H. Cole

Computer-operated X-Ray Laboratory Equipment

Abstract: Many instruments in research laboratories are now operated under varying degrees of computer control, not merely to accumulate and store data, but to obtain information about the sample sooner. The need for the scientist to interact with the computer is then as important as the instrument-computer interaction. This requirement leads to strong differences in implementation between laboratory automation and process control, and also suggests that the scientist must consider his over-all information needs as well as his instrument needs. A control computer shared by several people doing x-ray diffraction and fluorescence work is used as an example to illustrate some of these aspects of laboratory automation.

Introduction

The most widespread application of the computer in the scientific area, which originally spawned it, has been as a calculating machine in the computing centers. Use has spread from there into process control; into testing, quality control, and large analytical labs; and now, finally, into the individual research laboratories, where it is broadly referred to as "laboratory automation." This spread is schematically represented by the circle in Fig. 1, in an attempt to indicate some relative similarities but primarily to emphasize that the areas are different.

A gap that often exists between the computer center and the scientist is rapidly being closed through the growing use of conversational terminal systems (Fig. 1). Such a system permits one, within the privacy of his own area, to work at a console, to program and compute, to learn, and to make his own mistakes. Although these systems are becoming highly successful in implementation, it must be kept in mind that when a researcher sits at the terminal, with all his knowledge and plans, and with human time responses, he relieves the computer system of having to support many more complex system decisions. Even though different from computer-instrument requirements, a minimum form of this conversation ability must be built into any laboratory automation system.

Process control requires the attachment of non-computer-system input and output devices, some of which may well be complex scientific instruments. However, even though the process, its mathematical model, or the devices may be very complex, the main intent of the computer in the central control room is to minimize process fluctuations. It is a centralized operation under one boss, whose computer crew fine-tunes the system, and they are the only ones who converse with it.

The author is at the Thomas J. Watson Research Center, Yorktown Heights, New York

Testing, quality control, and large analytical or clinical laboratories, while often imposing the most demanding data handling specifications, are generally scheduled by the boss, even though the operations require a more flexible organization. Instruments are expected to make sizable excursions; the combination of instruments used may change on a daily, or even hourly, basis; somewhat independent but unchanging control programs, analysis programs, file searching, and report preparation need to be intermeshed. The environment in testing and quality control is characterized by the pressures of the immediate work, and the computer is added and used by the boss on the same basis of his using more instruments or more personnel. The environment of the research laboratory, however, is different from that of testing and quality control.

Research laboratory automation in general

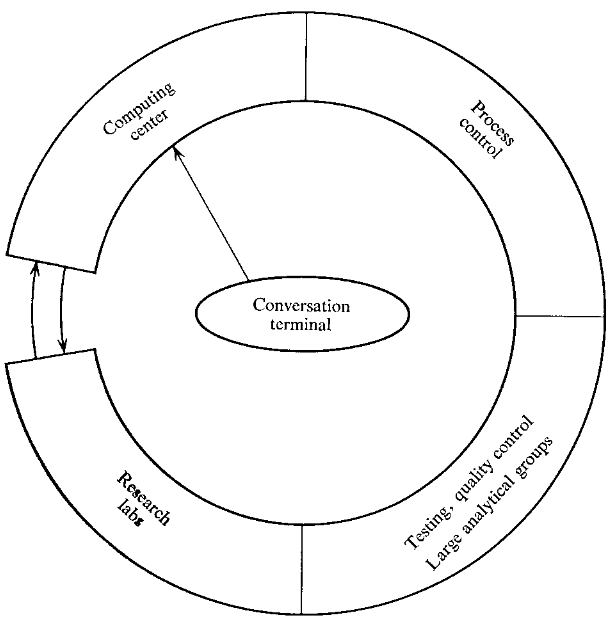
- *Environment*

In the research laboratory, where there is usually a collection of essentially independent researchers, each with his own problem area and experimental equipment, productivity is also a concern. But to use the computer to increase productivity here requires a shift in emphasis: researchers of equal importance but differing needs wish to reach into the computer, at their own convenience, rather than for a central authority to reach out with the computer. That is, "laboratory automation" in this context is assigning to the computer the role of a robot assistant. It helps with the data-taking, presents preliminary results for consideration, does calculations, and prepares plots. In the same sense that an experimental scientist's work day is often "unschedulable" but "responsive" to new thoughts, the computer system must also have these characteristics.

The scientific user may ask for other system capabilities, such as conversational computing, information retrieval, and connection with other groups working on similar problems and sharing a common data base; in this paper, however, we are concerned primarily with using the computer as a rapid, efficient robot. It is usually the computer plot, not the raw data, which contains the information in useful form. Taking the raw data directly into the computer, however, is usually a first step.

Computer-operated equipment can, of course, often work in ways that are beyond human capacity. However, even where the computer programs only copy the human operations, the increased willingness to use the equipment and the enhanced use of analysis techniques, because of the relief of tedium, increases professional effectiveness. Often laboratories which sense the justification of moving in this direction are then faced with the trying current question: how to implement? How can computer capabilities be distributed and used in close to an optimum manner to serve the experimentalist? Luckily, there is little that can be proved to be "wrong," and justification is sufficiently strong that optimization can wait, since there is apparently no single answer yet. Since it is not likely that each individual laboratory will wish, or get, a computer large enough to handle its infrequently occurring largest requirement, a close connection between these laboratory groups and the computing center can be very effective. This brings the circle in Fig. 1 back to a close, to emphasize this connection.

