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BULLETIN

NRCC

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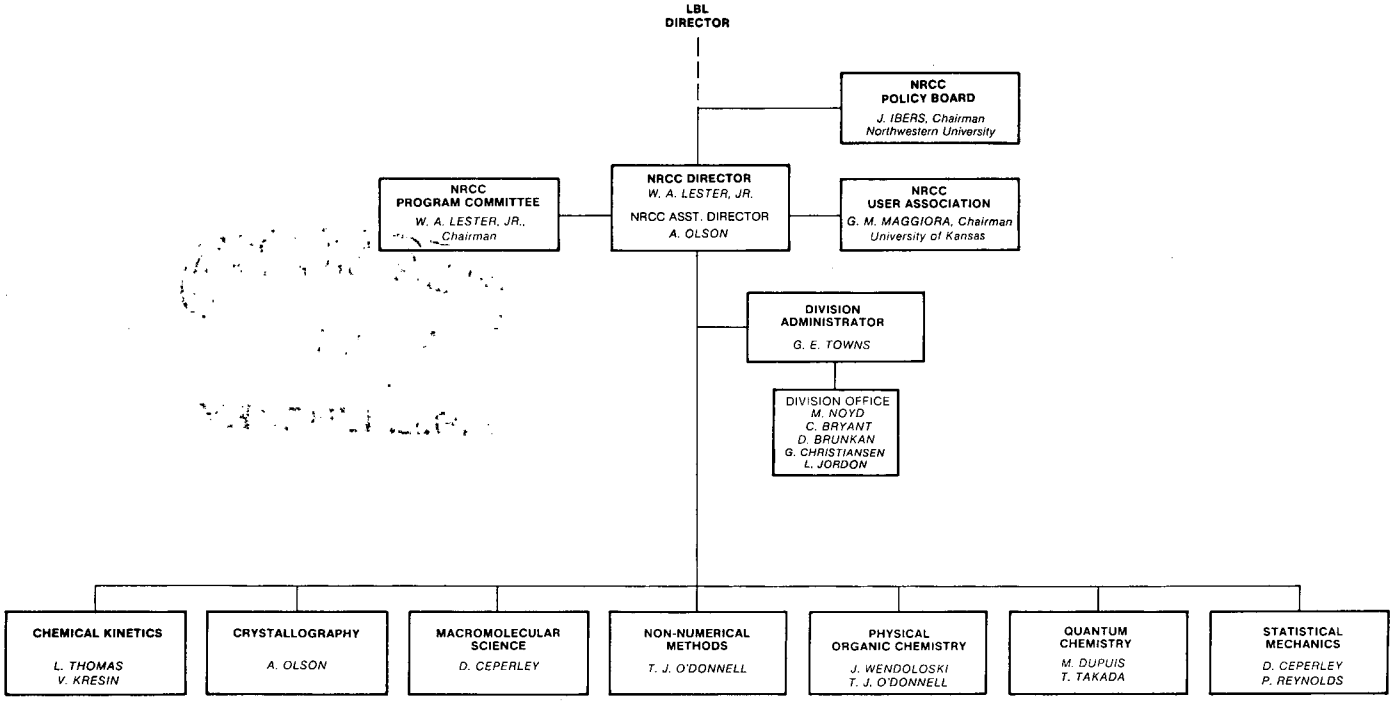

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Bulletin Editor,
John J. Wendoloski

ON THE CLOSING OF THE NRCC

William A. Lester, Jr.

Because the NRCC has been instructed to terminate operation on September 30, 1981 and this is the last NRCC Bulletin for the duration, I would like to reflect on our brief past as an organization, discuss our projected activities for the remaining months, and comment on the future of computational chemistry in this country.

First, I thank those people who have worked hard to build the NRCC, helped support it, and given it a record of accomplishment of which we can all be proud. Indeed, I feel quite strongly that, within the time and budget constraints set by the funding agencies, the NRCC has made remarkable progress in fulfilling the mission set out for it by the Wiberg and Bigeleison Committees. We of the NRCC take pride in the numerous workshops which we have held and in the various research and software development projects which they have spawned. We believe that the NRCC Software Library that we have developed, assembled, catalogued, and distributed is a significant contribution to the chemistry community. In addition, I feel that the outstanding record of the scientific staff both in service and in their own research activities should not go unrecognized. Certainly the burden of establishing the service component of the NRCC's activities (workshops, software library, user assistance) has made the research efforts of these computational chemists all the more impressive. Needless to say, I am deeply disappointed by the decision of the DOE and NSF to halt funding of the NRCC. I feel that, given the record of the NRCC during its short existence and the growing need within the chemical community for just this type of activity, the decision is an unfortunate and untimely one.

