the message concentrator could gain privileged real-time access to the monitor for high-speed data transfers. To protect experiments from the inevitable "crashes" and times when the full large machine was unavailable, a message concentrator capable of temporarily storing large data and program files was installed. Files would be moved forward at appropriate times. It was further hoped that the message concentrator could support some locally shared devices such as a line printer, a digital plotter, etc., which are either too expensive or inconvenient to install in the laboratory. A schematic of the system is given in Figure 2.

COMMUNICATION SYSTEM

The communication system used to support transfer of data between laboratory computers and the message concentrator was initially conceived as point-to-point when the number of remote processors was envisioned as below 5. This estimate was low by a factor of 3, and now it is desired that no practical upper boundary be placed on the number of experiments simultaneously supported. The communication system best suited for these requirements is that proposed by Farber (Farber and Larson, 1972; Far-

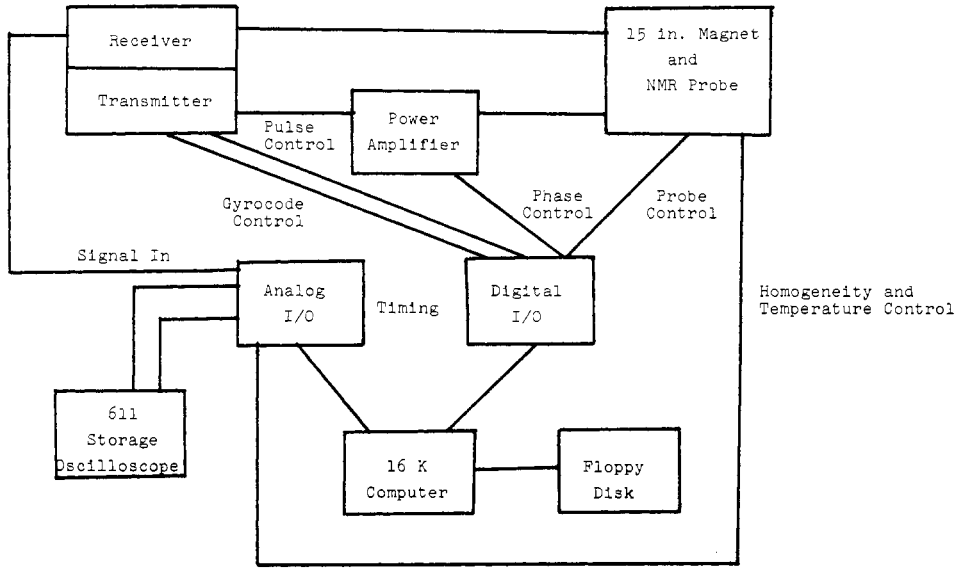

Figure 4. Nuclear magnetic resonance system.

ber *et al.*, 1973) and others, which makes use of a single ring as a data path to all laboratory computers.

The main advantage in this approach is that only one interface is required at the message concentrator no matter how many units are attached to the ring. Adding a new device requires only installation of a simple ring interface. Since each of these interfaces acts as a repeater on the ring, the line driving problem is also greatly simplified. The ring interface is very simple, and costs less than $100 complete with power supply and enclosure. The ring interface feeds a communications controller which is computer dependent, but for most machines costs about $250 to construct. The data rate supported in both the data lines will be determined by the speed of commercial communications controllers, but the devices currently in use operate at 640K Baud, or 40K words/sec for each line. This rate is sufficient for nearly all laboratory applications. A diagram of the interconnections in the ring is given in Figure 2.

Communications with the large campus computer are accomplished at 500K Baud over lines 3000 ft long. Although current technology would allow an increase in this rate, it seems sufficient at this time for chemical applications.

The above gives one example of the implementation of a hierarchical laboratory computing system. It is still under development, and represents one approach to total laboratory automation. Other systems of comparable and greater complexity are being implemented in other laboratories.

LABORATORY COMPUTER

The most striking recent advances in computer hardware technology are in the area of manufacture of inexpensive processors and low-cost bulk storage. Even with a hierarchical system for providing large scale computer power, it is now almost unavoidable to provide high-level power directly at the laboratory computer. Even the least expensive modern computers or microprocessors provide more power than older large scale computers. This means that elaborate high-level languages and extensive instrument control are now easily provided. This evolution of capability can be illustrated by examining changes in function in an electron spin resonance facility at the University of Oregon.