Figure 1 The various areas of use for scientific computers.



• *Functional needs in the laboratory*

Since the emphasis is on the experimentalist and effective use of his instruments, a first requirement usually is to get his instrument data, and possibly instrument control, into a computer. This leads then to an *instrument-interface* need. Sometimes this can be implemented in a step-wise fashion, from logging data in machine readable form from an instrument output or two, to finally completing a closed-loop computer control of a majority of the experiment parameters. Certainly the computer system should be prepared to handle the move to this last stage. This arrangement does not imply, however, the lack of human intervention, although it may make sense in some cases, but rather human operation of all aspects, instrument and analysis, of the experiment through the computer.

The instrument-interface mode brings concern for the elements tabulated in Table 1: data rates, timing, communications, analog-to-digital conversion or vice versa, shaft position control, multiplexing, interrupts, demand/response, channels, codes, expected use time, etc. In fact, most instruments are much alike: a voltage output is produced as a result of a turning shaft. This is reflected in the number of x–y plotters in use. So the basic questions are ones which deal with data rates, critical timing, total data, and storage capacity. Systems decisions have to be made, such as whether to make use of a multiplex channel, which can be told to take in N words on a demand basis; or interrupt responsiveness, to take in each word on command; or polling, on a periodic basis, to sample the output of the instrument. These questions usually require consultation with a systems group or have been partially answered by instrument makers through features that can be bought for the instrument. An interface usually requires signal conditioning, since few signals are compatible with computer inputs and large elements, such as multiplexors. The more unique logic elements in the interface, the more the interface itself becomes a small computer.

Obviously, the use of such an interface does little good unless computer programs are generated to handle the data, and later the instrument, and do some analysis. At a very minimum, "analysis" must proceed to the point where some aspect of the data, or results, is presented to the operator for his use. This need for *applications programs* is usually satisfied by programs developed or borrowed and debugged off-line, and then stored in the system and used when called for by the operator. The routines for data taking and information extraction grow to include smoothing, peak finding, curve fitting, convolutions, formula solutions, plots, interrupt handling, control procedures, file searching, etc.

On the other hand, a true *conversational mode* reflected in a minimum-hardware console, and supported by a stored program, is needed with each instrument to give

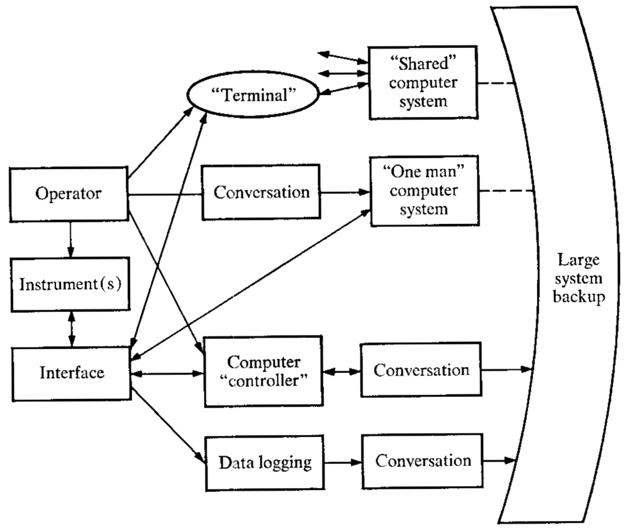
Table 1 Function needs in the laboratory.

I. *Instrument interface*
  - Data acquisition
  - Instrument Control
    - Data rates, timing, total data, communications, analog-to-digital conversion, multiplexing, shaft position control, interrupts, channels, codes, etc.

II. *Applications programs*
  - Data analysis
  - Control procedures
    - Smoothing, peak finding, statistical tests, deconvolutions, curve fitting, formula solutions, plotting, listing, control decisions, interrupt handling, file searching, etc.

III. *Conversation*
  - Operator input
  - Displays
    - Sign-on, input parameters, program selection, linking, display plots, status messages, on-line program modification, etc.

Figure 2 Options for implementing laboratory automation.



the user control over his operation. This is an obvious point but is often overlooked in the concern for the first two items indicated in Table 1. Sign-on, selection of sequences of programs, computer status, experiment status, instruction reminders, messages, lights, lists, plots or CRT display of intermediate or final results, and, of growing importance, on-line program modification, are needed. If a minimum capability to "converse" is not thought out and provided, the experimenter has every reason to expect his main worry to become a reality: namely, that the computer has taken over his instrument, which is no longer easily accessible to him.

Graphic display is becoming of particular importance since the computer can then present information in a form which humans can assimilate easily. Control is easily done with digital input from the operator, but "things to think about" are best displayed as plots or figures, rather than as lists of numbers.

If possible, use of the conventional manual controls, under a manual mode, also adds to the flexibility. This is not for protection in the case of computer down time, since the added productivity of computer-controlled instruments is such that reaction to down time is to fix the system rather than return to manual data-taking, but to give another measure of conversation. What the control program is expected to do after such manual intervention has to be considered, or the operator must converse with the program to reflect the changed instrument status due to use of the manual override.

