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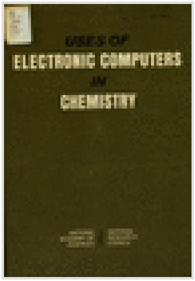

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USES OF ELECTRONIC COMPUTERS IN CHEMISTRY

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Division of Chemistry and Chemical Technology

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January 1967

14

Conference on Uses of Electronic Computers in Chemistry

Organizing Committee

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Herbert S. Gutowsky, University of Illinois
Walter M. Macintyre, University of Colorado

Panel Chairmen

Berni J. Alder, Lawrence Radiation Laboratory
Peter G. Lykos, Illinois Institute of Technology
F. A. Matsen, The University of Texas
Robert G. Parr, The Johns Hopkins University

Division of Chemistry and Chemical Technology

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I
INTRODUCTION

In response to a proposal generated at the January 1965 Sanibel Island Symposium on Quantum Chemistry, and presented by Professor Robert G. Parr, The Johns Hopkins University, to Dr. F. A. Long, then Chairman of the Division of Chemistry and Chemical Technology of the National Academy of Sciences - National Research Council, Dr. Long designated Professor Harrison Shull, Indiana University, to organize a representative group of users to identify the problems created by the growing use of electronic computers in chemistry and to explore channels through which enduring solutions might be developed. The need for and functions of a standing committee to deal with these problems were among the questions to be considered.

With the support of a contract between the Academy-Research Council and the National Science Foundation (Contract NSF-C310 T.O. 106) a conference of 25 invited participants was held November 1-2, 1965 at Indiana University, Bloomington, Indiana. Sessions were devoted to several topics of general interest and to four specific problem areas: (1) financial support for computing; (2) organization of computing centers and their use in research; (3) publications; (4) education. The closing session was devoted to the formulation of conclusions and recommendations, summarized in the final section of this report of the conference transactions. It was the general consensus that the high cost of computers, the difficulty of obtaining large amounts of computer time, the potential but still unrealized impact of computers on education, and the complex interactions of the great variety of user groups, were creating problems of broad concern to chemists.

1. THE ACADEMY REPORT ON USES OF COMPUTERS

Professor F. A. Matsen, University of Texas, led off the discussion of general topics by reviewing the status of the Academy's report on Digital Computer Needs in Universities and Colleges.[1] This report had been in preparation since 1962 by an ad hoc Committee on Uses of Computers, of which he had been a member. The Committee, headed by Dr. J. Barkley Rosser, had been under the aegis of the Academy's Committee on Science and Public Policy. The origin of the report is explained in its foreword as follows:

For half a dozen years the use of computers in universities and colleges has been growing very fast. Not counting government-supported laboratories, such as Livermore Laboratories, Lincoln Laboratories, and the Jet Propulsion Laboratory, expenditures and utilization of computers in the academic institutions of the country reached a total of nearly 100 million dollars for 1963. About half of this was supplied by aid in various forms from at least eight federal agencies. Prominent among these was the National Science Foundation, whose director, Dr. Alan T. Waterman, felt that the time had come "to take stock of the status and likely growth of computer uses in order that the federal agencies may proceed in an orderly way to develop plans for the future support of this important adjunct of science." In June of 1962, he requested the National Academy of Sciences - National Research Council to undertake a study for this purpose. A committee was chosen by the Academy-Research Council to make the study. This is the report of the committee.

The Committee recommendations (as they appear in the final, published report) are as follows:

1. THE 1964 CAMPUS COMPUTING CAPACITY SHOULD BE DOUBLED BY 1968. By doubling capacity we mean doubling annual campus computing budgets. To help accomplish this end, the federal share should rise from $65 million in fiscal 1964 to about $180 million in fiscal 1968. This overall doubling should be allocated about as follows:

a. Nearly double capacity to handle research needs of faculty and graduate students. (About 85 per cent of campus computing effort is now devoted to solving problems arising in research.)

b. More than double the number of undergraduate students trained annually to use the computers in their later professional work. (Such training now accounts for about 10 percent of campus computing effort.)

c. Increase as rapidly as possible the number of students trained annually as computer specialists and the support of pioneering research into computer systems, computer languages, and specialized equipment. (Such activity now accounts for about 5 per cent of campus computing effort.)

2. Government agencies should cooperate in helping a number of strong campus research efforts in computer science to grow at an expanded rate and to develop into regional centers. These centers may supply computing service for their own and for nearby institutions and can experiment with several currently attractive ways of providing this service. The research groups at these centers, with several directions of emphasis, would play major roles in originating and developing new programming systems and languages (software), new ideas for auxiliary and remote equipment (peripheral hardware), unified planning of hardware and software (coordinated design), and particularly the

[1] Later issued as NAS-NRC Publication 1233, February 15, 1966.

advanced education of computer specialists. Equipment of specialized and advanced design must be made available to research groups of these kinds. Estimated costs for strengthening about half a dozen such efforts and purchasing advanced equipment should build up to a total of at least $10 million per year within the next four years above and beyond any costs of providing service computing.

3. General support is needed to provide computing for novel, unforeseen research activities that are not part of established and continuing programs and are therefore as yet unsponsored.

4. The eight or more federal agencies already making major contributions to the support of campus computing must carefully coordinate their support. They must further join with the universities to:

a. Work out satisfactory funding and auditing procedures. Specifically, mechanisms must be found: (1) to eliminate some present practices that effectively deflect special support (e.g., National Science Foundation facilities grants and manufacturers' educational contributions) away from its intended use; and (2) to permit realistic amortization and depreciation practices.

b. Work toward rapid implementation of recommendations 1,2, and 3.

5. Planning should begin now for the long-range cooperative effort between federal agencies and universities and colleges extending beyond 1968:

a. To make effective and efficient use of future generations of computers,

b. To plan continued expansion of computer use in instruction, and

c. To enable the universities to perform their role as trailbreakers in new areas of knowledge and practice as increasing areas of science, engineering, commerce, and health activities grow to depend on computers.

In response to questions concerning the report, Professor Matsen offered the following personal comments and opinions: (1) the recommended doubling of present computational capacities implies an increase in the level of annual expenditures to $300 million by 1968, with the federal government continuing to assume about half of the total; (2) the survey and the recommendations apply to colleges and universities, only, and do not take into consideration the government-supported laboratories; (3) the Committee on Uses of Computers is not a standing committee and is expected to be discharged upon publication of the report; (4) the report went through at least six drafts and its publication had been delayed because of a division of opinion; (5) chemistry use had not been realistically estimated; (6) no consideration had been given to computer needs for storage, retrieval, and processing of information.

2. THE ACADEMY SURVEY OF CHEMISTRY

Professor Shull discussed the treatment of computer usage in the survey of chemistry sponsored by the Academy's Committee on Science and Public Policy.[2] The Committee for the Survey of Chemistry, headed by Professor Frank H. Westheimer, had originally expected to rely on the report of the Committee on Uses of Computers for data on use of computers in chemistry, and hence had not included this item in the questionnaire sent out to university chemistry departments. Subsequently, about half of the universities, carefully

[2] Chemistry: Opportunities and Needs, National Academy of Sciences - National Research Council Publication 1292, issued November 28, 1965.

selected to provide a representative sampling, were interviewed by questionnaire and telephone as to how many hours, on what type of computer, had actually been used by their chemistry departments in one year. The results, scaled up for all 125 universities that granted Ph.D degrees in chemistry between 1960 and 1963, are shown in Table 1.

