Planning the Proposed National Resource for Computation in Chemistry†

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Received June 11, 1975

In response to interest expressed in the possibility of federal support for a National Resource for Computation in Chemistry (a user-oriented center dedicated to solving important chemical problems for which the needed computational technology exists, or could be developed, but is now inaccessible to the majority of well-qualified investigators), a study has been conducted and a report prepared by a committee commissioned by the National Academy of Sciences to explore in detail questions relating to the facilities, accessibility, and site requirements for such a resource, the control of its scientific policy, the management, the initial level of funding, and the growth rate. The conclusions reached in this study are outlined, and attention is called to a forthcoming symposium at which they will be reviewed and further discussed.

In March 1974, the National Academy of Sciences (NAS) published a report[1] prepared with support from the National Science Foundation (NSF) by a study group chaired by Kenneth B. Wiberg. This study was the culmination of a series of earlier discussions and conferences on problems relating to the impact of the electronic digital computer on the conduct of chemical research, focused particularly on theoretical chemistry. The Wiberg study showed, however, that the needs extended to many areas of chemistry, including especially applications of theoretical chemistry to the design and interpretation of experimental investigations. Attention was directed, therefore, to the feasibility and desirability of a national computing center that would include personnel and facilities dedicated to solving important chemical problems generally for which the necessary computational technology existed, or could be developed, but was not accessible to the majority of well-qualified investigators.

The two-year study was widely publicized in the chemical community, and approximately 50 individuals from various areas of chemistry, computer science, and research administration directly participated in it. It led to the following recommendations:

"1. We recommend the establishment, as a national resource, of a computational center with facilities and personnel dedicated to advancing chemistry and related sciences through widespread, innovative, and intensive use of high-speed computational equipment. This mission is to be accomplished by making appropriate facilities available to a wide group of scientists, by providing and developing software to expedite and upgrade computer use, by encouraging and supporting research efforts to build new and more effective computational methods, and by carrying out an informational and educational program to bring the benefits created through the center to the widest possible scientific public.

2. We recommend that a committee responsible to an appropriate contracting organization (perhaps the National Academy of Sciences) be commissioned to bring this national resource into being."

Public discussion of the questions at issue was engaged through a symposium sponsored by the new ACS Division of Computers in Chemistry at the September 1974, National Meeting of the American Chemical Society in Atlantic City. The symposium, in which members of the NAS study group participated, was well attended and evoked favorable comment.

Meanwhile, in the spring of 1974, Los Alamos Scientific Laboratory had drafted a proposal to implement the recommendations of the Academy's report by utilizing the Laboratory's existing computational facilities. In June 1974, Argonne National Laboratory (ANL) and Argonne Universities Association (AUA) jointly sponsored a two-day workshop for interested individuals and representatives from interested organizations to develop recommendations that would provide a basis for writing proposals on behalf of ANL/AUA to establish such a national resource, hereafter designated as a National Resource for Computation in Chemistry (NRCC). Later, additional national laboratories supported by the Atomic Energy Commission (now ERDA) indicated a strong interest in making their expertise and facilities in computing available to this Resource, and drafted specific proposals concerning their roles in such an organization.

Consequently, on July 1, 1974, Dr. John M. Teem, Director of AEC's Division of Physical Research (now Assistant Administrator of the Energy Research and Development Administration), addressed a letter to Dr. Philip Handler, President of the NAS, in which he expressed the clear conviction of AEC that NRCC would serve important national goals. He requested that the Academy follow up the implications of the above recommendations. In particular, he requested detailed recommendations on the following questions:

1. The scientific policy and management of a proposed Resource.

2. The appropriate structure under whose auspices the Resource will operate. The organization should be capable of contracting in a responsible way for funds and overall management of the Resource, but it should be left sufficiently flexible to benefit from actual operating experience.

† Support for this project was provided by the National Science Foundation under Contract No. NSF-C310, Task Order 303, and by the U.S. Energy Research and Development Administration under Contract No. E(11-1)-2518.

