thing was a constant, it was eventually proved to be so. For example, a decade ago researchers were looking for efficient ways to find the median of a sequence of n numbers. At first a method was found that required $n \log \log n$ steps. This was succeeded by a method requiring $n \log \log \log n$ steps. Finally, a method was found that required a constant times n steps.

The new way of testing for primes also is intriguing to mathematicians because of the relation prime testing bears to the harder and more practical problem of factoring. Factoring and testing for primes are twin problems, says Pomerance, although it is not clear how to go from the first to the second. "To me, it [the new prime testing algorithm] gives evidence that it may be possible to find a polynomial time algorithm for factoring," says Graham.

If such a factoring algorithm could be discovered, it would have important implications for cryptography. A code which was developed by Adleman together with Ronald Rivest and Adi Shamir of MIT and which has attracted widespread interest is based on the problem of factoring a very large number. If factoring were somehow made easy, the code would be insecure. Adleman points out that the close relation between testing for primes and factoring illustrates that the difference between what is basic theoretical research and what is research that is directly applicable to cryptography can be quite small.

—GINA BARI KOLATA

Plug Pulled on Chemistry Computer Center

After an unusually brief trial, NSF and DOE decide to phase out chemists' first try at big science, the National Resource for Computation in Chemistry

The National Science Foundation (NSF) and the Department of Energy (DOE), joint sponsors of the National Resource for Computation in Chemistry (NRCC), have decided to terminate the not yet 3-year-old organization. The agencies have requested the Lawrence Berkeley Laboratory, home of the NRCC, to prepare a plan for phasing out the computational chemistry center by 30 September 1981. Although a compromise that would permit some NRCC activities to be continued has been proposed, agency officials say that doubts about the need for an NRCC coupled with tight budgets make it certain that the phase-out will occur as scheduled.

The NRCC was established to be a place where computational chemists could do things not possible in their own laboratories, such as solving problems requiring the use of a state-of-the-art supercomputer and developing and standardizing new software for community-wide use. Headed by William Lester, a quantum chemist on leave from IBM, and governed by a 12-person policy board comprising chemists of varied specialties, the NRCC has been a division of the Lawrence Berkeley Laboratory (LBL) since its birth in October 1977.* The organization has an annual budget of about $1.75 million.

When the NSF and DOE set up the NRCC, the agencies made its continued existence contingent on a favorable review after a 3-year trial period. Earlier this year, the agencies selected a ten-person review committee to evaluate the NRCC and make recommendations as to its future.† Under the chairmanship of William Goddard of the California Institute of Technology, the review committee this April reported serious shortcomings in the NRCC, but nonetheless recommended its continuation as an experiment for two additional years. According to Goddard, it was "too early to terminate the NRCC." To remedy the shortcomings, the committee also recommended some major changes in the organization that would eliminate all of the NRCC's professional staff and reduce its budget to just over $500,000 per year (excluding overhead).

Specifically, the review committee said that the NRCC should no longer fund grants for either internal or external computing time, should abandon its in-house software development activities, should leave all software distribution to the Quantum Chemistry Program Exchange at Indiana University, and should not buy its own central computer. On the positive side, the review committee said the NRCC should continue a series of highly successful workshops it has been holding and should establish an external postdoctoral program to replace in-house software development.

Perhaps in a gamble aimed at preserving a whole loaf rather than just a half, the LBL director, David Shirley, told NSF's Chemistry Advisory Committee that the skeleton NRCC that would remain if the review committee's recommendations were accepted would have little intellectual content and would not be appropriate for a scientific research laboratory. Shirley sketched out what he considered to be a minimum acceptable NRCC, one that would be comparable in staffing and scientific content to that existing now.

By the end of July, the two agencies had made up their minds. According to James Kane, Director of Basic Energy Sciences at DOE, the agencies construed the review committee's report as "a strong recommendation that the NRCC was not worth continuing as it was set up." Agency officials told *Science* that their already negative reading of the report and a unanimous recommendation by the NSF Chemistry Advisory Committee to close the NRCC combined with Shirley's position left them no choice but to terminate the experiment.