Automation began with a vendor-supplied "turn-key" system which was capable of giving single-minded attention to any one of the three spectrometers in that laboratory. Before long the limitations of this approach became obvious. New experiments were rather difficult to design since program changes in assembly language were necessary, and work was sometimes delayed because only one spectrometer could be used with the computer at a time. We then expanded the system to allow processing in a high level language which can support multiple tasks in a rather small core computer (Klopfenstein *et al.*, 1972). The system now in use is shown in Figure 3. Programs are coded in the language CLASS by laboratory chemists just before the experiments are to be performed, and the data are either processed locally, transferred to the large machine, or both, for further manipulations. This same language is used in several other of our research laboratories.

The Nuclear Magnetic Resonance Laboratory has also expanded much beyond its original scope, and now includes a disk for acquisition of large data files at high data rates. The system is shown in Figure 4, and provides a high level of sophisticated instrument control as well as complete data acquisition capabilities. Again, data are transferred to the larger computer for certain manipulations. For instance, developing a program for calculation of a 16K double precision Fourier transform required only 2 days work on the PDP-10, whereas probably several months of effort would have been required to develop the same program for execution on the minicomputer.

These two examples illustrate the level of automation available at relatively low cost today, that would have been prohibitively expensive just 3 years ago. We can ex-

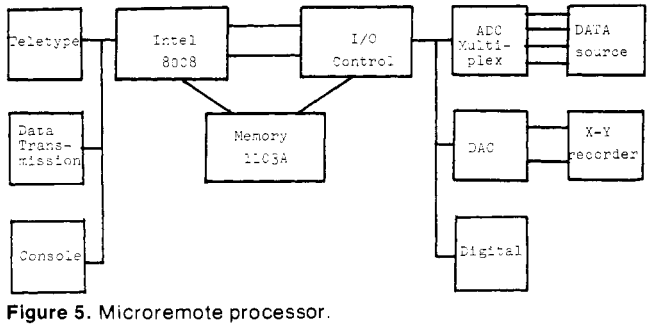

Figure 5. Microremote processor.

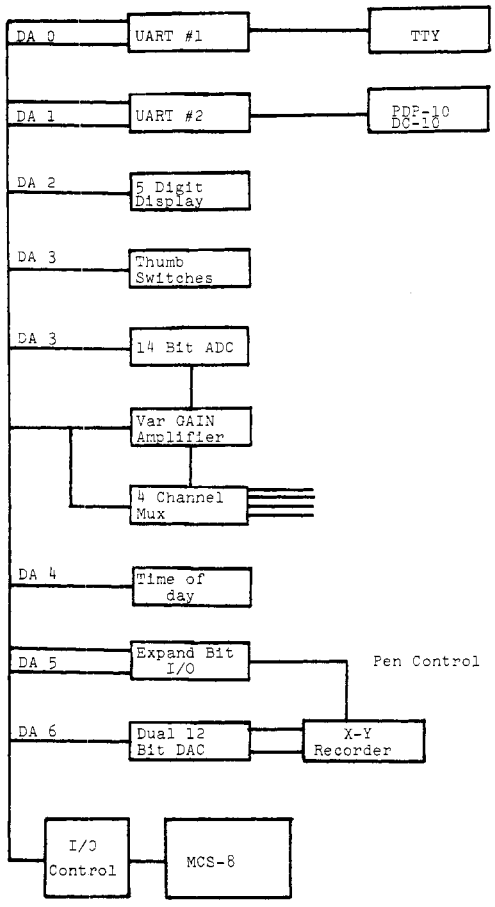

Figure 6. Microprocessor data terminal.

pect even greater power in the laboratory as the "computers on a chip" described below become commercially available, and actually included in the design of new instrumentation.

RECENT ADVANCES

Striking advances have been made recently in the production of massive scale integrated circuitry. Entire processors are now available in single packages. Some of these processors are designed to be used as calculators, others are true computers. The Intel 8008 and 8080 are in the latter category, and provide multiple instruction computers when combined with memory and I/O devices.

The difficulty in using these devices as remote processors is that they are by themselves too slow for program-controlled data acquisition from even medium speed instruments. To satisfy these needs a separate port to memory would be required similar to direct memory access features in larger systems. This added complexity raises costs of course, and at some point these miniprocessors cease complete price performance with "nude minis." A possible configuration for a microremote processor of this type is given in Figure 5, with which data collection can occur at any rate, using local processing for control functions, and possible transmission of data to a larger computer for further processing and archival storage.

Another possibility is given in Figure 6. Here the microprocessor and associated peripherals could replace some of the discrete electronics common in most laboratory instrumentation. Base-line correction, stepper motor driving, ratio calculations, recorder control, digital integration and differentiation, and automatic instrument parameter optimization are but a few of the possible functions a microprocessor could provide in addition to supplying communications to large computers.

As the technology continues to advance, faster processors and memories capable of even more complicated functions will become available. These components will eventually replace the standard integrated circuit systems in use today in our laboratories.

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