For the remaining period of its existence, we see two major objectives in the activities of the NRCC. First, we will direct every effort to see that NRCC-initiated projects will be brought to reasonable conclusion. These projects include NRCC sponsored research, publications, cooperative code generation projects, and workshops which have been scheduled to take place before close-down. In anticipation of the attrition that will occur in the coming months, we are in the process of transferring the NRCC Software Library distribution to other organizations. Most of our Library holdings will be forwarded to the Quantum Chemistry Program Exchange at Indiana University and to the National Energy Software Center at Argonne National Laboratory. The second major objective during this wind-down period will be the completion of research projects undertaken by the in-house scientific staff. It is clear that, to this point, the staff has put a disproportionate amount of effort into establishing a quality service component in the NRCC. In recent months, however, we had begun to move toward a better balance between service functions and research, and this thrust will be maintained. Thus, to the greatest extent possible within the constraints of the first stated objective, our remaining scientific staff will pursue research goals in computational chemistry.

Having the privilege of being a part of the nation's only center for computation in chemistry has given us a unique perspective from which to view a rapidly evolving and increasingly exciting symbiosis--that between scientific research and the computer. The nature of scientific information gathering, examination, and interpretation is changing dramatically. Computational technology is providing the tools that are effecting this transformation. Along with this changing environment have come new needs within the chemical community -- the need for information on, evaluation of, and access to rapidly advancing computational hardware; the need for access to ever expanding chemical data bases; the need for a means of sharing the increasing burden of software development; and the need for establishing standards to assure that developed software has a long, broadly useful lifetime independent of system hardware and software changes. Of course, individual research groups and organizations recognize what their computing needs are and will be; and they are taking individual steps to address those needs. Although a diversity of approaches to research level problems is healthy and should be encouraged, there are drawbacks inherent in a "cottage industry" attitude. There are an increasing number of computational "work-horse" tasks for which programs need not be reinvented or readapted at each individual laboratory or computer site. The amount of scientific manpower presently devoted to this duplication of effort is large, wasteful, and still growing. The need here is for a coherent national policy for this type of software development in the sciences, a policy that recognizes the costs and eases the burden on the individual investigator. Centralization seems to be the most cost-effective and equitable way of providing information on, evaluation of, and access to the newest computational equipment. As awareness of computational capability grows within the chemical community a wealth of research ideas will be generated. A mechanism for exploration must be available that depends upon more than happenstance of location or connection. Other countries have been addressing these problems and have committed proportionately far greater resources to solutions than has this country in the NRCC experiment. Notable are the Daresbury Collaborative Computing Projects in the United Kingdom and the Institute for Molecular Science in Japan. If the United States is to maintain state-of-the-art capability in the changing environment of scientific research it must not let its efforts to establish a coherent national policy on computational technology in chemistry end with the closing of the NRCC.

Chemical computing center will close

First effort in U.S. to provide chemists access to supercomputers will end because of critical review of its three-year performance

The National Resource for Computation in Chemistry (NRCC) will wind up its operations by Sept. 30, 1981, as instructed, despite last-ditch efforts by many computational chemists to save it.

The closing of NRCC, located at Lawrence Livermore Laboratory in Berkeley, Calif., ends the first effort of the U.S. chemical community to create a centralized research facility where chemists could gain access to equipment too costly for individual laboratories to buy and maintain. In the case of NRCC, the equipment was to have been computers big and fast enough to do massive calculations on problems at the forefront of research, backed by full-time scientific staff for consultation, program development, and in-house research.

The end came last July, when an interagency committee of the National Science Foundation and Department of Energy, the funding agencies, voted to cease support. As late as September, hope persisted that NRCC could be saved. The NRCC Users Association, headed by chemistry professor Gerald M. Maggiora of the University of Kansas, Lawrence, fired off a questionnaire to about 1200 persons to survey opinions about whether enough time had elapsed to evaluate NRCC's performance and in what form NRCC should continue.

In October, the users' association sent a report to NSF and DOE on responses of 230 people. The responses mostly supported continuation of NRCC for at least two more years in substantially its present form.

Actually, there never was any hope to keep NRCC open after the July committee vote. DOE's budgeting requirements forced officials there to make a final decision on funding at that time. NSF officials never had any intention of picking up NRCC's $2.2 million per year budget on their own.