TABLE 1. COMPUTER USAGE AND COSTS FOR 125 UNIVERSITY CHEMISTRY DEPARTMENTS*

YEAR[a]	COMPUTER[b] TYPE	HOURS USED	REAL VALUE $ MILLION[c]	HOURS PAID	$ MILLION PAID
1964[d]	B	8,800	4.0	1,500	0.38
	C	8,800	1.8	1,400	0.28
	D	18,000	0.6	1,700	0.06
1963[e]	B	5,700	2.6	1,300	0.32
	C	5,900	1.2	1,000	0.19
	D		0.4[f]		0.05[f]

[a]Either fiscal or calendar year, depending on local custom.

[b]As defined in the NAS-NRC report on Digital Computer Needs in Universities and Colleges, NAS - NRC Publ. 1233.

Type B: IBM 7094, CDC 1604, IBM 7090, Univac 1107, IBM 7044, IBM 7074, Burroughs B5000 or equivalent.

Type C: IBM 7074, IBM 7072, IBM 709, IBM 7070 or equivalent.

Type D: IBM 1620, IBM 1410, IBM 1401, Burroughs B220, Burroughs B205, SDS 910 or equivalent.

[c]Computed on basis of $450/hr for type B, $200/hr for type C, and $35/hr for type D. These figures are weighted average monthly rental × 1.5 (to cover partial overhead and staff costs) ÷ 176 (prime shift hours per month). We assume 35 type B, 35 type C, and 80 type D machines, as obtained from our direct replies together with the listing in the NAS-NRC report on computers. Some universities have more than one computer of these types in use.

[d]1964 data were obtained from 27 universities using type B, 18 universities using type C, and 26 universities using type D equipment.

[e]Comparative data for both 1963 and 1964 were obtained from 11 universities (U. Cal. at Berkeley, Duke, Harvard, Illinois, Indiana, Northwestern, Oklahoma, Pennsylvania State, Utah, Washington U., and Yale). The relative figures for 1963 and 1964 obtained from these 11 institutions have been used to scale the total 1964 results to produce the 1963 entries.

[f]No comparative data were available for type D computers. 1964 data have been scaled down in the same proportion found for type B and type C computers.

Enormous variation was shown from university to university, both in total computing time and in the percentage of total time charged to chemistry departments. Furthermore, the information was not broken down to indicate specific uses, which are known to vary widely. In some universities, usage by chemistry departments is negligible; at others, like Indiana University, where there are a number of individual large users, chemistry accounts for 30 to 40% of the total. Professor Shull's estimates prepared for the survey of chemistry are considerably lower than Professor Matsen's prepared for

*From <u>Chemistry: Opportunities and Needs</u>, NAS-NRC Publ. 1292, p. 101.

the computer report, but are based on actual computing times attributed to the chemistry departments by the university computing systems. They indicate a growth of 50% in value of computing time for the university chemistry departments between 1963 and 1964, in good agreement with the over-all annual increase of 45% in university use of computers estimated in the Rosser report.

Professor Shull commented on the large difference between the estimated $6.4 million of computing time used by the university chemistry departments in 1964 and the $0.7 million directly charged to them. The universities are indirectly subsidizing chemistry use to the extent of close to $6 million per year (through support from the computer industry, government support to the universities for general computing services, university subventions for auxiliary services, and other means). The Westheimer report recommends a growth rate in computing services for university chemistry of 35% per year over the next four years, the increase needed over the present (1964) $5.7 million of hidden university support to be funded in full by the federal government through research grants and other methods of funding. The recommended figure for 1968 totals $19.8 million, including $14.5 million from government sources.

In reply to a question whether, in view of the growing use of computers in education, support should continue to be charged so exclusively against research funds, Professor Shull felt that with increased efficiency of time sharing by the new, large computers educational use will come to occupy a smaller and smaller fraction of the total time available. Furthermore, the computing power of the large computers is so great relative to their cost that the largest computing centers will almost completely dominate the scene in any forecast for the future. No projection is yet feasible for computers of Type A (such as CDC 6600), since not enough of them are in use or even in existence for reliable assessment of their capabilities.

3. FEDERAL INTERAGENCY COMMITTEE ON COMPUTERS

Dr. Geoffrey Keller, Director of the Division of Mathematical and Physical Sciences of the National Science Foundation, commented briefly on the Foundation's computer program which, for organizational purposes, is in the Mathematical Sciences Section of his Division, though intended to support computer needs of all disciplines. His agency is faced with the problem of what the government's response should be to the recommendations in the Rosser report. An interagency committee has been set up, involving 8 or 9 federal agencies, to review the recommendations and to ascertain whether they represent the considered opinion of the best thought in the scientific community.

With regard to the recommended specific rate of increase in government support for computers, it will be essential to know where are the present sources of support. A trial questionnaire is being designed to elicit from 9 selected universities how much it costs in all respects to operate their computing centers, and the sources in detail of their revenue (how much from major grants or contracts intended primarily for direct support of computer activities, and how much from recharges against research grants and contracts, or other sources). If the questionnaire is successful, it may be sent out to other universities, or at least to a representative sampling of them. Such information is prerequisite to any detailed planning. The problem of support for computer services is particularly complex because of the extremely broad variety of projects and users, the exponential growth in use and projected use, and the rapid pace of technological developments in the computers themselves. At the same time, computers are exceedingly expensive, and require a long lead time in preparation for their financing. It is the worst kind of situation in which to make plans, but one that desperately calls for planning.

4. THE CHEMICAL INFORMATION PROGRAM

Mr. Paul D. Olejar, Head of the Chemical Information Unit in the Studies and Support Section, Office of Science Information Service of the National Science Foundation, introduced the topic of use of computers in chemical information services, with particular reference to the developing Chemical Information Program (CIP) of the federal government. The CIP is an interagency program supported by the National Science Foundation, the National Institutes of Health, and the Department of Defense, and cooperating with Chemical Abstracts Service (CAS) of the American Chemical Society. It is intended to modernize existing chemical documentation services and to develop new concepts and tools for handling chemical information on a large scale. Current activity consists primarily in a two-year contract for about $2 million with the American Chemical Society, announced on June 3, 1965, under which CAS is to set up a large registry system for filing information about chemical compounds and to conduct allied research.

Although not all the proposed research is necessarily directly allied to the registry system, the intention is to create a file of sufficient size to test many problems of utility, sericeability, and economics of the operation of such a system on a national scale. The background of the present contract is a series of research projects funded jointly by the American Chemical Society and by various government agenices. The federal government had expended about $1.5 million on this research (mostly through National Science Foundation grants) and CAS an approximately equal amount. Much of the effort had gone into problems of nonconventional chemical notation systems adaptable to mechanization and into development of some of the newer services at CAS, such as Chemical Titles, and Chemical-Biological Activities.

The registry system, the main subject of the present contract with CAS, is an interrelated set of files through which information about a chemical substance can be associated with a unique 9-digit registry number for the substance. Entry into the system can be by structure, name, or cipher. A connection table will provide an atom-by-atom inventory of the molecule, showing each atom, the atoms connected directly to it, and the types of connecting bonds; mass number, valency, coordination number, and charge will be shown whenever required for exact identification. The molecular formula and bibliographic references will also be provided. With this hard core of information, other data can eventually be provided. The registry number of the substance will provide the bridge to such specialized files as, for example, toxicity, drug-reaction, and sources of supply. Magnetic-tape records of various areas of information are currently being received and distributed to cooperating agencies for testing and evaluation.

