Foreword

A colleague of mine started his physics experiment at 4:30 p.m. the other day and went home. For the next twelve hours a digital computer controlled the apparatus and recorded the data. In the morning these data in their refined and reduced form were available for interpretation. In another laboratory analytical chemists have attached a number of digital computers to their instruments for more reliable and faster analyses. These are only a couple of examples which illustrate possible benefits from laboratory automation. The anticipation of automated biological and physical laboratories in space and data acquisition from instruments for the comprehensive care of critically ill patients have been discussed in the press and are reportedly being developed and implemented. Today, the capability for many exciting possibilities of laboratory automation exists. Laboratory automation with a digital computer can readily be done for many experiments. We therefore felt that it would be useful to devote an issue of the *IBM Journal of Research and Development* to the subject. These are reports of original work in the field of experimentation aided by digital computers. They include descriptions of functioning systems involving some aspect of data acquisition, open and closed loop control, and real-time data analysis through the use of devices such as an interactive graphic terminal. Needless to say, this is not the first mention or discussion of advanced topics in laboratory automation. A partial bibliography of recent literature is included at the end of this Foreword. Note that most of the works cited are from 1966 on and indicate the emergence of the field. With the references from the papers in this issue, the papers themselves, and this bibliography, a worker interested in the subject should have a good start. The rapid advance of the field precludes much more than that.

For the novice, the two most frequent questions asked are "Why should I connect a digital computer to my experiment?" and subsequently, "How do I connect a computer, including details concerning the interface hardware and the systems and applications programs?" For the first question the increase in experimental data and the more efficient utilization of some experimental apparatus initially comes to mind. But after further reflection, quality, not quantity, should be the expected result. Indeed the experiences of myself and my colleagues have clearly shown this to be the case in our computer controlled experiments. The accuracy is improved, the signal-to-noise ratio is improved, and the data are stored digitally for further processing, i.e., there is the opportunity for searching for hidden correlations which are the bases for new advances in understanding. Further, the tedium of long experiments is removed so that a search can be conducted at high sensitivity for long periods of time with the experimentalist released for creative thought.

If this were all, laboratory automation would no doubt be used by many; however, there is an even more compelling reason to consider computer-instrument operations. Experiments previously thought impossible are now feasible. The papers by McCann and Birnbaum et al. illustrate this point. The amount of data is enormous, the speed of acquisition is very fast, and the detailed course of the experiment cannot be anticipated. The latter difficulty is being currently solved in both cases with interactive graphic terminals which allow the experimenter to monitor and modify his experiment in progress by timely observation of the results in a variety of ways.

Let us now turn to the second question—"how is the computer connected to an experiment?" In all cases of which I am aware the completion of the total system required detailed direction and supervision at the working level by one person. That is, the first step is to appoint some one individual to be responsible for the interface design, the selection or writing of systems and application programs, and getting the whole system built and into operation.

After the decision has been made to automate and the responsible leader identified, the desired objectives and their priorities must be determined. Trite as they may sound, the scientific and engineering goals must be stated in rather specific terms. If data logging is all that is desired, one must not try to do everything in sight at first or to estimate the data rates by the composite total. Usually much lower rates than expected are sufficient, and the cost of an all-inclusive system would rapidly become prohibitively high. If a complete control system is sought, one experiment should be done at a time with a complete plan for the remainder. For example, if one desired to automate a chromatographic laboratory, he should first select only one chromatograph. He should then address the problems of ranging, number of points over a line (probably about one-fifth the initial estimate), base line correction, accuracy required for peak separation, methods to accomplish it, method to calculate areas, and the extent of results to be presented to the user. Fortunately most of these tasks are relatively independent and can be accom-

plished with few cross references. In general, the electronic and mechanical interface devices must be designed, and the programming must be planned and executed to accomplish the desired tasks. Although it may be possible to utilize the prior work of others, at the present time this has not been practical. Either the computer has been different or the desired results different—that is, each group of individuals seems to approach the problem differently. Hopefully this situation will not always prevail and one will be able to select from a catalog the desired features and have them delivered. Finally, the capabilities and limitations must be understood. Laboratory automation is not the panacea for poorly conceived or executed experiments; under these conditions it merely collects more bad data. Hopefully the papers presented here give a good summary of the better approaches from which readers can profitably learn.