The event that propelled NRCC toward the brink was an April report by a review committee, chaired by chemistry professor William Goddard of California Institute of Technology. This review of NRCC was built into the center's establishment in October 1977. The Goddard committee praised some NRCC activities, but concluded that some other activities could best be carried on outside the center. The committee's final recommendation was that NRCC should continue, shorn of its scientific staff and certain operations, running on a budget of $550,000 yearly.

The Goddard committee praised NRCC's workshop program in particular, in which chemists met to work out problems in specific areas. Subjects ranged from introducing chemists to computational chemistry to developing a portable program for crystallographic calculations that could be put onto almost any computer.

The workshops could continue beyond NRCC. James Kane, DOE director of basic energy sciences, says his group will look into continuing them under the aegis of Lawrence Berkeley Laboratory or elsewhere.

Kane says that DOE also would make grants for research that go along with the department's mission and that require use of a supercomputer. The Goddard committee had recommended that a smaller NRCC continue to make its CDC 7600 scientific computer available to chemists as well as give occasional access to a supercomputer. Supercomputers such as the Cray-1 and the soon-to-be-introduced CDC Cyber 205 not only function extremely rapidly in usual linear operations, but for added speed also, on instruction, select out certain numbers to process in parallel by the

Rise and fall of NRCC

1974	National Research Council study ("Wiberg committee") reports computation needs of theoretical and applied chemists exceed resources and recommends establishing a national chemical computational center.
1975	Second NRC study ("Bigeleisen committee"), commissioned by National Science Foundation and Energy Research & Development Administration (now incorporated into the Department of Energy), makes specific recommendations on how to establish national chemical computational center.
October 1977	NRCC begins operation at Lawrence Berkeley Laboratory with three-year budget of $5.3 million, split equally between NSF and ERDA; review of activities and recommendations for continuation to occur three years hence.
February 1978	William Lester takes leave from IBM Corp. to become NRCC director; Lester gains one-year extension of initial phase activities but no new funds; review of NRCC still set for 1980.
January 1980	Review committee ("Goddard committee") begins evaluations.
April 1980	Goddard committee recommends two-year extension of NRCC with $550,000 per year budget and reduced scale of activities; Workshops and chemists' access to computers should continue, but NRCC grants for computing time, employment of in-house scientific staff, and distribution of programs should cease.
July 1980	Lawrence Berkeley Laboratory director David Shirley pronounces truncated NRCC unacceptable; NSF chemistry advisory committee votes to end NRCC funding; interagency committee of NSF and DOE votes joint withdrawal of funds, asks for plan to phase out NRCC by October 1981.

Workshops: The jewel in NRCC's crown

Subject	Date	Location
Computational methodology in crystallography	June 1978	Asilomar, Calif.
The minicomputer and computations in chemistry	July 1978	Lawrence Berkeley Laboratory, Berkeley, Calif.
Numerical algorithms in chemistry—algebraic methods	August 1978	University of California, Santa Cruz
Post Hartree-Fock: configuration interaction	August 1978	Lawrence Berkeley Laboratory, Berkeley, Calif.
Algorithms and computer programs for atomic and molecular quantum scattering theory	June 1979 October 1979	Argonne National Laboratory, Argonne, Ill. (part one) NRCC, Berkeley, Calif. (part two)
Stochastic molecular dynamics	July 1979	Woods Hole, Mass.
Software standards in chemistry	July 1979	University of Utah, Salt Lake City
Computation methods for molecular structure determination—theory and techniques	August 1979	Indiana University, Bloomington (joint with Quantum Chemistry Exchange Program)
Cooperative computer program generation for crystallography	November 1979	NRCC, Berkeley, Calif.
The problem of long-range forces in computer simulation of condensed media	January 1980	Menlo Park, Calif.
Quantum chemistry data interface	January 1980	Berkeley, Calif.

same operation. Many respondents to the Maggiora survey had doubts about whether chemists could learn skills needed to put their problems into a supercomputer without consultations with experienced in-house staff, however.

The review committee also recommended that NRCC stop developing programs, and instead fund postdoctoral fellowships for this purpose at locations apart from NRCC. The committee also recommended that NRCC stop distributing programs and leave this function to the long-established Quantum Chemistry Exchange Program, centered at Indiana University, Bloomington. In addition, it recommended that NRCC no longer fund research grants itself, but leave this to NSF and DOE.