Shirley, Lester, and the NRCC policy board have since come up with a compromise proposal and have secured the blessings of Goddard's review committee, but Richard Nicholson, Director of NSF's Chemistry Division, and Elliot

*The NRCC policy board members are: Bruce Berne, Columbia University; Charles Bender, Lawrence Livermore Laboratory; Mary Good, Louisiana State University; William Guillory, University of Utah; James Ibers (chairman), Northwestern University; Carroll Johnson, Oak Ridge National Laboratory; Martin Karplus, Harvard University; Herbert Keller, California Institute of Technology (resigned in 1979); William Miller, University of California at Berkeley; John Pople, Carnegie-Mellon University; Anessur Rahman, Argonne National Laboratory; and Kenneth Wiberg, Yale University.

†Members of the review committee are: Allen Bard, University of Texas at Austin; John Brauman, Stanford University; William Busing, Oak Ridge National Laboratory; Marshall Fixman, Colorado State University; Willis Flygare, University of Illinois; William Goddard (chairman), California Institute of Technology; Dudley Herschbach, Harvard University; Daniel Kivelson, University of California at Los Angeles; Howard Simmons, DuPont; and John Tully, Bell Laboratories.

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Pierce, Director of Chemical Sciences at DOE, recently advised LBL that phase-out of the NRCC is still the official plan.

Once established, institutions tend to endure, not fall. What made the NRCC one of the few organizations that failed to survive its infancy? The answer seems to be that the NRCC never had the full support of the chemistry community, having been controversial from the day it was first discussed 15 years ago. In its short lifetime, the NRCC was never able to convince the skeptics of its merits. The funding agencies appeared to be quite concerned that the organization be fully accountable to the chemistry community as a whole and not just to computational chemists. One agency official admitted that "it is fair to say that the decision to discontinue the NRCC was as much due to attitudes within the chemistry community as it was to actual performance."

Most scientific research is carried out by individual investigators with their own research grants or contracts, in contrast with a few traditional "big science" disciplines such as high energy physics or astronomy that require centralized facilities and the sharing of resources. But in several fields of science an increasing amount of research is being carried out in a centralized fashion, as exemplified by the popularity of synchrotron radiation and neutron diffraction centers. While not turning their backs on such facilities, chemists may have rushed a little more slowly than workers in other disciplines to take advantage of these and other new tools. As chemists' first try at big science, the NRCC seems to have become the focus of much of the resentment stirred up when times change and long-accustomed habits have to follow.

The idea of a national center for computational chemistry was born in 1965 when Indiana University's Harrison Shull (now Provost at Rensselaer Polytechnic Institute) suggested it at a meeting of quantum chemists. In the ensuing decade a series of meetings held by committees of the National Academy of Sciences gradually refined the concept and came up with a specific proposal. Shull recalls that there was considerable division among chemists about the wisdom of establishing a centralized computational chemistry facility. Internal disagreement among members of the academy's committees and within NSF's Chemistry Advisory Committee reflected what was apparently a highly polarized chemistry community.

Opponents of the concept of a centralized facility tended to fall into two groups. The first consisted of those who genuinely felt that the objectives of computational chemists could be more efficiently met by traditional funding patterns, that is, by support of principal investigators. But a sizable contingent feared that the main effect of the establishment of such a center would be to drain funds away from the research pool and opposed the concept for that reason alone. The review committee established by NSF and DOE to evaluate the NRCC contained members drawn in part from both of these groups, as did the NRCC policy board itself.