Much has been said here and elsewhere concerning the relative merits of small dedicated computers, medium sized time-shared computers, and satellite computers attached to larger computers. It is not my desire to enter this quagmire but merely to state that each approach has its proponents. Only after a study of all the papers in this issue and the bibliography and a mapping of these accomplishments on expectations can a meaningful conclusion be drawn for a specific case. Our experience at San Jose has been with a medium sized time-shared computer; although the results have been very good, I am reluctant to say this is ideal or correct for everyone.

Finally before setting the stage for the included articles I wish to make two points concerning data rates. Experiments fall into the classifications of fast, slow, time independent, and those requiring computation between data points. The first point is that to satisfy all these requirements simultaneously in a single system is a complicated and involved procedure. Fortunately many experiments are either slow experiments or time-independent experiments, the latter being the common spectroscopic experiment where wavelength, frequency, or magnetic field are the independent variables. A commonality among experiments exists, leading to a real ease in handling. The second point worth making on timing is the question of hierarchy—for example, should the computer control the instrument or should the instrument demand service by the computer? In my opinion, for flexibility, the device with the most logic capability should be controlling, with the possible exception of time-dependent phenomena such as radioactive decay. Further, with the reliability of current circuits, most computer-instrument systems are not hampered by much down time. In fact, should the computer be down, rarely does the user shift to local control because of the difficulty of running the experiment the "old way."

Let us now consider the current issue before us. Nuclear physicists have the honor of being, from necessity, among the first users of computers in their experiments. This fact is reflected both in the number of papers and, in general, the sophistication of the approaches. Most of these papers involve multichannel analyzers for spectral peaks from nuclear species. The papers by Bevington, Wilburn and Coffin, and Fryklund and Loveland treat data acquisition and analysis for pulse height spectra. A small computer, 8K storage, is used in each case. The systems, present and planned, described by Mollenauer represent somewhat more complicated ones with two CPU's. Bell and Øverås catalog all the systems at CERN, the data acquisition scheme from an array of scintillators with a System 360/44 being the most interesting from the laboratory automation point of view. Finally, Birnbaum et al. relate the details of their interactive graphic system that permits the user to sample various sections or part of his results and subsequently modify the experiment in progress, this approach being one of the most advanced to date.

On the other end of the spectrum, the life scientists use the computer in their experimentations probably the least; McCann and his associates, being exceptions, use a graphic display terminal to study neural systems. This allows a study in depth with the ability to correlate signals for meaningful interpretation and analysis. The modeling and understanding of neural systems requires sophistication in order to start to unravel the complications of the sensory and information processing mechanisms of living things.

Chemistry and solid state physics experiments currently present great expectations. Many diverse methods and approaches are described in the papers and in the references. Cole's work is some of the earliest in computer control of an X-ray diffractometer to record and analyze the data from crystals. Although many others are now doing this, pioneering work is summarized in his paper. Reich and Konnerth present novel uses of a terminal, though slow, for data acquisition from NMR and light emitting diodes, respectively. In the latter example, the drudgery of recording the data of many lifetime tests is much relieved. Okaya gives an account of the uses of a computer in a university chemistry department for research and instruction, and Byerly and Fahidy simulate the kinetics of a chemical reaction for better understanding and extrapolation to difficult experimental conditions such as high temperature or pressure. Herd and Davis describe a much improved technique for lens testing. On the higher rungs of the ladder of complexity we have the systems of Gladney and Sederholm. Both are time-sharing in the sense that they permit concurrent sampling and control of several different instruments; and both permit considerable flexibility in usage which facilitates the implementation of software interfaces. Application of these systems for electron paramagnetic resonance spectroscopy is illustrated in Johnson, Kuga and Gladney; for optical spectroscopy

by Grant and by Hannon, Horne and Foster; and for mass spectroscopy, nuclear magnetic resonance, and chromatography applications by Lusebrink and Sederholm. The reader should find these two groups of articles at an advanced state of the art most informative and instructive.

Finally, I wish to acknowledge my appreciation to my secretary, Mrs. Shannon, who did much of the organization and correspondence, and the Research library for their bibliographic assistance.

Hopefully these papers will engender in the reader as much enthusiasm for the subject as I have found.

J. D. Swalen
Guest Editor

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