Mr. Olejar made the following points in reference to the CIP:

(1) The technical feasibility of registering information on organic compounds in a computer-based file has already been demonstrated at a number of places, including CAS.

(2) Refinement and extension of the registration techniques were needed in a setting of handling data on a large scale, to test the economic feasibility and operational efficiency for a system of national scope. Such development called for a project of sufficient size, which came out to be roughly 10% of the estimated 3 million compounds now on record, and of sufficient duration, up to 2 years, to permit orderly evaluation and a valid sampling of user feedback. This is the aspect now being handled through the contract between CIP and CAS.

(3) Requirements for a national chemical information system, or systems, are not presently known. However, the registry concept does provide each compound with a unique address, as a common link to all related information as needed. The second part of the CIP program will look into extension of the registry concept to substances other than defined organic compounds, and will provide for handling associated data and documentation as needed. This work will be done by various agencies besides CAS, including academic institutions, private contractors, and industrial concerns.

(4) Results of the two foregoing activities will provide bases for decisions as to how far and in what direction further research and development may be supported by federal funding, and will permit scientists and engineers, individually and through their organizations and professional societies, to assess values and services they may wish to support if an operational system is to be developed. It is expected that systems concepts and design will be under way and perhaps completed within the three-year period through FY 1969.

Dr. Fred A. Tate, Deputy Director of CAS, contributed some details of the CAS program. The basis of the registry system is the ability to put into the computer and retrieve either the complete structure, uniquely identified with the compound, or the substructure (any basic subset of atoms within the molecule)—all the detail that is recorded in a two dimensional diagram plus all the third dimension that is recorded in the connection table. A scanner is on order from IBM that will read hand-drawn structures and automatically convert them to a machine cipher for recognition. The machine record will permit a search on any subset of atoms within the structure.

The contract with CIP calls for CAS to put into the registry system all compounds indexed in Chemical Abstracts for 1965 and 1966—some 450,000 to 500,000 structures during the first 12 months of the contract, plus an additional 400,000 during the second 12 months. The structures are prepared by chemists from the original publication and can be put into the system simply by clerical effort beyond the structure-drawing point, either by tabular inventory, based on a connection table, or by typing the structures and having the machine record and convert them to tabular form. Alternatively, the structures can be typed directly from the diagram. The computer programs convert these entries to a unique, linear cipher, which is searchable for subsets, within the machine. The system is designed to take eventually the full 3 million compounds now known, plus the additional 75,000 new compounds which come into the literature each year. It is set up to include references in publications, and about 15 to 20 million references are indicated if organized on the basis of compounds.

One of the major problems has been that chemical information services do not get sufficient attention at present in the colleges and universities. There is a substantial amount of effort in industry and in governmental circles, but within the academic institutions information services hardly exist. It would be desirable to increase the flow of information between academic institutions and other sectors of the chemical community. A great many problems are faced in getting the kind of computer support at the universities that will allow them to utilize chemical information services on a practical basis. Furthermore, there are problems in getting support for CAS's own programs and in gaining the interest of hardware manufacturers in developing equipment suitable for other than computational and business applications. The equipment commercially available has not been designed with information purposes in mind, and it is only recently that the expanding size of the market has begun to have an effect. In due time, this demand will influence hardware design, so that the task of accumulating and disseminating the basic published data of chemistry can be carried on more efficiently.

Discussion of Mr. Olejar's and Dr. Tate's presentations brought out that university chemistry departments are just beginning to become aware of computer-based information activities. Dr. Tate added that CAS expects to convert all of Chemical Abstracts to computer-based composition over the next three to four years. The operating budget for 1966 will be about $8 million, to which about $1.5 million for research and development should be added; the estimated annual total by the end of 1970 will be $16 to $17 million. It was also brought out that the registry system number is actually a quite flexible concept, and does not commit the user of information to any fixed method of classifying the substances; the registry system does assign each distinct substance a distinguishing number, which can then be used as that substance's address for information purposes in any way the user sees fit.

II FINANCING PROBLEMS

Professor Robert G. Parr presided over the session devoted to this topic, assisted by Professor Don L. Bunker, Dr. Enrico Clementi, and Dr. Jerome D. Swalen, constituting a panel to review the discussion and formulate recommendations.

Dr. Glenn R. Ingram, Associate Director of the Computer Science Program in the Mathematical Sciences Section, Division of Mathematical and Physical Sciences of the National Science Foundation, outlined the Foundation's computer science program. The two principal components are research grants and computational facilities grants. Research grants have totaled about $800,000 per year. Among examples of the kinds of research that have been supported are research on pattern recognition, on numerical analysis and algorithms, on approximation theory, and on advanced techniques in hardware and software (such as on-line processing, time sharing, and image processing). A particular example of a technique interesting to chemists is the representation of three-dimensional molecular-orbital wave functions on a fluorescent screen by means of varying degrees of intensity in the X-Y plane, from calculations carried out directly on an IBM 1410.

The facilities grants are in response to proposals submitted by the institutions, and justification is based primarily on interdisciplinary research needs. For the past three years, the level of support has been about $5 million per year, but during the current fiscal year (1966) it has been increased to about $9 million.

Dr. Ingram touched on government auditing practices as they affect NSF grants. In the past, any NSF support was first subtracted from the total cost of operating the university computing center, and the balance, only, was used in determining the hourly rate. Thus, for a computing center costing $500,000 per year and providing 5,000 hours of computing time, if the center received an NSF grant of $100,000 the auditors for other agencies would take the view that a proper charge was at the rate of $400,000/5,000 hours or $80 per hour, instead of the actual rate of $100 per hour. Negotiations are under way, with some success, to convince the other agencies that they should allow charges for computer time at the actual rate, thereby permitting all of the NSF grant to be applied to reducing the cost of unsupported time to the individual research user. Thus, if 2,000 of the 5,000 hours in the preceding example were expended on Department of Defense contracts at $200,000 instead of $160,000, the NSF grant would reduce the cost of the remaining 3,000 hours of unsupported time to $200,000, and the individual research user could be charged $67 instead of $80 per hour.

Professor Shull mentioned another aspect of the uniform rate, that it encourages the university to shut down the center at all times except during funded operations, in order to keep the rate up. This attitude tends to freeze out small, experimental, unfunded operations. Dr. Ingram pointed out the auditor's view, that if the university were to increase user time by encouraging unfunded users, the sponsored users should get the benefit of the lower rate since all users are getting the same service. One possible solution, suggested by Professor Parr, would be to have a sliding scale of rates, uniformly applied, by which higher rates would be charged to heavier users; the presumption is that the heavier users are likely to be able to afford the higher rates. Another possibility, mentioned by Professor Shoemaker, would be to charge different rates for different computing installations available at the same university.

A question from Professor Wahl brought out that the auditors apparently are not concerned about differences in computing charges at different universities. This is a point of real concern, however, to the Chemistry Panel of the NSF and to the Petroleum Research Fund Board in allocating funds for computing time in research grants, since rates can vary from one university to another by a factor as much as 10. It is almost impossible for the review panels to determine what is a reasonable amount of computing time in a given research proposal, and what is a reasonable charge for that amount of computing time, particularly when there is keen competition from other proposals requesting funds for instrumentation.