Lawrence Berkeley Laboratory director David Shirley met with NSF's chemistry advisory committee in July and said that such a reduced NRCC would not be viable. The advisory committee unanimously recommended closing down NRCC. These actions set the stage for the final decision by the interagency committee.

NSF officials were moved not only by the negative tone of the Goddard report and Shirley's counterproposal to keep NRCC essentially as it was, but by the amount that NRCC took away from funding other research. The NSF share of more than $1 million annually was already 1.7% of its total chemistry budget of $59 million for fiscal 1981.

Shirley patched up a compromise with the Goddard committee, in which NRCC would have kept its in-house staff. Many computational chemists feel that an in-house staff is essential to organizing high-quality workshops and easing outside chemists' work on advanced computers. But DOE had passed the budgetary point of no return at the time of this August development, and the compromise never had a chance of acceptance.

Ironically, one important upshot of NRCC's brief, four-year existence might be its catalysis of improved computational chemistry in other countries. Peter Lykos, chemistry professor at Illinois Institute of Technology, says that establishment of NRCC served notice to the rest of the world that the U.S. regarded a centralized computing facility as crucial to its scientific and technological advance.

Indeed, at the Second Chemical Congress of the North American Continent held in Las Vegas last August, Lykos chaired a symposium on supercomputers in chemistry at which Martyn Guest of the Daresbury Laboratory of Britain's Scientific Research Council, Warrington, England, and K. Hijikata of the University of Electro Communications, Tokyo, presented papers on progress in making supercomputers available to their nations' computational chemists at research facilities such as NRCC was to have been.

Steve Stinson, New York

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 phaseout 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

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The preceding two articles pertaining to the closing of the NRCC appeared originally in the pages of Chemical and Engineering News and Science magazine. They have been reproduced with the kind permission of the publishers.

SOFTWARE DISTRIBUTION

All programs which the NRCC has been distributing have now been released to the Quantum Chemistry Program Exchange (QCPE) and the National Energy Software Center (NESC).

After March 1, 1981, requests for software should be directed to these organizations. Their addresses are:

The Quantum Chemistry Program Exchange
Department of Chemistry
Indiana University
Bloomington, IN 47405 USA

National Energy Software Center
Argonne National Laboratory
9700 South Cass Avenue
Argonne, IL 60439 USA

BULLETIN SCHEDULE

The current issue of the NRCC BULLETIN will be the last regularly scheduled issue. Current information on such subjects as NRCC workshops and software will be communicated by separate mailings.

PROPOSALS FUNDED

The NRCC is pleased to announce awards totaling $33,000 for proposals funded from the sixth NRCC proposal review. A brief description of the funded proposals follows:

Thomas F. George, Department of Chemistry, University of Rochester, "Laser-Stimulated Surface Processes." Supports computational studies of laser-stimulated surface processes. ($10,000; terminates September 30, 1981).

Warren J. Hehre, Department of Chemistry, University of California, Irvine, "Development of Computationally Efficient Split-Valence Basis Sets for Third-Row Elements." Develops a computationally efficient 3-21G split-valence basis set for both third-row main-group elements and first-row transition metals. ($20,000; terminates September 30, 1981).

Irwin D. Kuntz, Jr., Department of Pharmaceutical Chemistry, University of California, San Francisco, "Applications of Distance Geometry to Conformational Analysis." ($3,000; terminates September 30, 1981).

WORKSHOPS FOR 1981

Four major workshops are planned for FY 1981. They are in the areas of (1) Computer Simulation of Organic and Biological Molecules, (2) Effective Potentials in Electronic Structure Determination, (3) Non-numerical Methods, and (4) Perturbation Theory for Many-Body Problems.

Computer Simulation of Organic and Biological Molecules

This workshop was held January 5-8, 1981, at Asilomar, California, and was organized in association with Dr. Arnold T. Hagler of the Weizmann Institute, who is on sabbatical leave to the University of California, San Diego. The goal of the workshop was to define the desired capabilities of software for the titled purpose. Thirty leading workers in this field participated. The workshop was built around presentations that summarized the research efforts and interests of the participants, with emphasis on those areas where computer simulation plays a significant role.

Effective Potentials in Electronic Structure Determination

Planning for this workshop is being carried out jointly with Drs. Jeffrey Hay and Willard Wadt of Los Alamos National Laboratory (LANL) who have contributed significantly to the development and application of effective and pseudo-potential methods for molecular structure determination. Our interest in pursuing a workshop on this topic is prompted in part by enthusiastic response to a questionnaire mailed to twenty of the most active workers in the field to ascertain their interest in participating in such a workshop, and to obtain for consideration a listing of subtopics of maximal interest. The workshop is tentatively planned for the week before the American Theoretical Chemistry Conference, June 17-19, 1981, at LANL.