Table I. Planning Committee for a National Resource for Computation in Chemistry

Jacob Bigeleisen (Chairman) University of Rochester	Howard E. Simmons E. I. du Pont de Nemours & Co., Inc.
Bruce Berne Columbia University	Lawrence C. Snyder Bell Telephone Laboratories, Inc.
F. Albert Cotton Texas A&M University	Kenneth B. Wiberg Yale University
Harold A. Scheraga Cornell University	W. Todd Wipke University of California, Santa Cruz
Staff	
William Spindel Staff Director	Martin A. Paul Consultant

3. The composition, size, and responsibilities of a policy board of prominent scientists drawn from a wide spectrum of interests in chemistry and computing, which will be responsible for ensuring that the Center's performance is directed in the interests of its scientific mission, with due consideration of scientific, social, and technological relevance to national needs.

4. The relationships of a policy board to the operating structure of the Resource, to the Atomic Energy Commission and possibly other Federal funding agencies, and to the user groups.

5. Desirable priorities, growth rate, and levels of funding and operation for the first several years.

6. The issue of charge structure as it relates to academic, government, and industrial users, to the health of regional and university computing centers, and to the general fiscal policies of the Atomic Energy Commission.

7. Facilities, access, and site requirements for such a Resource.

The NSF through its Assistant Director for Scientific Research, Dr. Edward C. Creutz, also expressed interest in such further detailed recommendations concerning NRCC.

In response to those requests Dr. Handler, with the approval of the Governing Board of the National Research Council (NRC), and upon recommendations from the Executive Committee of the Assembly of Mathematical and Physical Sciences, appointed a study committee to examine the questions raised. Its composition was selected to be broadly representative of all areas of chemistry with an interest in computation. The members are listed in Table I.

In carrying out the task assigned to this NAS–NRC Committee, the members as a whole, in smaller groups, and individually sought out the opinions of a wide spectrum of users and organizations interested in chemical computation. An extensive questionnaire was prepared requesting input information on computing hardware, communications, communications environment, software, system performance, rate structures, potential availability of hardware and software to NRCC, and administrative organization. This questionnaire was distributed to five ERDA laboratories and two university-based computation centers. After compilation of the returns, site visits were made to those six institutions that had responded in time to meet the Committee's operating schedule. A questionnaire concerning user needs was also distributed to approximately 500 college and university chemistry departments, 340 industrial research laboratories, and 600 individual research scientists who make extensive use of large computers.

During the study, the Committee learned of the existence of the Atlas Computer Laboratory operated by the Scientific Research Council of Great Britain. The Atlas Laboratory has played a role in Britain similar to that NRCC would play here and seems to have contributed much to the growth and quality of scientific research in several important areas of chemistry. The Director of Atlas met with members of the Committee to alert them to problems encountered by Atlas in its formative years.

The Committee has recently completed a report[2] which incorporates recommendations based in part on the responses to the questionnaires, in part on information gained from the site visits, and in part on information regarding the experiences of the Atlas Computer Laboratory. The report recommends that the National Resource for Computation in Chemistry (NRCC) be organized as a user-oriented facility, with hardware and personnel dedicated toward serving the needs of the broadest chemical community. The prime function of the Resource would be to give impetus to the solution of important chemical problems by providing enhanced computational opportunities and capabilities not presently available to individual research investigators throughout the nation.

The Committee envisions a centralized Resource serving the community by making available the potential to be derived from systematic, collaborative attention to software development, documentation, and improvements in computational procedures as applied to chemistry, as well as by making available the benefits of increased computational hardware. In view of the study's finding that facilities can be made available at existing federally supported laboratories, in a suitably rich scientific environment, NRCC can be established without an initial major capital investment. The Committee is convinced that the enhanced computational efficiency of such a National Resource will be more cost-effective than a further increase in the application of computers as presently practiced, and will in time make important contributions to the solution of important current national problems.

The report suggests ways in which NRCC could uniquely contribute to the enhancement of chemical research. The availability of a human resource of computer scientists and chemists working together would permit the systematic documentation, testing, and improving of existing programs, the development of more efficient algorithms, the generalization of computer programs for recurring chemical problems, the development of new computational methods, the design of specialized hardware, software, and languages particularly suited for the chemical community, and the establishment and updating of important data bases. A dedicated staff would bring about improvements in means of remotely accessing computers, including the possibility of efficiently utilizing a nation wide computer network for chemical research. The NRCC would stimulate interaction via workshops among groups and individuals sharing common computational interests to establish priorities for important and yet unsolved computational problems. Through visitor programs, it would bring together outstanding scientists at the NRCC for periods ranging from weeks to months so that they could interact with each other, and with the in-house staff.