A question was raised concerning the funding of computer research in chemistry through the Computer Science Program of the NSF. Dr. Ingram pointed out that although the Computer Science Program is in the Mathematical Sciences Section, it is by no means restricted to mathematical aspects of computer research. Proposals are entertained from a broad spectrum of fields, which presently include biology, mathematics, physics, and even music. No grants are presently in force to professional chemists, but neither have any formal proposals been received from them. Substantial indirect support of computer use in chemical research is provided, of course, through the facilities grants, which total much more than the direct research grants.

Questions of funding small, departmental computers for laboratory research were discussed. Professor Gwinn commented on the problems his group had confronted in purchasing such computing equipment. By local decision, the expenditures had been confined to state funds so as not to compete with federal funding of the university computing center. He had had difficulty also in negotiating research proposals that involved both the purchase of small computing equipment, to control data-collection and computer-assembly programs, and the use of computing time at the large central computing system. Dr. Ingram and Dr. Keller expressed the opinion that the question of funding equipment and computing time for a specific research proposal would be regarded at the NSF as completely unrelated to the question of support for the local, central computing system.

Professor Shull raised the question of departmental grants to cover computers for department-wide use. Dr. Keller felt that the specific need of chemists for departmental computers would have to be argued, and that the case would certainly be considered if chemists felt that it was an issue of major concern.

There was discussion of the economic advantages of large compared with small computers. Power and economy of operation are increased if the funds are put into one large installation rather than several smaller ones, provided that the system is used efficiently. Indirect costs related to preparation and programming stay about the same.

Dr. Tate was questioned about costs to university chemistry departments of the chemical information services under development by Chemical Abstracts Service. Both custom services and direct access from the user's own facility are contemplated.[3] The costs will depend greatly on the extent to which government support for the requisite hardware can be assured. Considerable support for the information services is expected from chemical industry.

Accounting practices of government auditors and the universities met with further criticism. The idea of closing down a computer center during time free from sponsored computation, so as to maintain an artificially high hourly rate of compensation, struck many of the conference participants as particularly repugnant. No definite conclusion was reached, but it was felt that the facility should be made available somehow at low cost to research users with restricted funds.

[3]After the conference, Professor Peter G. Lykos arranged for a cooperative venture between Illinois Institute of Technology and Chemical Abstracts Service to explore the use of <u>Chemical Titles</u> and CBAC magnetic tapes by undergraduate students in IIT's course in chemical literature and by faculty members.

III
ORGANIZATION OF COMPUTING CENTERS AND USE OF COMPUTERS IN CHEMICAL RESEARCH

The chairman for the session was Professor F. A. Matsen, assisted by a review panel consisting of Professor William D. Gwinn, Professor Stanley Hagstrom, and Professor John A. Pople.

Professor Matsen described briefly the organization of the computing center at the University of Texas. The center is supervised by an active, interdisciplinary committee which meets several times a month to consider policy questions. The director of the center is a mathematician, Dr. David M. Young. The center has on its staff 6 or 7 faculty members having joint appointments in the center and in the disciplinary departments (chemistry, education, electrical engineering, linguistics, mathematics, psychology). This has proved to be an effective way to maintain liaison. The chief difficulty confronting the center has been a shortage of personnel experienced in systems research. Professor Matsen emphasized the importance of keeping the university adminstration informed of prospective developments and costs on a continuing basis.

There was some discussion of the role of computer science departments in producing trained personnel. At present, there is a tendency for the graduates to run into difficulty gaining acceptance in mathematics departments and in other academic positions, though they have no difficulty in finding employment at computing centers. The difficulties are attributable at least in part to the newness of the field.

Professor Macintyre described the organization of the computing center at the University of Colorado. There is a separate computer science department with six joint appointments in computer science and other primary fields. The computing center itself is run as a non-academic service division of the graduate school, under a director who is not a professional programmer but a scientist intimately concerned with the application of computers to some other primary field. The technical operations are in charge of a manager responsible to the director.

Professor Gwinn expressed reservations concerning the use of joint appointments, because of the possibility that neither department would give its full support to the man involved. The consensus was that joint appointments are coming to be acknowledged as a necessary and useful device, along with area studies and other interdisciplinary activities.

Professor Shull stressed the need to keep the computing center as a separate operation from computer science. He commented on the psychological disadvantage of handling computer facilities grants through the Mathematical Sciences Section of the NSF. He went on to raise the question of satellite installations and how determinations are made concerning the tying in of such installations to the computing center. Professor Hagstrom expressed his strong belief that the advisory committee controlling the center should be dominated by users equally well qualified in computer science and in their own disciplines. He also mentioned the need for each center to have complete control over its own programming system, independently of conditions determined by the manufacturer. There is a growing rift between industrial users and university users, and the manufacturers are naturally more in tune with the needs of industrial users. Furthermore, each active university center tends to develop its own ideas, which frequently are not compatible with those of other centers.

Professor Macintyre commented on the value of operating the center with a small number of quite different systems which can be switched in and out, each having its special strong point, rather than with a single, universal system for all classes of users. Professor Pople pointed out the need for standardization of systems, so that users in the same field at different universities can reproduce each other's results.

Dr. Clementi raised the question of whether a specific computer program developed through a government grant can be copyrighted. The general impression was that it could not be; the government agency would require that the program be in the public domain. Professor Shull mentioned that the systems programs developed by Indiana University have been copyrighted to prevent their misuse; no royalty is demanded for their use.

The question of exchange of information about computer hardware[4] was raised by Professor Shull. It was the consensus that no media for the exchange of such information among chemists now exist, but that the need was great in view of the rapid proliferation of new equipment.

Satellite operation came in for considerable discussion, but no specific conclusions were reached. Professor Hagstrom felt that the design and maintenance of satellite hardware was a major problem for the user. He mentioned a sophisticated satellite operation in use at California Institute of Technology

[4]In computer terminology, "hardware" covers the mechanical, electrical, magnetic, and electronic devices from which a computer and its accessory equipment are constructed. "Software" denotes computer programs and collections thereof, including compilers and assemblers which can be used to generate other programs; it includes also executive and diagnostic programs used to schedule and test other programs.

for monitoring nerve impulses; the satellites are relatively simple in design, mission adapted, and tied up during any given experiment. He mentioned a difficulty in getting the manufacturer of a leased central computer to provide interfaces for specialized satellite installations; there usually is no difficulty when the computer is a purchased one.

Professor Matsen raised for discussion the general question of prejudice against computation, found on the part of many scientists. He attributed this to two sources: a feeling that a computer solution is neither as general nor as elegant as an analytical solution, and the fact that many second-rate problems have been put on computers. Now that computing is becoming more widespread and highly expensive, those chemists who are leading the demand for better computing facilities are faced with the necessity of justifying the worth of computational methods to science and to society. To emphasize the seriousness of the problem, Professor Matsen quoted recent remarks of Professor Peter Debye's, depreciating computation, in an interview published in the September 1965 issue of International Science and Technology.[5] He mentioned other examples of disparaging comments heard from influential scientists on the value of numerical computation, and expressed concern as to how such attitudes affect the funding of research involving computation.