Non-numerical Methods

At the November 1-2, 1980, NRCC Policy Board and Program Committee meeting, there was strong sentiment expressed that a workshop in this general area would be timely because of recent advances in the field and the need to make chemists aware of this progress. In order to best focus the direction of the workshop, a planning committee was formed consisting of Policy Board member, Dr. Carroll Johnson of Oak Ridge National Laboratory, Program Committee member, Dr. W. Todd Wipke, University of California, Santa Cruz, and the NRCC Director. Current planning is directed towards a broad-based workshop with a tutorial component in addition to the usual research emphasis. Subareas that will be more fully explored include symbolic manipulation, organic synthesis by computer, and graphics.

Perturbation Theory for Many-Body Problems

This topic also arose out of Policy Board and Program Committee discussions as one strongly meriting consideration in our final-year program. Planning for the workshop is being coordinated by Dr. Ernest Davidson of the University of Washington. The workshop is planned for the week of July 6, 1981. It will emphasize state-of-the-art research directions.

Further information regarding these workshops may be obtained by calling or writing the NRCC workshop coordinator, Gervais Christensen.

SYMPOSIUM ON SUPERCOMPUTERS AND CHEMISTRY

A symposium on Supercomputers and Chemistry was held in Las Vegas as part of the National Meeting of the American Chemical Society during the week of August 24-29, 1980. This symposium was jointly sponsored by the ACS's Divisions of Computers in Chemistry and Physical Chemistry and by the NRCC. Co-chairmen for the symposium were Dr. Isath Shavitt of Batelle Columbus Laboratory and Professor Peter Lykos of the Illinois Institute of Technology, Chicago, Illinois.

The symposium was highlighted by discussions of the state of the art and future trends in large scale scientific computers. Representatives of several major computer manufacturers outlined both present and planned capabilities. A novel approach to large scale computing utilizing a user-made micro vector processor was also described.

Several experiments in the conversion of codes to vector processing machines were discussed by representatives of Daresbury Laboratory and the NRCC. They found that, while a significant increase in speed over non-vector machines could be obtained without major rewriting of programs, a much larger factor was possible by redesigning and improving existing algorithms.

Many applications of vector processing machines were also described. A major conclusion of these talks was that there are several areas of computational chemistry, such as artificial intelligence and graphics, where the real-time use of high-speed vector processing machines were critical.

Proceedings of this symposium are being prepared by the ACS and should be available early in 1981.

USER ASSOCIATION NEWS

The Executive Committee of the NRCC User Association convened the second annual meeting of the User Association August 25-29 in conjunction with the fall meeting of the American Chemical Society in Las Vegas. During this meeting of the American Chemical Society in Las Vegas, the situation at NRCC was discussed. The view was expressed that the NRCC User Association was the mechanism for grass roots input into the operations of the NRCC by the user community and that, if those assembled supported the continuation of the NRCC, the User Association's first priority should be to express this support. It was felt by those present that the views and needs of the users were not properly analyzed in the Ad Hoc Review Committee's report. It was also noted that many users in the chemical community were appalled by the NRCC's situation and that they wanted to make clear their desire for continuation of its funding at an adequate level.

A motion was made and passed that the Executive Committee should write to the appropriate agencies expressing their disagreement with the NRCC Ad Hoc Committee's Report and that a poll of the User Association members be conducted and analyzed.

The motion passed at the User Association meeting has been implemented by the Executive Committee, and has been distributed in a separate mailing to everyone on the BULLETIN mailing list. A separate letter, summarizing the results of the User Association poll, was also prepared by the members of the Executive Committee and submitted to SCIENCE. The text of this letter, as published in the November 14, 1980 issue of SCIENCE (Vol. 210, No. 4471), is reprinted below.

Chemistry Computer Center

As representatives of the community most affected by the decision to scuttle the National Resource for Computation in Chemistry (NRCC) (Research News, 26 Sept., p. 1504), we feel compelled to make our view public regarding this example of public science policy in the making. Our own examination of the issue indicates that the decision of the funding agencies (the Department of Energy and the National Science Foundation) is at odds with the general sense of the chemistry community and, indeed, we find that the decision-making process has essentially ignored community input. In the interest of possible future ventures into "big science" in chemistry, we feel that the scientific public should become aware of the nature of science policy decision-making and how it reflects on performance and politics.