• *Approaches to implementation*

The functional needs of the laboratory may be implemented in a variety of ways. The easiest step is to log data from the instrument into punched paper tape, punched cards, or magnetic tape. This, of course, still requires an interface on the instrument. The data and programs are then taken to the computing center.

A very small computer may be built into the instrument and dedicated to the instrument. It can successfully carry out a data taking operation programmable within its capacity; and its data output is again carried to the computing center for data justification and analysis. It's capabilities are usually limited to that of "controller."

In each of these operations a time gap of hours or days still exists in the flow of information to the operator about the results of the experiment. This may be quite acceptable in many operations. On the other hand, approaches which offer more nearly "immediate" information responsiveness are: the small computer system in each individual lab, the sharing of a moderate size computer system by several labs, or the terminal operation into a really large system, usually in the computing center. The various approaches are represented by the blocks in Fig. 2.

Most of the approaches are in use in this laboratory. We have instruments, which, through digital interfaces, log intensity and shaft position into punched cards. The data cards are then taken, with the appropriate program, to the computer center as a batch job. This has reduced the personnel time spent in data taking and first analysis, but the turnaround is still long. We also have digital interfaces which operate through the IBM 1050 terminal and send data to the conversational system (APL based in an IBM 360/50) over standard telephone lines.* Since this system is very popular and still growing, although it is very

* See paper by K. L. Konnerth, this issue, page 132.

powerful, all lines may be busy, or the system may be scheduled only for certain hours. An 1130 is used by an individual scientist, and an 1800 is shared by several independent groups. The experimenters on the individual IBM 1130 computer, and on the shared IBM 1800 system use the systems to obtain the "immediate" responses desired for several aspects of their work.

The individual laboratory computer system, characterized by the IBM 1130, is dedicated to a scientist, and is used by him to perform more than just instrument operations, and is used by him to operate more than one of his instruments. This computer, with an 8K core, one disk (500K words), card reader-punch, printer and plotter, has a digital interface through which is attached a single-axis x-ray spectrometer and a 400-channel multichannel analyzer. It is being used to develop instrumentation and analysis program techniques for x-ray fluorescence and x-ray energy powder pattern diagrams. Since the computer "belongs" to the scientist just as do the other instruments in his laboratory, he is responsible for its total operation. Any monitor system program in the computer can then be quite minimum (system I/O, foreground and background task) since only one individual is concerned with the flow of its operations. It has, however, sufficient capacity to perform a variety of instrument and computational tasks, often intermeshed. With its interchangeable disks, it can also be used for stand-alone computing or file searching. The researcher, however, must be willing to learn its operation, and be responsible for its programming. Interfacing with external logic is also required, since only a channel is available. Nontheless it is sized so that it is attractive for individual operations.

Up to this point the individual scientist can and usually does initiate the implementation. Beyond this level, the approach is to *share a larger system* among a group of individual laboratories, acting in concert. The advantages sought, in addition to those listed above, are the sharing of system costs, e.g. a high-speed printer, and the availability of a large-capacity system for each user on an as-needed basis. There is also the possibility for greater flexibility as users enter and leave, as the nature of their research changes.

The sharing of a system generally requires the creation of a new group. That is, if the x-ray, NMR, GLC, and Mass Spectroscopy labs are to share an 1800, a fifth lab is needed, namely the 1800 lab. The reason, of course, is that the shared system has system demands that no one of the users may wish to be responsible for. There must clearly be a more elaborate system monitor program which keeps all the system actions sorted out and performs them in some organized sequence. It must keep each user from interfering with any other (what's to prevent user A from operating user B's equipment?); it must be adjusted to give reasonable priorities and responsiveness; it must reflect the changing hardware items and programs and their method of use; it must provide recovery procedures and inform each user of unusual conditions. Each user may also need help in learning how the system works, how to structure his programs, and how to interface his equipment.

The system programs supplied with computer hardware go a long way toward providing these operations, but just as the mix of hardware reflects the needs of the local situation, particular modifications or emphasis in the system monitor can also be expected because of the local mix.

To complete the picture, it is clear that the IBM 1130 or IBM 1800 computer may be attached, by cable or by teleprocessing, to a larger computer, and thus become "terminals." If the user is in a separate part of the building, he will also require a terminal at his location to provide solutions to the functional needs of instrument interface and conversational mode.

Shared computer/x-ray experimentation

In order to show the possibilities discussed here we shall describe a shared system now in use.

Hardware. An IBM 1800 is shared by several groups doing x-ray diffraction and fluorescence work. Attached to the computer at the present time are a four-axis x-ray diffractometer for crystallographic data-taking;[1] a single-axis "pole figure" spectrometer; a single-axis x-ray fluorescence spectrometer; and a single-axis microdensitometer for reading films or plates. Single-axis spectrometers for powder pattern work and line-shape analyses are being attached.