Professor Parr discounted the significance of such remarks, and felt that the new generation of scientists of all kinds are accustomed to using computers when they need them. Professor Wahl pointed out how numerical calculations on model systems frequently provide feedback necessary in the development of the model, so that numerical values and properties of the actual system not directly accessible through experiment can be derived through computational means. Professor Shull expressed concern over the slowness with which the budget for the computer program of the National Science Foundation had been increasing over the years, and felt that if scientists influential in top-level decisions were insensitive to computational needs, there could be a seriously detrimental effect on all fields dependent on modern computation. Professor Gwinn suggested that in the teaching of quantum chemistry attention should be paid to the power and utility of accurate numerical solutions, wherever such solutions are needed and can be obtained. Professor DeTar emphasized the growing complexity and increased sophistication of experimental research, whether in chemistry, physics, or biology, and pointed out that problems not otherwise even considered can now be attacked by means of computers; he cited as a general example the kinetics of chemical reactions involving complex mechanisms. Dr. Swalen felt that misuse of computers on poorly conceived computations was a potential source of difficulty in relations with other scientists. Varying degrees of concern were expressed by other participants over proper recognition of the value of modern computational methods, though no definite consensus could be reached on an appropriate course of action.

[5] "Density of Discovery. Thinking Ahead with Peter Debye," International Science and Technology, September 1965, p. 55.

IV
PUBLICATION PROBLEMS

The chairman for this part of the conference was Professor Berni J. Alder, and serving with him on the review panel were Professor D. F. DeTar, Professor Walter Macintyre, and Professor David Shoemaker.

Professor Alder led off the discussion by commenting on the lack of publication media for articles dealing specifically with computational aspects of theory and experimentation in chemistry and physics. He then described plans for a new Journal of Computational Physics, to be issued quarterly beginning January 1, 1966. This publication is an outgrowth of a series of (annual) books entitled "Methods in Computational Physics," which for some years have presented important computational material, consisting partly of declassified projects from certain Atomic Energy Commission work, such as in hydrodynamics, but covering all fields of physics. Each book is devoted to a specified area. Pressure had come from a number of investigators who wished to submit original manuscripts in this series, so the editors decided to explore the feasibility of founding a journal. The Journal of Mathematical Physics had become too specialized in mathematics to serve the purpose, whereas the Review of Scientific Instruments, another possible medium, was too diluted with other material. The question had been discussed with the American Institute of Physics, but without success. Present plans call for publication on a commercial basis by Academic Press. An effort will be made to use fully automated printing, and there will be no page charge to authors. The subscription charge to the individual subscriber ($10.00 per year) will be initially lower than to institutional subscribers, including libraries, for a trial period of three years. The first few issues will contain a number of invited papers.

The members of the Editorial Board are:

Editors:

Berni J. Alder, Theoretical Physics Division, Lawrence Radiation Laboratory
Sidney Fernbach, Computation Division, Lawrence Radiation Laboratory
Manuel Rotenberg, University of California, San Diego

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Zevi W. Salsburg, Department of Chemistry, Rice University
Philip D. Thompson, National Center for Atmospheric Research
George H. Vineyard, Brookhaven National Laboratory
M. H. Wrubel, Department of Astronomy, Indiana University

The editorial policy has been stated as follows:

The policy of the Journal of Computational Physics is to publish articles concerning computational techniques developed in the solution of problems describing physical phenomena. The emphasis in this journal is more on the techniques than on the results, that is, on the techniques evolved in the numerical solution of mathematical equations as well as in automated data reduction. These techniques need not necessarily be proved to be mathematically rigorous, but a practical demonstration is desirable.

By publishing the detailed description of computational techniques, it is hoped that even better techniques will be developed, that computers will be used more effectively, and that further analytical developments will be encouraged. Furthermore, the policy of publishing on any subject of interest to the physical sciences should lead to a fruitful interchange of ideas in the numerical solution of related problems in various branches of science.

In response to questions, Professor Alder stated that Communications of the Association for Computing Machinery (ACM) was not sufficiently oriented toward physics to serve the purpose of the new Journal, that the Journal would find it generally impractical to publish detailed computer programs, that letters and short notes would be acceptable, that the main interest was in methods of computation, and that many details of policy still remain to be worked out on the basis of experience.

Professor Shull commented on QCPE (Quantum Chemistry Program Exchange), an informal serial newsletter now in its third year, prepared and circulated by the Chemistry Department of Indiana University with financial support from the Directorate of Chemical Sciences, Air Force Office of Scientific Research. This periodical announces computer programs that have been sent in by contributors and are available on request from the Exchange. The programs are tested to make sure that they will reproduce the stated output, but otherwise are not screened or edited. The supporting documentation is distributed to anyone asking for it. However, to introduce critical screening and refereeing in a uniform way, as in a formal journal, would be beyond the capacity of the present effort. Professor Shull expressed doubt whether computer programs should ever be published in detail in permanent form.

Professor DeTar described plans for the publication in book form by W. A. Benjamin, Inc., of complete computer programs in the field of chemistry. He made the point that just as modern chemists do not all design their own instruments, so they should not all be expected to design their own computer programs. The programs under consideration for the proposed series of volumes are fairly general ones that have been tested and found applicable in stable, finished form to various kinds of routine chemical measurements and theoretical calculations, such as the interpretation of NMR spectra, the handling of chemical kinetics data, and basic quantum chemical calculations. The publisher has agreed to make tapes of the programs available at cost, through a data-processing concern. Preparation of the tapes will be supervised by the editorial board, presently consisting of Professor DeTar, Professor Kenneth B. Wiberg, and Professor Andrew Streitwieser. The project differs in purpose from QCPE in that the programs will be refereed on the basis of their general and lasting interest to chemistry.

Professor Pople commented on the value of having programs in published form. The publication affords the user general familiarity with what has been done and what is available, aside from specific use of the published material. Professor Alder felt it would be sufficient if the author of a program were merely to announce that the program was available; he felt that the lifetime of a typical active computer program was short compared with the time required for publication. Professor DeTar remarked that programs in the experimental stage were not under consideration for the series of volumes he was editing; the objective, rather, was to assemble programs for well-established calculations that nevertheless have to be repeated routinely.

There was spirited discussion of how best to exchange information concerning computer programs. Professor Shull thought he had reason to believe that QCPE was performing a needed service in announcing and making available any contributed program that passed the test of performing what the authors claimed. The number of requests for programs had been in the hundreds during the past two years. The programs were supplied at no cost to those requesting them, and the entire operation was supported by a modest grant from AFOSR. He felt that the method was flexible, provided the user with what he individually wanted, relieved the author of supplying programs, and was far less costly than any method based on publication of the programs. The number of users for any one program is likely to be small; few programs are widely used, and most of them have short lives. Professor Shull raised the question whether such a service would be useful in other fields besides quantum chemistry, such as spectroscopy and x-ray crystallography. Professor DeTar favored a comprehensive program exchange to cover chemistry generally, and expressed the belief that the contemplated series of published programs would not cover many of the programs available and desirable for exchange purposes. He viewed program publication and program exchange as complementary projects serving different needs.