Compounding the effect of this built-in ill will was the short review period. A 1975 academy study had recommended a 3-year trial, a so-called phase one, before a large commitment of funds for a permanent NRCC with its own large computer would be made. But the selection of Lester as NRCC director did not take place until the organization was already over 4 months old, and the DOE's lengthy budget preparation cycle required an evaluation to be completed 18 months ahead of any new budget outlays. Lester was able to get a 1-year extension, but the NRCC still had only 2 years between the time Lester arrived at Berkeley and the first visit of the review committee. Chemists sympathetic to the NRCC say that it did not have time to demonstrate its value to anyone except those who were already interested in the organization and that, with such a broad-based review committee, it was almost a matter of chance that the NRCC might have accomplished something of interest to any given member.

Measuring the NRCC's performance by the usual yardsticks was not possible because the principal products of the organization were tools for chemists to use in their research rather than research results in their own right, comments Edward Hayes of NSF. This unusual characteristic probably did not help the review committee to appreciate the NRCC in a time when tight budgets are causing the funding agencies to reject many otherwise meritorious proposals.

The NRCC's most highly praised activity, for example, was the running of a series of workshops that examined several areas of computational chemistry where well-defined problems existed. In one such workshop, a group of ten crystallographers gathered at Berkeley for a week to create a computer program that could be run on any large or medium-sized computer, provided that the data were cast in a standardized format. Because of idiosyncracies between one computer and another, most programs can be run on only one machine. Creating such "portable" programs is increasingly being considered an important activity because so much time is lost when researchers have to rewrite programs to be compatible with their own computers.

Software development is a similarly dull-sounding but nonetheless important activity. By collecting programs, making them easier to use, and incorporating them as building blocks in larger program systems, the NRCC could make readily available major software tools that would be prohibitively expensive to develop from scratch each time they were needed. But it is not the sort of product that is itself an advance in chemistry. Some staff members did start research projects of their own, but the press of running workshops and establishing a software library limited this kind of activity.

One way that the NRCC could have been the progenitor of new computational chemistry was by providing access to a state-of-the-art supercomputer. Prior to the mid-1970's, one of the biggest problems for computational chemists was access to such a machine. Since calculations of the electronic structure of molecules, the dynamics of collisions between molecules, and so on, required the use of such machines, the early discussions of a computational chemistry center focused on the issue of a central computer. By the time of NRCC's inauguration, however, chemists had discovered that advancing computer technology made it possible for them to accomplish almost all of their presently envisioned computational tasks on so-called super minicomputers costing about $250,000. Moreover, it was argued, the cost of using the super mini was less than that of using a central computer, such as the one at LBL. When NSF began approving requests to purchase the smaller machines, it satisfied very nicely chemists' natural inclinations to work in their own laboratories and reduced their interest in a large, centralized facility.

Further diluting their interest was the chemists' discovery that NRCC would not be able to provide large blocks of free or nearly free computer time at LBL, in part because of an Office of Management and Budget ruling requiring DOE laboratories to charge rates that reflect actual costs. The NRCC budget was not big enough to support many users at the mandated rates. Moreover, the technology of supercomputers was also advancing, and LBL's machine was no longer considered to be in the supercomputer class. And, finally, some chemists complained that LBL's computer was difficult to use. Since most

NRCC grantees did their computing at LBL, the organization was stuck with offering a machine that the few chemists needing a large computer did not want.

In a guest editorial in the May 1978 issue of the *Quantum Chemistry Program Exchange Newsletter* that chided the NRCC for not getting off to a faster start, Peter Lykos of the Illinois Institute of Technology wrote that to be continued into phase two, the NRCC "must convince the reviewers and cognizant bureaucrats that significant progress has been made in research on important problems in chemistry which likely would not have happened were it not for the NRCC." For a variety of reasons, mostly beyond its control, the NRCC was unable to do this. As a result, an experiment to see whether chemists from different specialties were at long last ready to cooperate on a large project of the type that would benefit other chemists as well as themselves is dying.

Chemists overseas may be doing better in this regard. In the United Kingdom, the Science Research Council's Daresbury Laboratory is making its supercomputer (a CRAY-1) available to participants in six SRC-sponsored projects that focus on different aspects of computational chemistry, each lasting 5 years. And, in Japan, Hitachi is building a huge scientific computer for delivery in 1983 to the Institute for Molecular Science in Okazaki (midway between Tokyo and Osaka). In accepting a few dozen super minicomputers scattered around the country in place of the NRCC, American chemists may have settled too cheaply.