At the Las Vegas meeting of the American Chemical Society (28 August 1980), the NRCC User Association decided to poll its membership (1700 scientists on its mailing list) regarding the report and recommendations issued by the ad hoc committee appointed by the funding agencies to review NRCC performance. It was felt that such a questionnaire was necessary because the report had recommended drastic changes in the nature of the NRCC, and yet the community to be affected had not even been informed of the recommendations.

The first question asked was if enough time had elapsed for a reasonable judgment to be made on the future of the NRCC. The second was whether the NRCC should continue in its present form for a longer time before critical decisions are made regarding its operation. The third question was whether the respondent agreed with each of the five recommendations of the ad hoc review committee.

Of the 200 members who returned their questionnaires within 2 weeks of mailing, 68 percent felt that not enough time had been allotted for proper judgment and 69 percent felt that the NRCC should continue as originally constituted for a period of 2 to 3 more years before review. The strongest disagreements were with the recommendations that suggest substantial changes in the way the NRCC now operates (79 percent were against switching software development away from an in-house scientific staff to an external postdoctoral program; 73 percent were against transferring software distribution to the Quantum Chemistry Program Exchange; and 53 percent were against stopping support of both internal and external computational research).

Shortly after the questionnaires were mailed out, a decision regarding the fate of the NRCC that goes beyond even the review committee's recommendations was reported in the pages of *Science*. However, no official announcement has been made, and no stated rationale for the decision has been made public by the funding agencies. Not only did the disclosure in the *Science* article emphasize to us the necessity of making our findings known as quickly as possible, it highlighted the manner with which this public policy issue has been handled since its beginning.

We have sent the detailed results of our questionnaire to the funding agencies and have urged them to reconsider continued funding for the NRCC. We have also asked them to issue a public report detailing the rationale for any decision that is made regarding NRCC's future.

We see a real danger when funders, effecting decisions concerning a national scientific resource, do not fully regard the community being served. There are unmet needs within the chemical community that will grow without a cogent national policy on computational technology. Beyond the immediate harm of eliminating an organization whose focus was to address some of these needs, the larger danger exists of stigmatizing any future efforts in this area.

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SEMINARS

Dr. Jonathan N. L. Connor, University of Manchester, England, "A New Method for Obtaining Information of Potential Energy Surfaces from Experimental Data," August 19, 1980.

Prof. David R. Yarkony, Johns Hopkins University, "MCSCF Wavefunctions, "August 20, 1980.

Dr. William Furey, University of Pittsburgh, "Array Processors and Crystallography," September 5, 1980.

*Dr. Roger Miller, University of Waterloo, Canada, "Infrared Laser Molecular Beam Spectroscopy," September 29, 1980.

Dr. Felix Smith, SRI International, "Modified Heliocentric Coordinates for Molecular Fragments with One Heavy Center," October 15, 1980.

Dr. Lester Shipman, Argonne National Laboratory, "Applications of Quantum Chemistry to Problems in Chemical Mutagenesis and Photosynthesis," October 16, 1980.

Dr. Reinhard Schinke, Max-Planck Institut fur Stromungsforschung, Federal Republic of Germany, "Rotational Rainbows in Inelastic Scattering," October 22, 1980.

*Prof. Donald L. Thompson, Oklahoma State University, "Formation and Decay of Quasi-Bound Clusters of Ar Atoms," October 24, 1980.

*Prof. James Farrar, University of Rochester, "Crossed Beam Studies of Proton Transfer Reactions at Low Energy," October 27, 1980.

*Prof. J. Peter Toennies, Max-Planck-Institut, Federal Republic of Germany, "Beam Scattering Experiments on Rotational and Vibrational Excitation, November 17, 1980.

Mr. Alan Lipkus, University of Rochester, "Laser Dissociation of Iodine and the Cage Effect," November 17, 1980.

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*Joint seminar with the Materials and Molecular Research Division, Lawrence Berkeley Laboratory and the Department of Chemistry, University of California, Berkeley.

NRCC STAFF PUBLICATIONS

D. M. Ceperley, NRCC, Lawrence Berkeley Laboratory, "The Relative Performances of Several Scientific Computers for a Liquid Molecular Dynamics Simulation."