The configuration of the computer is shown in Fig. 3: 32K of core, two disk drives, card reader-punch, plotter, console. The digital front end has 16 16-bit words of output (closures), 24 16-bit words of input (on-off signal lines), 6 16-bit words of interrupts (demand signals from equipment). There is a channel adapter and an experimental connection to an IBM 360/67 in the computing center. The three 1053 printers are for remote output at experiment locations. A CRT storage oscilloscope is used at the computer for output. It is, of course, a disk oriented system, with system programs, application programs, and data files on disks.

There is no analog I/O. That is, although a central analog-to-digital converter with a multiplexor is available with the computer, it was not ordered because most of the devices on x-ray equipment are already digital (shaft encoders, scalers for counting pulses from detectors, and timers). Where analog/digital conversion (ADC) is required (e.g., from the photomultiplier of the film reader) it is done locally (at the terminal), and only digits are transmitted to the computer.

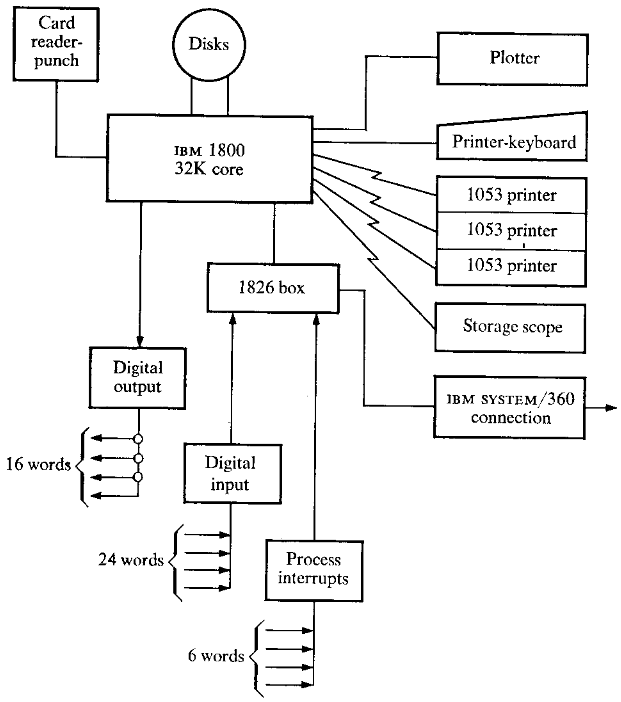


Figure 3 IBM 1800 computer features.

In addition to the remote printers, a numerical keyboard and a 3 × 4 array of lights at each instrument gives minimum conversational capability.

Most instrument signals go directly to the computer contacts (after appropriate amplification or shaping); but some multiplexing is done at certain instruments, i.e., bits in a computer are used to select a particular instrument readout to be put on a common set of lines to a computer input word. The desire, however, is to keep this to a minimum. Where external devices, with logic, such as a presettable scaler, are readily available; however, they are used instead of performing the function in the CPU.

System software. The TSX-II monitor system, supplied with the 1800, is used. The skeleton, that set of systems programs which are core resident, uses approximately 12K of core. This includes COMMON regions, in the skeleton, for each experiment; interrupt service subroutines pertaining to each experiment; several in-house written skeleton routines used for scheduling; and, of course, the supplied system routines.

One of our in-house routines, the LAB DIRECTOR routine, gives use of the 20K of variable core (core not assigned to the skeleton) to the different experiments, or to the time-share (regular batch computer jobs initiated from the card reader). The LAB DIRECTOR, which is called as the proper exit from all programs, assigns use of the variable core on the basis of who next in the list of users has a request in. If no experiment program is requested, the nonprocess jobs (time-share) are given use of the core. This arrangement is an attempt to give equal priority in the use of variable core to all those using the system at any one time, independent of any hard-wired priorities associated with their interrupt signals.

There are unavoidable hardware priorities in any system, which is then intermixed with software modification. The computer hardware is built so that "cycle stealing," the momentary halting of processing for a device on a data channel to insert a word in core or take a word out, has the highest priority. The forced halting and branching to an interrupt service routine in response to arrival of interrupt signals, which, among themselves, have hard-wired priorities, is next. Use of variable core as assigned by the LAB DIRECTOR is next. And use of variable core by nonprocess batch operations is last. Any experiment will generally have activities associated with each of these priority operations.

The interrupt service routines, which are in the skeleton, give "immediate" response (several hundred microseconds, or longer, depending on the state of the machine) to the information conveyed by the arrival of the interrupt, from a sign-on signal, to intermediate experiment operations, to sign-off. These are short programs which may initiate an action, but they do not transfer control. If more response is required, the interrupt routine may set bits in the LAB DIRECTOR's table. The LAB DIRECTOR will then bring into core and give control to the indicated experiment program when the LAB DIRECTOR next has control, and the bit set by the LAB DIRECTOR is the next one on in the list. Any experiment program being processed is halted during the execution of any interrupt service routine from any experiment, but it is not aborted. It continues to be processed after the interrupt is serviced. Control is returned to the LAB DIRECTOR by the experiment program in variable core at appropriate points in time. Any non-experiment program, however, being run under time-share, is stopped and stored on disk if an experiment program is requested through the LAB DIRECTOR. When no further experiment programs are requested, even though interrupts may be occurring and are being handled, the LAB DIRECTOR, through the TSX system programs, restores the saved batch job to core, and its processing continues. Figure 4 is a schematic representation of this system behavior.