Professor Shoemaker mentioned that the crystallographers, through a Commission on Crystallographic Computing of the International Union of Crystallography, of which he had been chairman, had gone so far as to circulate a listing of available crystallographic computer programs, so that individuals interested in acquiring programs could write directly to the authors. This scheme had put the burden of supplying programs on the authors, but had worked rather well. He saw merit in expanding the QCPE type of operation to include crystallographic programs, if feasible. He also raised the question of whether the American Documentation Institute (ADI), which has been handling information on microfilm, might expand its services to include the storage and reproduction of information on magnetic tape. Dr. Tate, who is a member of the executive board of ADI, thought that this could be done without much difficulty, and undertook to explore the question with ADI.

Professor Shull noted that as computer facilities are updated, the older computers are inherited by other users. One of the goals of QCPE had been to serve as a repository for programs no longer useful with the newer equipment, so that inheritors of the older equipment could take advantage of them. He had seen no evidence, however, that such program exchange had actually been effected through QCPE.

In reply to further questions concerning Professor Shull's stand against publishing programs, he reiterated his belief that publication is an expensive way of accomplishing something attainable by a less costly method. The transitory nature of computer programs, in view of the exceedingly rapid pace of computer developments, is all the more reason not to give them permanent form and shelf space.

It was suggested that a possible role for an NRC committee on uses of computers in chemistry might be to develop a general computer-program exchange for chemistry, similar in function to QCPE.

V EDUCATIONAL PROBLEMS

The chairman for the session was Professor Peter G. Lykos, and serving with him on the review panel were Dr. Franklin Prosser, Professor Donald H. Secrest, and Professor Arnold C. Wahl.

Professor Lykos opened the discussion by describing the experiences growing out of his introduction of the use of a computer in a laboratory exercise in undergraduate physical chemistry at Illinois Institute of Technology. He had devoted the first half of one six-hour laboratory period to programming in machine language for the Univac 1105, and the students had then proceeded to write a program for a least-squares, linear treatment of their vapor-pressure data, experimentally determined for a pure liquid as a function of temperature. Out of this beginning had grown three flourishing developments: (1) a course for high school students and their teachers throughout the Chicago area; (2) a general one-credit introductory course on computer use for undergraduates; (3) a sequence of undergraduate courses providing some degree of specialization in uses of computers (in connection with a major program pursued in one of the traditional disciplines).

1. THE HIGH SCHOOL PROGRAM

Three years ago Professor Lykos, invited to address a computer club in a Chicago high school, had chosen to offer the students the same experience he had given routinely to his students in physical chemistry. These high school students turned out to be highly motivated and quite capable of coping with the material. As a consequence, he recommended to the IIT administration that the same kind of experience be offered on a wider basis in the Chicago area, using the IBM 1401 computer. In response to letters addressed to 200 high schools, nearly 700 applications were received for a program intended initially to accommodate 150 students. The program has since continued to grow in size and scope until at present four courses are being offered regularly on Saturdays for high school students in the greater Chicago area. Over 6,000 students have now participated.

The first of the courses consists in three full days of introduction to FORTRAN. The students are then screened by examination, and, depending on their performance, are invited to participate in subsequent phases of the program. The second course is five half-days of introduction to a symbolic machine-oriented language, enabling the student to communicate in a direct manner with the computer (IBM 1620). In the third course, ten half-days of computer applications involve model building, simulation, numerical analysis, matrices, critical path method, and other selected topics. The fourth course, introduced this year, associates the student for a semester with a professional adviser, who tutors and counsels him on the working out of a special project involving computation.

The high school teachers sought a similar experience, so, in the Fall of 1963, an additional workshop was set up for them. Teachers completing the workshop were invited to select up to 10 of their own high school students to take through the course themselves. At present, 70 teachers are participating in workshops of six full days, and over 500 teachers have gone through the program. A set of 25 problems has been developed requiring little mathematical sophistication but offering, through selection, a range of programming experience. By the end of five days, these teachers are quite at home in using the computation center facilities, and on the sixth day are bringing in problems of their own to program.

Of particular interest, growing out of the teacher program, has been the discovery that high school teachers are only a subset of a larger group of professional people who feel that their lives are being touched by the computer and who wish to know more about it. Professors from the IIT staff have enrolled. An important factor in the success of these workshops is that they are self-contained; there is no homework. Apparently this feature is essential to a busy professional person.

The high schools are developing an interest in calling on the IIT computing facilities for assistance in their adminstrative and educational programs. The Illinois Bell Telephone Company is willing to solicit connections and set up teletype lines whereby remote stations can hook into the IIT facilities. There are about 500 high schools with one million students within a radius of 100 miles of IIT. As an estimate, these might be accommodated with two IBM 360/67's and five hundred consoles, at a cost of $40 million for a five-year program (including a building and staff, and support for one full-time-equivalent professional in each of the 500 high schools).

2. INTRODUCTORY COURSE FOR UNDERGRADUATES

The experience with the physical chemistry students demonstrated how successfully the use of the computer could be introduced in a disciplinary context, where its value was manifest. Accordingly, a recommendation was made to the IIT administration that a one-semester-hour course in computing be offered in the junior year to teach elementary programming and numerical techniques. Thereafter, the students would have available to them the computational facilities, free of charge, to support them in their course work, the only restriction being authorization by an officer of instruction. The reason for the restriction was two-fold: (1) to elicit the interest of the teaching staff, and (2) to put a damper on those students who otherwise might let their enthusiasm for the computer run away with their discrimination in its use.

A number of key punches were rented and distributed over the campus, including the undergraduate dormitories, to make clear to the students that the computing equipment was indeed meant for their use. Ultimately, an IBM 7040 was procured with the aid of a grant from the National Science Foundation. The Computation Center itself serves the entire academic and non-academic IIT community. It has four distinct activities: operations, systems development, applications to research and teaching, and applications to school administration.

One interesting development was that in the initial phase of operation with the 7040, elementary problems that had previously been in use on the 1620 took as long in real time (two minutes or so) as on the 1620. This turned out to be due in part to input/output errors made by the students when they first started out but mainly to inefficiencies in IBM's FORTRAN. A student-oriented compiler called IITRAN was created by William S. Worley, Jr., of the IIT Computation Center, with which the 7040 computer time per problem (in the set of 25 test problems previously mentioned) was cut to less than one second, at a cost of less than 10¢ per problem. The students now buy IITRAN punched identification cards at 25¢ a piece, good for a time limit of 12 seconds access to the computer. The student probably uses on the average about six seconds per problem. This pay-as-you-go plan is a simply administered and effective departure from the usual, more formidable, procedure of opening an account and receiving bills based on internal accounting. The IIT program has thus demonstrated that a properly oriented system can take advantage of the power of modern large hardware and provide computer support for education at a nominal cost. Furthermore, it has demonstrated that people can be trained at entirely different stages of education to use a computer, so that the complexity and cost of these machines is no barrier to their widespread use in support of educational goals.

3. UNDERGRADUATE SPECIALIZATION IN COMPUTATION

There appears to be a severe shortage of people thoroughly knowledgeable in computational methods, at the level of professional competence in computational science. The IIT Computation Center has attempted to cope with the problem by the creation of a sequence of courses available to undergraduates.

The first course is a one-semester-hour introduction to computers, intended primarily for liberal arts freshmen. It covers the machine-language structure of computers, FORTRAN-type language, and an introduction to programming, enabling the student to use the Computation Center facilities. He will have used an algebraic compiler at least once, and he will have had some general discussion about classes of computers and their characteristics.