Abstract: A statistical mechanics simulation package "CLAMPS" has been tested and timed on four scientific computers: CDC 7600, VAX 11/70, VAX 11/70 with FPS array processor 120B, and CRAY-1. The simulation used for the timing studies was a molecular dynamics calculation for the Stillinger-Lemberg potential of water. The author will discuss the ease of programming the various machines to achieve high efficiency and the type of simulation for which, in his opinion, each computer is best suited.

S. A. Hagstrom, NRCC, Lawrence Berkeley Laboratory, "Vector Computers in Computational Chemistry."

Abstract: Performance evaluations of the CRAY-1 have been conducted for several large portable Fortran programs currently supported by NRCC on the CDC 7600 at Lawrence Berkeley Laboratory. The purpose of the study was to determine the extent of existing program vectorization and resulting improvements in performance as a function of problem size. The programs considered ranged from completely scalar to highly vectorizable, from I/O limited to thoroughly compute bound. Local fine-tuning and insertion of BLAS's (Basic Linear Algebra Subroutines) where appropriate was done, but no major re-writes of scalar sections were attempted. Quantum chemistry programs studied included a multi-configuration, self-consistent field code (ALIS), a general purpose atomic CI package (ATOMIC), Slater integral routines (DERIC, ERIC), and several special purpose routines from the linear algebra area. In the chemical kinetics area, the principal program investigated was VIVS, a variable-interval variable-stop size integrator for the coupled sets of second-order differential equations arising in quantum mechanical inelastic molecular collision theory.

W. A. Lester, Jr., and A. J. Olson. NRCC, Lawrence Berkeley Laboratory, "The National Resource for Computation in Chemistry."

Abstract: The National Resource for Computation in Chemistry (NRCC) is the first national effort for the systematic advancement of computation methodologies in the field of chemistry. The NRCC functions to:

- Make information on existing and developing computational methodologies available to all segments of the chemistry community.
- Make state-of-the-art computational facilities (software and hardware) accessible to the chemistry community.
- Foster research and development of new computational methods for application to chemical problems.

A presentation will be made of current NRCC activities and publications.

L. D. Thomas, Max-Planck-Institute fur physik and Astrophysik, 8046 Garching near Munich, West Germany and NRCC, Lawrence Berkeley Laboratory and W. P. Kraemer, G. H. F. Diercksen. Max-Planck-Institute fur Physik and Astrophysik, 8046 Garching near Munich, West Germany. "Rotational Excitation of CO by He Impact."

Abstract: To study rotational excitations of CO by He impact, configuration-interaction potential energy surfaces have been computed with two different basis sets. The surfaces are compared to one another, to an electron-gas surface, and to an experimentally determined surface. In addition, converged close-coupling calculations of the collision cross sections have been done on these surfaces for energies up to 100 cm^{-1} and compared. On the most accurate CI surface, cross sections have been computed using the infinite-order sudden (IOS) and quasi-classical methods as well.

L. D. Thomas, M. H. Alexander, B. R. Johnson, W. A. Lester, Jr., J. C. Light, K. D. McLenithan, G. A. Parker, M. J. Redmon, T. G. Schmalz, D. Secrest and R. B. Walker, NRCC, Lawrence Berkeley Laboratory, "Comparison of Numerical Methods for Solving the Second-Order Differential Equations of Molecular Scattering Theory."

Abstract: The numerical solution of coupled, second-order differential equations is a fundamental problem in theoretical physics and chemistry. There are presently over 20 commonly used methods. Unbiased comparisons of the methods are difficult to make and few have been attempted. This report compares 11 different methods applied to three different test problems. The test problems have been constructed to approximate chemical systems of current research interest and to be representative of the state of the art in inelastic molecular collisions. All calculations were done on the same computer, and an attempt was made to do all calculations to the same level of accuracy. The results of the initial tests indicated that an improved method might be obtained by using different methods in different integration regions. Such a hybrid program was developed and found to be at least 1.5 to 2.0 times faster than any individual method.