Generous use of interrupts in an experiment is encouraged, not as panic conditions, but as convenience, or "action completed," signals. The experiment is stepped then, in real time, on the basis of the arrival of such interrupts. On the other hand, the pessimistic point of view is taken towards hardware, that every device that can will "stick" and no interrupt signal will arrive. Thus, wherever possible, two actions are initiated, the desired

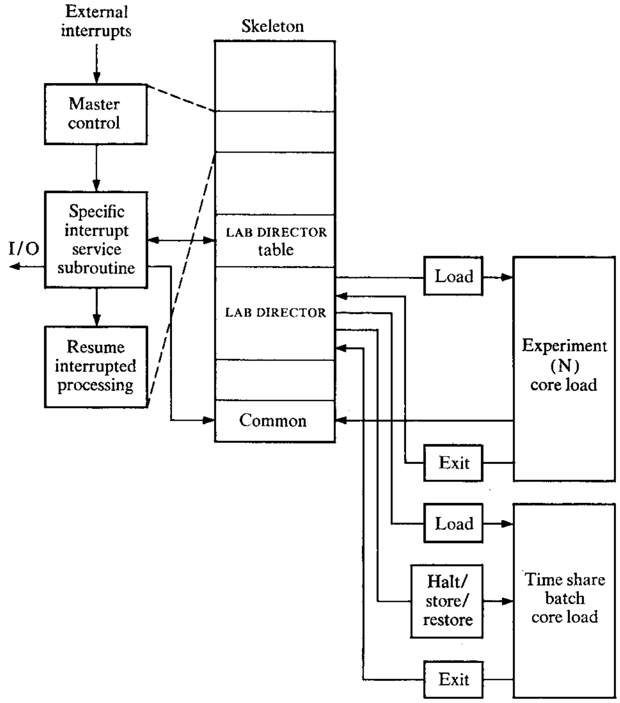


Figure 4 System monitor for the IBM 1800.

one and a watch-dog one. The interrupt service routines, or the experimental program, must then be able to decide that the device is "stuck" and how to try to free it. This leads to another general point, namely that good records must be kept in the programs of all experiment status and requested actions currently under way. Otherwise the arrival of a "noise," or unexpected, interrupt, or an indication of a "stuck" device will cause the computer programs and the real actions of the experiment to get out of step.

It is still possible for conditions to occur which require a restart, or reload, of the computer, i.e., to bring in a fresh copy of the skeleton from the disk. In order to prevent loss of the contents of the COMMON regions in the skeleton, we also use an in-house routine which saves INSKEL COMMON on disk before the reload, and then restores it afterwards. Each user should have a recovery program of his own to check over his own experiment when the system undergoes a reload. This again is part of the "conversational" requirement: the system should inform each user, and each user may want to "converse" with his operations.

Experiments

• *Four-axis x-ray diffractometer*

This instrument is used to measure the x-ray diffraction intensity and angular positions of several thousand Bragg reflections from a small single crystal. These intensities are then used, with sizeable analysis programs, to deduce the arrangement of the atoms in the molecules of which the crystal is composed.

Input devices from the experiment include four absolute reading, brush, shaft angle encoders, each giving a reading of five decimal digits; a six-digit pulse counter, or scaler; a six-digit timer; indicators of open/closed status of eight shutters, filters, and attenuators. Control signals are given by the computer to four motors, each with stop/start, two speed selections, and two drive sense choices; stop/start, reset, and preset signals to the scaler and timer; open or close signals to the eight filter-attenuator-shutters. Interrupts are generated by certain encoder conditions; by overflow (reaching preset value) of scaler or timer; by open or close action complete from the filters, attenuators, and shutter; and by actuation of limit switches. A block diagram of the experiment hardware is shown in Fig. 5.

This experiment is in the same room as the computer. The operator can turn to any of the system I/O units for interaction with the computer. One of the experiment program routines even permits the 1816 keyboard to be used as a manual control panel to manipulate the hardware items. Even so, a set of 16 switches, as input, and a set of 16 lights, as output, on the instrument, have been very useful in stepping the experiment along and indicating which current operation is going on.

Given these basic hardware functions, the experimenter develops, through programs, the particular mode of data-taking he desires. For example, the programs, given the approximate orientation of the crystal, move the shafts to the calculated settings for a Bragg reflection; a search is made to locate the peak; the peak is stepped through (position shafts, then expose) or scanned through (expose while shaft moves continuously); filters and attenuators are adjusted concurrently; data are scaled and stored on disk; several options exist for order of sequence of reflections to be studied; blocks of data can be processed for application of correction factors, preliminary statistics, and plots; certain peaks can be returned to on a periodic basis for calibration; and so on.