In order that NRCC make a unique contribution to chemical computation and software development, it would require access to the most advanced and powerful computational equipment. A computer having the speed and memory of a CDC 7600, an IBM 370/195, or equivalent, is the minimum with which the NRCC could fulfill its function. Such equipment is now rarely available for chemical research, though its effectiveness has been demonstrated. In order to permit optimal participation by and benefits to chemists throughout the nation, communications facilities would need to be available for convenient and equitable remote access. A good scientific library readily available to staff, visitors, and users would be an essential part of the site requirement.

The Committee has recommended that the NRCC be established at one of the federally supported institutions where the needed major computational hardware is cur-

Table II. Proposed Personnel Levels

Personnel	Year		
	First	Second	Third
Scientific staff[a]	8	10	12
Visiting scientists[b]	2	4	6
Workshop leaders[b]	1	1.5	2
Joint appointments[b]	1	1	1
Consultants[b]	1	0.5	0.5
Secretarial–clerical	2	3	3
Total, man-years	15	20	24.5

[a] In-house chemists, computer scientists, programmers. [b] Full-time equivalent.

Table III. Budget Projections[a]

	Year		
	First	Second	Third
Staff[b]	440	575	700
Visiting scientists	80	160	240
Consultants	40	25	25
Workshops	50	75	100
Program review and Policy Boards	40	40	40
Equipment	150	200	200
Communications	100	100	100
Computing[c]	400	650	1000
Total	1300	1825	2405

[a] In thousands of 1974 dollars, including indirect costs estimated at 50% of salaries. [b] Includes joint appointments, postdoctorals, and all scientific, professional, administrative, secretarial, and clerical staff. [c] Calculated at $400/hr for a fourth-generation computer.

rently available for utilization by the NRCC during Phase I (first three years) of its operation.

The operation of NRCC presents some unique organizational problems. NRCC would be a relatively small organization committed to serving its external user community and would require identity and independence.

If it is to function effectively when folded into a large, existing organization, the management structure must be such as to nurture the growth and utilization of the Resource without detriment to the functioning of the host institution. Phase I should be capable of fostering the growth of the NRCC to Phase II, when the Resource could independently justify acquisition of its own major hardware, or when it would be desirable to affiliate with more than one federally supported institution. Operation under the management of two institutions would clearly be impossible.

A careful examination of the above considerations has led the Committee to conclude that NRCC must function in one of two modes: either as a division within a currently existing institution or as an independent nonprofit organization. In either case it must have a large degree of autonomy in establishing its scientific goals, priorities, and budget: its policy should be set by a cross section of individuals from the disciplines of chemistry, computational science, and research management. Cogent arguments are presented in the report that the needs of NRCC could best be met in the latter operational mode.

In either mode, NRCC would require a Policy Board which would establish scientific and management policies to be carried out by the Director. The latter would be the executive officer of the organization and would serve at the pleasure of the Policy Board. A Program Committee is necessary to review the scientific content of all major activities proposed to NRCC, and to recommend within guidelines established by the Policy Board relative priorities among competing programs and proposals. A Users Committee, representing outside users of the Resource as well as the in-house scientific staff, would provide feedback to match NRCC operations to user needs.

Personnel levels and budget projections recommended by the committee for the first three years of operation are presented in Tables II and III, respectively.

The Committee is cosponsoring jointly with the ACS Division of Computers in Chemistry a symposium on August 27, 1975, at the 170th meeting of the American Chemical Society in Chicago. A detailed program of the symposium is published elsewhere in this journal.

LITERATURE CITED

(1) A Study of a National Center for Computation in Chemistry, K. B. Wiberg et al. (National Academy of Sciences, Washington, D.C., March 1974). Available from Office of Chemistry and Chemical Technology, National Academy of Sciences, 2101 Constitution Ave., Washington, D.C. 20418.

(2) The Proposed National Resource for Computation in Chemistry: A User-Oriented Facility, J. Bigeleisen et al. (National Academy of Sciences, Washington, D.C. July 1975). Available from Office of Chemistry and Chemical Technology, National Academy of Sciences, Washington, D.C.