At the junior level, for scientists and engineers, there is a course on introduction to the digital computer. This consolidates previous program experience and involves the student in numerical methods of a non-trivial kind, such as have importance enhanced by the advent of the computer. It introduces the student also to a general-purpose systems simulator, in order to develop his thinking in terms of model building on the computer, especially for systems characterized by properties that cannot be predetermined.

Three courses follow. One introduces the student to basic techniques of programming and the logical description (using the Iverson notation) of a complex assemblage of hardware and software. A second is concerned with computer languages and how the supporting translators are created. The third deals with system analysis and simulation. The undergraduate sequence permits a student majoring in a traditional discipline to develop a fairly strong minor in what can be called Computer Science.

At the graduate level, there are presently two courses. One is on the design and use of large-scale computers. The other, offered as a sequel to an introductory course given by the Language Department, is concerned with computer techniques of information storage and retrieval.

The September 1965 issue of Communications of the ACM describes preliminary recommendations of the ACM Curriculum Committee on Computer Science for a major program appropriate, when suitably augmented by material from the other disciplines, for a degree of Bachelor in Computer Science. The IIT Computation Center feels that an undergraduate program of this sort is the next greatest need to be filled.

Following his presentation, Professor Lykos invited comments from the conference participants. Professor Matsen felt that the applicability of the computer to sophisticated model building should be viewed as an important cultural element in the educational program, and proposed the need for an elementary course open to all undergraduates, whatever their field of interest. Dr. Swalen questioned the need for a special battery of courses in computer science, in view of the rapid obsolescence of knowledge; he favored a closer tie between training in the use of computers and a field of application, where the student would attain his major professional competence. Professor Lykos pointed out that obsolescence is a danger faced by engineering education generally, and that an intense study of the problem is under way by the American Society for Engineering Education. According to preliminary thinking, there would be no specialization in the first two or three years of the engineering curriculum, but instead, a combination of basic sciences and mathematics appropriate for all students.

Professor Shull asked whether a chemist could best learn computing in a chemistry course or in a computer science course. Dr. Swalen felt that a close tie with application was necessary, but that a separate course in computing of sufficient character (such as FORTRAN) could be given in several weeks. Professor DeTar questioned the extent to which computers are being used in physical chemistry courses. Professor Shull noted that the computer was not yet being used appreciably for this purpose at Indiana University, but would be, as soon as a satellite could be installed in the chemistry building. The lack of a satellite is the main barrier. A computer is presently used in the physical chemistry courses at the University of California, Berkeley, and at Harvard University, and its use is offered as an option at the University of Colorado. California Institute of Technology is using one in its introductory physics course. Professor Macintyre felt that computer instruction for undergraduates has to be followed up quickly by actual experience in the use of a computer for real problems, preferably problems of a new type not approachable except with a computer. Professor Lykos expressed the view that if elementary instruction spreads throughout the high schools, undergraduates may arrive seeking out the computer. He thought it important to motivation that the computational facilities be wide open to all qualified undergraduates. He further noted that in the physical chemistry experiment previously described the students were first directed to fit a few of their points with a straight line using conventional least-squares hand calculation; then, as a class exercise, they developed a computer program for the purpose and found that all the points obtained by the entire class could be fitted in a few seconds. The object lesson was thus brought home.

There was considerable discussion of the kind of experience needed in computer use by prospective chemists, and of how to bring this experience into the educational program. Professor Gwinn made the point that in a large university it was not feasible to give many undergraduates unlimited access to the computer because the facilities would soon be tied up. He felt, however, that a most important experience in the undergraduate physical chemistry or instrumentation course was an exercise involving direct data reduction—the signals developed by some measuring device should be digitized and transmitted directly to a digital computer for processing. Professor Secrest felt that programming did not present a real problem, but that the undergraduates' deficiency in numerical analysis did; he suggested that training in basic numerical methods at an early stage would have more lasting value than training in programming. Professor Macintyre thought that the entire mathematical training of chemists needed study and revision, and that the American Chemical Society's recommendations on undergraduate training in chemistry were deficient in this respect. Professor Shull felt that a more fundamental and difficult problem was how chemists could effectively influence the mathematics program. Professor Lykos thought that the threat of an independent department of computer science was one means of bringing pressure to bear on unresponsive mathematics departments.

Professor Lykos raised also the question of short courses in computer use, such as the short courses developed in other specialized subjects by the

American Chemical Society (offered recently in connection with national meetings of the Society).[6] Professor Shoemaker mentioned the short courses of one or two weeks duration offered at Massachusetts Institute of Technology several times a year, preceding or following one of the regular semesters. They are designed to introduce newcomers (including graduate students and staff members) to the computer, and take up programming, FORTRAN, machine language, time sharing, and specific uses of the facilities locally available; numerical analysis, which the students are presumed to know, is not included. Professor Secrest stated that the Chemistry Department at the University of Illinois offers a two or three-week course each semester and summer, with emphasis on machine language. Professor Lykos thought that the universities appear to be well prepared to introduce their students to use of the computer, but that they reach only a small fraction of the interested chemists who could be reached by short courses at the ACS meetings. Lack of sophistication in numerical analysis and in general mathematics sets limits to what can be accomplished in a short course devoted to computer use. Professor Wahl expressed the hope that in such a course, established standard mathematical techniques for solving various specific types of problems could be mentioned by name, at least, particularly where the techniques are well documented and available.

Professor Lykos introduced another question, whether the possibilities of simulation techniques for educational purposes were sufficiently realized. Professor Alder mentioned an educational film on computers in which he was participating. He thought that the physicists had made considerably more progress in this area than the chemists. For example, he had seen an admirable motion picture, intended for high school seniors or college freshmen, demonstrating computer-generated one-dimensional solutions of Schrödinger's equation. He himself had used the oscilloscope output of the computer to simulate the effects of changes in equilibrium conditions on the chemical thermodynamic functions, effects difficult to demonstrate in any other perspicuous way. Professor Wahl noted that he had found oscilloscopic demonstration a valuable educational tool for describing chemical bonding processes in terms of molecular wave functions now available for computation. He thought that computers are beginning to create a whole new area of detailed information about the structures of molecules that has not been attainable in any other way. He envisioned the student's controlling the computer (on a time-sharing basis) to experiment with simulated model systems involving new, intuitively useful concepts not otherwise accessible. Professor Matsen pointed to chemical kinetics as a field where computer simulation would be particularly useful for analyzing complex situations. Professor DeTar mentioned that he had a program capable of conducting such an analysis for reaction mechanisms of any degree of complexity.

[6]An ACS Short Course on "Computer Programs in Chemical Research" was later announced to be offered at the University of Maryland Computer Science Center, August 27-28, 1966. Co-sponsored by the University of Maryland and by the Maryland and Washington Sections of the ACS, it was to be given by Professor DeLos F. DeTar and his associate, Carleton E. DeTar.

Professor Hagstrom raised a question concerning meaningful laboratory experiments controlled by the computer. He felt that automation can be carried too far, to the point where the student may have no idea of what the output numbers mean or how they are generated. Such experience can be particularly detrimental when he later finds himself in a laboratory environment where such facilities are not available. The student should have a hand in setting up the automation and getting the experimental equipment on line.

Professor Lykos stated as a general conclusion that computing facilities are now becoming conveniently and easily available at most universities, and that chemists must try to learn how such convenient and easy access to these facilities can improve the teaching of chemistry. He pointed out also how in those institutions where graduate work is going on and where research is being conducted at the frontiers of knowledge progress has clearly been made in developing uses for computers. Such progress redounds to the advantage of the undergraduate educational program.