The programs consist of several small interrupt service routines (a few hundred words) which are in the skeleton at all times, and two core loads (approximately 15,000 words each) which are brought in from the disk through the LAB DIRECTOR, as needed. These core loads are themselves modular in nature, each major experiment operation (such as, "calculate settings," or "position shafts") being an independent subroutine, except for the sharing of COMMON. Although the sequence of their use is built into the program for continuous operation, this sequence can be broken into through use of the 16 switches, so the operator can break into the operation and continue from whatever point he desires, or skip operations that he doesn't want. Also, since this experiment runs con-

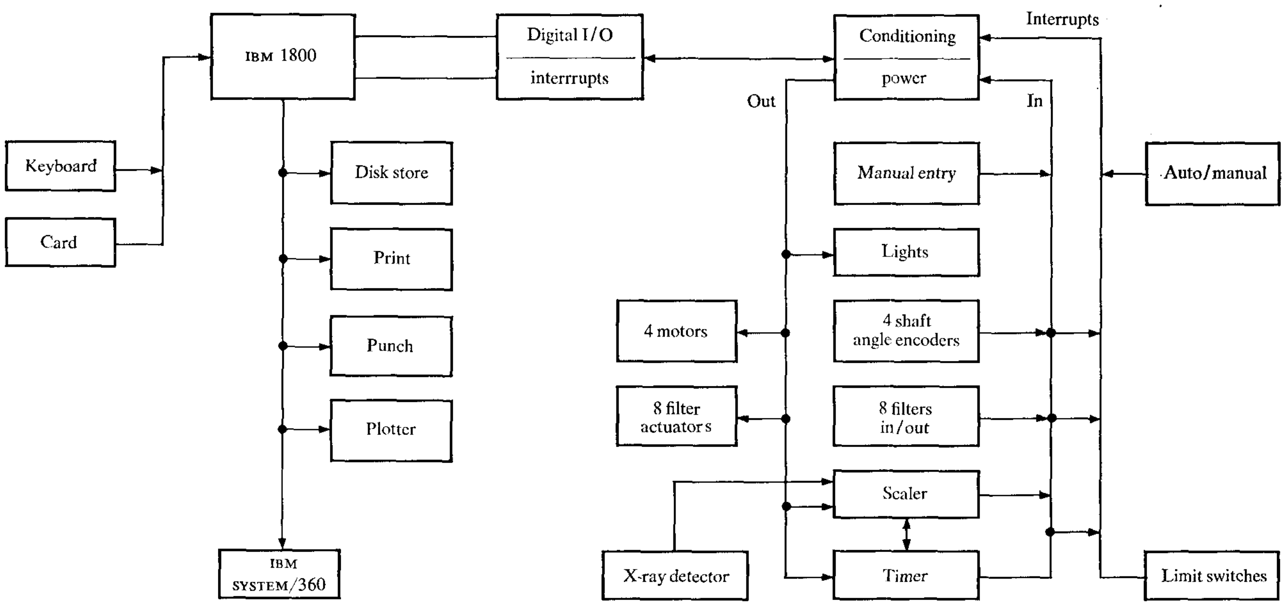


Figure 5 Diffractometer features.

tinuously (day, night and weekends) any trouble that is detected, even if corrected for, and a running summary of results (peak intensity and positions) is printed out on a local (1053) printer. Thus the operator can quickly bring himself up to date whenever he checks on the experiment.

The hardware of the experiment is such that it makes demands on the computer only about once a second. x-ray intensities and statistics are such that the detector and associated scaler and timer are usually operated for periods of several seconds, which requires no computer time if in a step mode, and only need to be sampled a few times if in scan mode. The motor speeds are such that, at highest speed, a shaft turns at a rate which changes the least significant digit of the encoder only a few times a second. The shafts are positioned by two schemes: if the desired position is far away, as determined by the shaft positioning routine, it will refer to a table of motor speeds and preset an 1800 timer and turn the motor on. The interrupt service routine started when the timer finishes and interrupts, stops the motor and asks the LAB DIRECTOR to bring in the experiment core load. The experiment core load reads the encoder and compares. Quite often the hit is acceptable; if not, but if it is close, it will activate the interrupts from the turning shaft encoders and set up an interrupt count in the appropriate interrupt service routine. It starts the motor and exits to the LAB DIRECTOR. The interrupt service routine counts the interrupts as they arrive and when the specified number of interrupts has been reached, stops the motor, and asks the LAB DIRECTOR to bring in the experiment core load, and so on.

If the interrupt level is momentarily masked, or some other experiment is using variable core, there is no loss of data in this experiment. If there were critical times, more elaborate use of the interrupt service routine, or agreement among the users that a certain experiment core load could keep control until the critical point were passed, could be tried.

The increased flow of crystallographic data, processing, and graphics output has permitted the same group of people to perform six times as many published studies per year as was done previously. Figure 6, for example, shows use of the drawing capability, which permits figures for publications to be drawn by a computer. The drawing and plotting function alone almost justifies the computer.

• *Pole-figure diffraction*

In pole-figure work a sheet of crystalline material is manipulated in a way that a normal to its surface traces out a section of a sphere. An x-ray detector is set in a fixed position to measure the reflected scattering. A contour plot of the detector readings on a projection of the spherical surface then indicates the distribution of the orientation of the grains in the sheet.