—ARTHUR L. ROBINSON

An "NRCC" for Industrial Chemists?

The failure of academic chemists to keep afloat the National Resource for Computation in Chemistry (NRCC) is made doubly intriguing by the growing interest in computational chemistry within industry. A case in point is the Battelle Columbus Laboratories, where computational chemists are trying to drum up support for the idea of establishing an industrial counterpart to the NRCC.

In industry, the current fashion is a renewed emphasis on technology to revive a flagging productivity. Computational chemists, says Battelle's George Wolken, believe computers can help because of declining costs and advancing technology. For $250,000 one can now buy a computer that has the number-crunching capability of a machine costing $2 million to $3 million not so long ago. At the same time, a gradual accumulation of progress in computational technique is allowing theoretical chemists to calculate the properties of molecules and the reaction rates between molecules about as accurately as they can be measured experimentally. Since experiments can be expensive and time-consuming, especially when large numbers of molecules have to be screened for the chemical properties of interest for a given application, simulation by computer provides a way to get the needed data faster and at lower cost. And some experiments are either too dangerous or not even possible in principle, so that computer simulation provides the only way to obtain the required information.

For 25 years, computational chemists have been proclaiming that "quantum engineering is just around the corner." It was said that quantum chemistry calculations would reveal new reaction pathways that would enable chemists to develop more efficient processes for such things as synthesizing chemical feedstocks or pharmaceuticals. Now, according to Wolken, the statement is really true, and he points to several examples at Battelle to back him up. In one case, Battelle theorists were able to select from a group of closely related organic dye molecules those that might be the most promising for synthesis and characterization as candidate materials for solar energy collectors. Wolken says that the computer enabled chemists to pick out the desirable molecules in about one-hundredth the time it would have taken to do the same job by experiment. The computational task was to calculate the energy stored in a molecule when the absorption of light induced a conformational change.

Precisely what form an industrial "NRCC" would take is still undecided. Battelle is taking things slowly until the number of sponsoring companies and the depth of their interest can be determined. There are at least two directions in which a center could go. One would be to function as a cooperative, generic technology center of the type that the President called for last October in his industrial innovation initiatives. (The Senate recently passed a bill that would establish several such centers.) A generic technology center would initially be largely federally supported, with the financial responsibility gradually shifting toward the cooperating companies. At the other extreme, an industrial computational chemistry center could operate as part of Battelle's array of services to clients. Whereas the information gained in a generic technology center would be available to all concerned, results of sponsored research projects would be considered proprietary and restricted to the sponsor. At present, Battelle offers a service to its clients called technical inputs to planning. The use of computer modeling in chemistry is now part of the service.

Another role for a computational chemistry center at Battelle would be the third leg of a triad formed by the Quantum Chemistry Program Exchange at Indiana University, the American Chemical Society's Chemical Abstracts service, and Battelle. The program exchange was organized in 1962 for the purpose of collecting and distributing computer programs relating to quantum chemistry, although that restriction no longer holds. Chemical Abstracts, located near Battelle in Columbus, is a national resource for information storage and retrieval. Taken together, the services offered by the three centers could make a rather neat package.

Wolken mentions several recent developments that suggest that industrial support for a computational chemistry center could be found. Some corporations, notably DuPont with a group of four computational chemists, are setting up their own research programs. Others mounting some effort in computational chemistry include Kodak, American Cyanamid, and Dow Chemical. Moreover, the Quantum Chemistry Program Exchange has begun to help industry learn how to use available computer programs. It has already held one workshop for this purpose and a second is planned for next year. The problem for Battelle at this point is to decide what sort of industrial computational chemistry center it wants to establish and then find federal or industrial support to operate it.—A.L.R.

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