Professor Hagstrom made a further point that two semester-hours of programming should be considered a bare minimum requirement for undergraduates. He felt that the introduction of such a requirement should be recognized as a sound educational principle, on a par with other required subjects. The merit of this proposition was discussed by several of the conference participants. There appeared to be a consensus that the introduction of computers had actually proceeded much faster than other changes in the traditional chemistry curriculum, and that a keen awareness and motivation was developing on the part of students to make use of available computing facilities.

VI
CONCLUSIONS AND RECOMMENDATIONS

The closing session, with Professor Shull presiding, was devoted to discussion of the conclusions and recommendations prepared by the panels that reviewed the four areas considered. The following summary represents a consensus of the conference.

1. FINANCING CONCLUSIONS AND RECOMMENDATIONS

(1) It is in the interest of chemists who use computers to coordinate their computing plans, in order (a) to provide economy in the use of available funds, (b) to provide continuous pressure on suppliers of computer hardware and software to satisfy the needs of chemists, and (c) to provide a focus for presenting dollar computing needs of chemists to prospective sources of support. To this end, we recommend the formation of an appropriate standing committee on the uses of computers in chemistry, for example in the Division of Chemistry and Chemical Technology of the National Research Council.

(2) Valuable specific advances in chemistry, pure and applied, are now being made through the use of computers. The uses range from ordinary small scientific calculations through large scientific calculations otherwise impossible, and encompass both laboratory automation and the mechanized handling of chemical information. We, accordingly, endorse the recommendation of the Academy Committee for the Survey of Chemistry[7] (the Westheimer Committee) that the universities be urged to ensure that adequate central computer facilities are available, and that the funding agencies accept substantial

[7] <u>Chemistry: Opportunities and Needs</u>, National Academy of Sciences - National Research Council Publication 1292, issued November 28, 1965.

charges for computer time as normal expeditures for chemical research. We endorse also the increase in financial support for computer time recommended by the Committee.

(3) Optimal use of computers entails maximum use of available computing time. It is of the greatest importance to establish university and government policies and auditing practices that encourage maximum use. In particular, auditing practices and policies for computer use should be designed to encourage the elimination of idle computing facilities. This is an urgent problem for early action by the recommended standing committee.

(4) Sharing of computing knowledge and experience of all kinds, from hardware through programs and systems, is economically desirable. Such sharing should be encouraged, and steps taken to promote it. Further study is needed on the development of compatible higher languages as they affect such sharing.

(5) The possible formation and support of regional, national, or international computer centers should be studied. It is not yet clear whether these combined facilities are economical or efficient, but the possibility that they might be desirable future developments should not be ignored.

2. CONCLUSIONS AND RECOMMENDATIONS ON COMPUTING CENTER ORGANIZATION, SATELLITES, AND RESEARCH

(1) Management: The management of a university computer center should be user oriented. It is essential that it work effectively with a strong faculty committee. The committee should be composed primarily of men who themselves are users and who are knowledgeable in various aspects of computing.

A staff of good systems programmers is essential for efficient operation. It is most important that some programmers be hardware oriented, and that their programs utilize the most advantageous features of the type of machine and its particular configuration. It should also be realized that a large staff of poor programmers can be a liability.

(2) Compatibility: Computing centers should have as much compatibility as possible. Each system will be different and systems programs will be different from one center to the other. It is unlikely that it will ever be possible or useful to attempt to transfer programs or sub-programs in machine language, but it is important that the higher source languages, such as ALGOL and FORTRAN, should each be compatible down to the sub-program level. However, it is extremely important that progress not be stifled for the sake of compatibility. The recommended standing committee should undertake a continuing study to establish desirable compatibility consistent with proper encouragement of individuality.

(3) Library: A good program library is important for an efficient system. It should be extensive and user oriented (that is, adapted to the problems of computer users and in a form ready and easy to use). The use of tape units for library storage is undesirable because if many programs are made available, then each tape search becomes excessively long. The program

library should therefore be stored on a disc file or comparable random-access device to permit ready availability of many sub-routines.

(4) Satellites: It is quite likely that the Chemistry Departments will have increasing numbers of problems involving analog/digital conversion. These problems should be resolved on a department-wide basis. Careful thought should be given before purchase of individual digitizing equipment. At present it may be more economical to have a single A/D converter with a multiplexer to convert various instruments. Satellite computers are useful also for input/output decentralization. If a department has a small computer for remote operation and on-line instrumentation, I/O devices may be added to make the satellite an I/O station for the central computer, an arrangement having many advantages. For example, if a long program were running on the central computer, producing intermediate output, and if it were not operating properly, the investigator by simply pushing a button at the satellite station could delete its subsequent execution.

I/O equipment is expensive at present and may cost as much as the satellite computer itself, but its addition to the satellite would not degrade the operation of the satellite for data reduction and communication to the Computing Center. It is recommended that chemistry departments make active plans for development of this category of computing facilities and that government granting agencies should take into account the almost inevitable rapidly increasing financial needs in this area.

3. CONCLUSIONS AND RECOMMENDATIONS ON PUBLICATION

(1) Program exchange facilities should be made available to specialists in each field. These facilities may be patterned after present, successfully operating exchanges, or new exchange techniques may have to be explored.

(2) The American Documentation Institute should be encouraged to accept adequately documented programs for their permanent files, the programs themselves to be filed in magnetic tape or disk-pack form.

(3) Editors of journals in individual fields and disciplines should be encouraged to examine the adequacy of references to computers and programs in their published papers. A major publication medium in each field should be encouraged to accept program abstracts and references to availability of programs submitted to ADI or other exchange facilities.

(4) The foregoing problems of program exchange and their extension to international science circles form suitable subjects for further investigation by the recommended standing committee.

4. CONCLUSIONS AND RECOMMENDATIONS ON EDUCATIONAL PROBLEMS

The rapid proliferation of the computer has created an educational vacuum. There is a need to introduce the computer as part of a general education program in order that people might know what these devices are, how they operate, and how they are affecting our society. There is a need to determine how the impact of the computer should affect chemistry curricula, and, in addition, a need to evolve appropriate programs of continuing education for the professional chemist.

Discussion brought out explicitly the following points:

(1) The computer is now readily available. There should no longer be a barrier to introduction of computers in the educational process at a feasible cost.

(2) There is a general need for training in basic elements of what a computer is and how it operates.

(3) There is a need for increased awareness of the power of numerical methods as well as a need for explicit instruction in their use.

(4) Computer-oriented problems should be incorporated in the chemistry curriculum.

(5) The use of on-line data-processing techniques is hampered by lack of training and lack of coordination in educational efforts.

(6) Teaching aids should be developed utilizing the simulation and display of abstract concepts such as chemical binding, evolution of a kinetic ensemble, and generation of thermodynamic functions.

(7) Model building techniques should be developed and utilized.

(8) Curricular materials are needed to support these educational ventures.

(9) Programs in continuing education should be encouraged. Within universities, apparently, such programs are already underway at the algebraic-compiler programming level. For the professional chemist, the ACS-sponsored workshops or related techniques should be encouraged.

(10) Information processing and retrieval in chemistry should be brought more closely to the operational level, particularly at educational institutions.

APPENDIX

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