In this operation on the computer there is no need for control of the mechanical motion, other than stop/start. The output of the detector is sampled periodically. Only an analog (rate meter and strip chart recorder) output was being used, so an ADC is used at the instrument to digitize the readings. (A scaler could have been used instead). After sign-on, entering the initial offset of the mechanical motion, and start, a cam-operated signal initiates an ADC reading and sends an interrupt to the computer about once a second. The ADC is then read into the computer and reset. If the computer does not get to the reading in time, a time-out occurs at the instrument which stops the motor. The computer resets this time-out. If a time-out occurs, the computer also starts the motor again. No data are lost, but if anything prevents response from the computer in time, the experiment stops and waits.

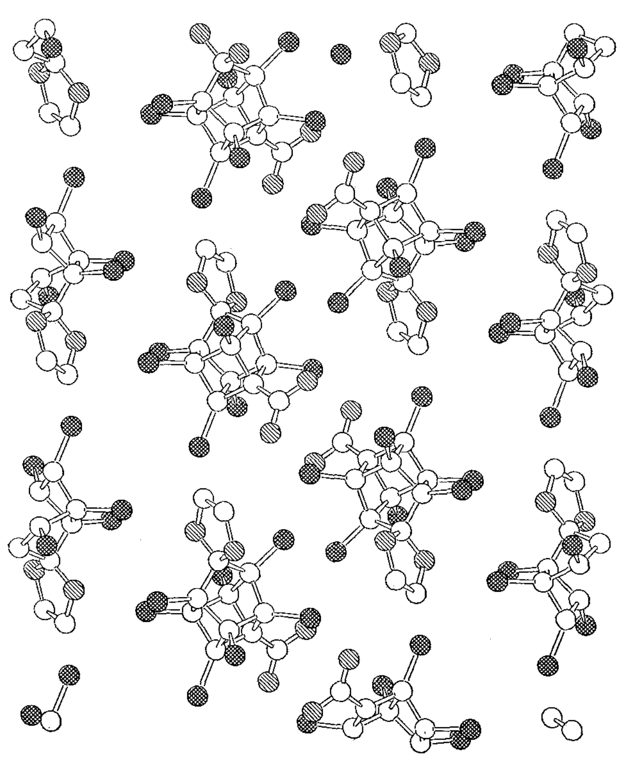
Some 15,000 readings are accumulated. These may be stored and plotted as raw data, but usually the data are smoothed point by point by fitting from five to nine points on both sides of the particular point to a parabola, and replacing the central point by the parabola point. The data are then contoured, those points which represent an intensity change from one contour to another are selected, and these points are indicated by symbols on a polar plot generated by a plot routine. The operator can draw in, easily and quickly, contours connecting like symbols, and can see the orientation distribution. Thus after placing the sample on the device and starting it, the next step the operator must take is to pick up the polar plot. An example is shown in Fig. 7. The elimination of the tedious data-taking and hand plotting has made this a routine tool in the laboratory, as opposed to a seldom used special technique.

A numerical keyboard is used, at the instrument, to provide at least minimum conversational input, since this instrument is remote from the computer. The operator can sign on, and enter a stream of numbers through the keyboard which are interpreted by this experiment core load; experiment parameters, options in analysis and plotting, and text feedback to the operator are possible. The printer in the area permits the computer to send messages to the operator. Also a set of lights at the instrument gives basic status information about the computer operation to the operator.

Figure 6 Illustrative example of the capability of the computer to prepare graphic material from crystallographic data.

C9 cage chlorocarbon acid $C_9CL_7 \cdot COOH \cdot (O_2C_2)$

Projection along **B**



○ Carbon ◍ Oxygen ● Chlorine Hydrogen not shown

- *X-ray fluorescence analysis*

The x-ray fluorescence spectrometer is used to determine the amount (concentration) of certain atomic species in a sample. The intensity of characteristic x-rays emitted by atoms in a sample, which is made to fluoresce by exposure to an initial x-ray beam, are measured by Bragg reflection from a crystal of known orientation set for the characteristic reflection angles. Since a fair amount of sample manipulation (inserting standards, blanks, and changing unknowns) is still required, operator-computer interaction is very high during the data taking.

The hardware items attached to the computer through the interface are a scaler, for counting the pulses for fixed periods of time from the x-ray detector, and a motor-encoder combination for reading and positioning the reflection angles. A numerical keyboard and local printer are provided for conversational needs, as well as a minimum set of computer status lights at the instrument.

There are several options in the data-taking procedure and data-analysis programs. For example, the operator may choose to follow a defined format of sample manipulation (low standard, unknown, high standard) with a defined format of intensity readings (low-angle background, peak, high-angle background), with the operator performing all settings, and thus the computer is used only to read the scaler when requested. Usually the computer repeats the reading at least three times at each position, to give information for use in the analysis program which checks derivations. An erase routine is also provided which causes the last set of readings to be removed from the data file.