L. D. Thomas, NRCC, Lawrence Berkeley Laboratory, to be published as a chapter in Potential Energy Surfaces and Dynamics Calculations, D. G. Truhlar, ed., Plenum Press, New York 1981. "Rainbow Scattering in Inelastic Molecular Collisions,"

Abstract: The role of rainbow scattering in inelastic collisions of atoms and atomic ions is well known and provides an important link between experimental observation and the theoretical potential energy curve which governs the dynamics of the colliding atoms. Only recently, however, has the analogous phenomenon in the case of non-spherical potentials and inelastic collisions been investigated. Based on a comparison between a classical trajectory calculation and experiment, it was suggested that rainbow-like structures might be observable in the distribution of differential cross sections vs. the (quantized) rotational angular momentum of a diatomic molecule after collision with an atom or atomic ion. Several experiments have subsequently revealed such structure. In the past 2 years numerous papers, both experimental

and theoretical, have appeared which discuss the subject. Different researchers have, however, arrived at different and sometimes conflicting terminologies and interpretations of the theoretical analysis. Indeed, it has even been questioned whether the rainbow analogy is proper in this case. It is therefore appropriate to begin with a brief history of the main physical and mathematical concepts in rainbow scattering. This will be followed by a classical analysis of coplanar scattering of Li^+ from CO. Finally, a brief review of the experimental and theoretical literature is given.

T. J. O'Donnell and Arthur J. Olson, NRCC, Lawrence Berkeley Laboratory, "GRAMPS--A Graphics Language Interpreter for Real-Time Interactive Three-Dimensional Picture Editing and Animation."

Key words: Graphics Interpreter, Vector Display List Processor, Picture editor, Real-time animation.

Abstract: GRAMPS, a graphics language interpreter has been developed in FORTRAN 77 to be used in conjunction with an interactive vector display list processor (Evans and Sutherland Multi-Picture System). Several of the features of the language make it very useful and convenient for real-time scene construction, manipulation and animation. The GRAMPS language syntax allows natural interaction with scene elements as well as easy interactive assignment of graphics input devices. GRAMPS facilitates the creation, manipulation, and copying of complex nested picture structures. The language has a powerful macro feature that enables a new graphics command to be developed and incorporated interactively.

Animation may be achieved in GRAMPS by two different, yet mutually compatible, means. Picture structures may contain "framed" data, which consist of a sequence of fixed objects. These structures may be displayed sequentially to give a traditional frame animation effect. In addition, transformation information on picture structures may be saved at any time and used to generate new macro commands that transform these structures from one saved state to another in a specified number of steps, yielding a transformation animation effect.

An overview of the GRAMPS command structure is given and several examples of application of the language to molecular modeling and animation are presented.

MANUSCRIPTS RECEIVED--RESEARCH PARTIALLY SUPPORTED BY THE NRCC

Marvin Bishop, Fordham University at Lincoln Center, David Ceperley, NRCC, H. L. Frisch, State University of New York at Albany, and M. H. Kalos, New York University, "The Need for Supercomputers in Time Dependent Polymer Simulations," to be published in the ACS Symposium of Supercomputers, Las Vegas, August 1980.

William F. Coleman, University of New Mexico, Michael G. Prisant and Richard N. Zare, Stanford University, "A Laser-Induced Transient Photovoltaic Effect Using Blocked Electrodes," J. Phys. Chem. 84, 2685 (1980).

Paul L. DeVries and Thomas F. George, University of Rochester, "Effect of Laser Frequency on a Collision-Induced Radiative Process," to appear in Potential Surfaces and Dynamics Calculations edited by D. G. Truhlar (Plenum, New York).

David A. Micha, University of Florida, "Few-Body Processes in Atom-Diatom Collisions," invited talk at the IX International Conference on Few-Body Problem, Eugene, August 1980. To appear in Nucl. Phys. (1981).

VISITORS

Herbert W. Jones, Division of Natural Sciences and Mathematics, Florida A M University, Tallahassee, Florida, June 30-August 31, 1980.

Lynn E. Lewis, Department of Chemistry, Clemson University, Clemson, South Carolina, July 9-30, 1980.

Marvin Bishop, Division of Science and Mathematics, Fordham University at Lincoln Center, New York, New York, July 14-August 29, 1980.

David Yarkony, Department of Chemistry, Johns Hopkins University, Baltimore, Maryland, August 4-September 1, 1980.

Alan H. Lipkus, Department of Chemistry, University of Rochester, Rochester, New York, August 11, 1980-August 18, 1981.

Jeff H. Nichols, Department of Chemistry, Texas A M University, College Station, Texas, August 15-25, 1980.

Delos DeTar, Department of Chemistry, Florida State University, Tallahassee, Florida, August 18-September 18, 1980.

William Jackson, Department of Chemistry, Howard University, Washington, DC., September 1-30, 1980.

William L. Jorgensen, Department of Chemistry, Purdue University, West Lafayette, Indiana, November 20-24, 1980.

PUBLICATIONS REQUEST FORM

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