Another operation being implemented causes the computer to read the shaft encoder as well as the scaler as the operator goes through the data-taking steps the first time, and thereafter, as long as this option is indicated from the

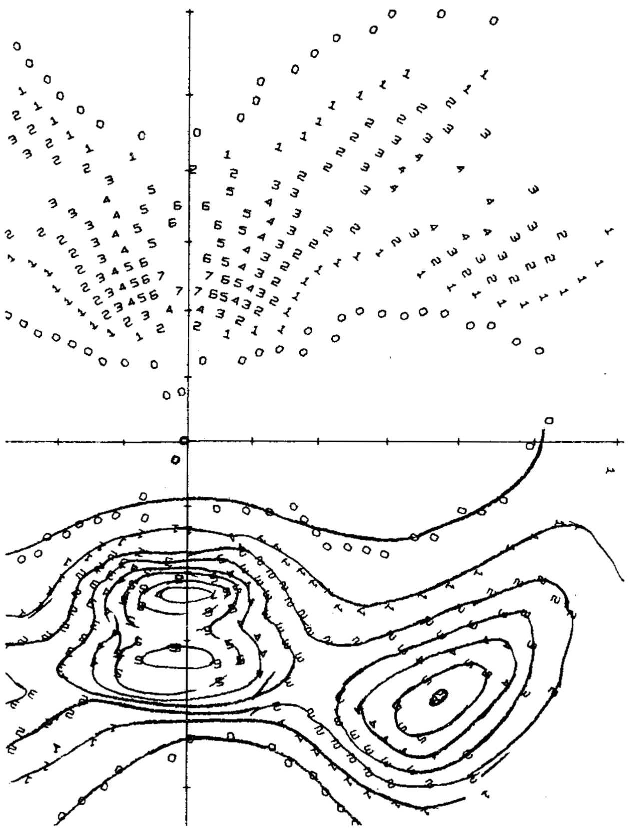


Figure 7 Example of computer-prepared contours derived from pole-figure x-ray diffraction data for polycrystalline sheet.

keyboard, the computer will position the shaft to these locations in the same sequence and take the data. The operator is concerned thereafter only with sample manipulation and monitoring, which are indicated by text messages from the program in the computer. Thus the conversational mode is of utmost importance if the human operator and the computer are not to get out of step.

The analysis programs, which are called for after the formatted, or tagged, data file is completed, may check deviations and flag questionable points; fit the readings of the unknowns to a curve determined by the standards; or calculate concentrations on an absolute scale, using certain algorithms; and plot, or tabulate, results on output devices.

Data rates are obviously low, but responsiveness is very important. Since the operator is so involved, the system must give some response, even if it is a "hold," before the operator might proceed impatiently to operate the keyboard. The importance of the system to the operator is that analysis can be finished while the samples are still immediately available, if not still in the spectrometer. Thus the answers are not produced days later after some other intervening work but are "immediately" available.

- *Film reader*

The densitometer on the computer is used primarily for reading x-ray powder pattern films and mass spectrometer plates. The carriage has a little over 25 cm of translation possible with a minimum increment along the plate of 50 microns. A motor-encoder combination permits the program in the computer to read the position of the carriage and move it in either direction to a new position, with a variety of speeds. An integrating ADC is used to digitize the voltage output of the photodetector. The intention was to use the ADC to average the light transmission over areas of the film before bringing the reading into the computer, but in practice, data are taken on the finest possible grid and all data manipulations are done by programs in the computer. A numerical keyboard and a set of status lights, plus a local printer (shared with the pole-figure operation) give operator interaction with the remote control computer.

A film is placed on the carriage by the operator and the light and optics adjusted. The table drive can be activated through manual switches at the instrument. The keyboard is used to sign on to the computer, select the options, and enter any information about the film. The computer manipulates the table, activates the ADC, and takes intensity and position readings. An x-ray powder film can be read in about three minutes. Programs are available for smoothing, locating peaks, and determining peak heights, with text output back to the instrument and plots at the computer. In progress are more analysis programs, for example, for routine powder pattern identifications of unknown compounds, the selection of the strongest lines, verification by the operator that this is not a "suspicious choice" (again a requirement for extensive decision programs, or good conversational interaction), and file searching of the ASTM file for suggestions for identification. Reading of plates associated with other instruments would obviously require a different set of analysis programs.

- *General*

Whenever possible, commercially available hardware items have been used, although no vendor supplied a complete package. Thus engineering assistance is required to assemble the items into an operating whole. The programs were largely written by each user for his own operation. The programs are mostly in FORTRAN and are constantly being revised as more use is made of the computer. Certain routines are sharable, such as "calculate settings for Bragg reflections," or "smooth data in file on disk by parabola fit"; others are very specific for the I/O of a particular instrument or device, such as a particular make of shaft-angle encoder attached to a particular set of computer I/O words. We are constantly rebuilding programs, so compiling is an important capability for the system to have, and it runs as a time-share (non-process) job. The skeleton is rebuilt as new or changed interrupt service routines are required. Although the FORTRAN routines, not specific to an I/O operation, can be used in any system, our core loads exit through the LAB DIRECTOR. This routine, however, can be incorporated without changing the TSX monitor supplied by IBM.

Summary

A computer system has been shared by several x-ray groups doing independent work. The "pay-off" for some is the steady, around-the-clock data taking and cross checking; for others it is the immediate analysis of the results on each sample. In each case, the need for operator communication with the computer is as great as that for data acquisition and instrument control. Plotting and display are important elements. Even with all experiments operating, time is available for larger batch calculations or analyses. Attachment of the IBM 1800 to the central IBM System/360 is expected to give larger capacity for data storage, file searching and large scale calculations.

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