

Lawrence Berkeley National Laboratory

LBL Publications

Title

Bulletin Vol 3 No 1

Permalink

<https://escholarship.org/uc/item/54r608wn>

Author

Lawrence Berkeley National Laboratory

Publication Date

1980-02-01

Copyright Information

This work is made available under the terms of a Creative Commons Attribution License, available at <https://creativecommons.org/licenses/by/4.0/>

DISCLAIMER

This document was prepared as an account of work sponsored by the United States Government. While this document is believed to contain correct information, neither the United States Government nor any agency thereof, nor the Regents of the University of California, nor any of their employees, makes any warranty, express or implied, or assumes any legal responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by its trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof, or the Regents of the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof or the Regents of the University of California.

NRCC

NATIONAL
RESOURCE
FOR COMPUTATION
IN CHEMISTRY

Lawrence Berkeley Laboratory
Building 50D
Berkeley, California 94720
415/486-6722
FTS 451-6722
800/227-0198 (Toll free outside California)

3470
Bulletin No. 7 Vol. III Winter 1980
BULLETIN

For Reference

Not to be taken from this room

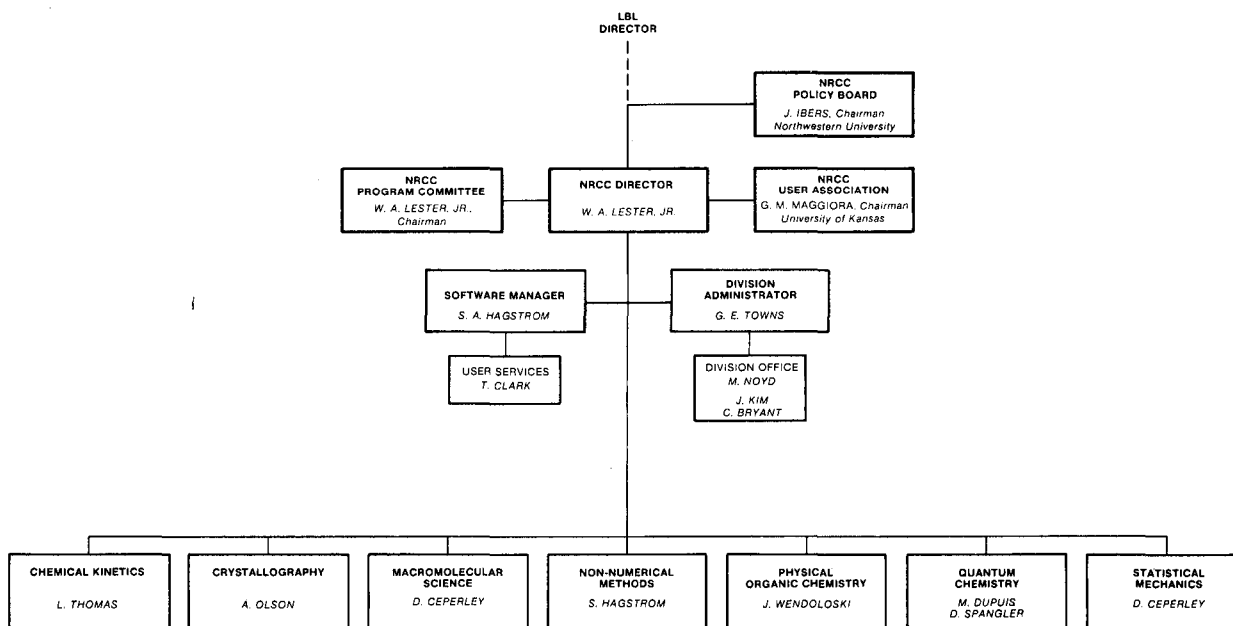
TABLE OF CONTENTS

NRCC Organization Chart.....	2
NRCC Staff Telephone Numbers.....	2
NRCC Bulletin Schedule.....	3
New Home for the NRCC.....	3
National Theoretical Effort on Combustion.....	3
New Software Announcement Policy.....	4
NRCC to Publish Computers in Crystallography Newsletter...	4
Call for Proposals.....	4
NRCC Minicomputer Delivered.....	7
Array Processors.....	8
Scattering Theory Workshop.....	8
Stochastic Molecular Dynamics Workshop.....	9
Conference on Software Standards in Chemistry.....	9
Computational Methods for Molecular Structure Determination: Theory and Techniques.....	10
NRCC Holds Workshop to Develop Portable Crystallographic Code.....	10
NRCC Scientific Staff Activities.....	10
Personnel Changes.....	11
Daresbury Laboratory Interactions.....	11
Visitors.....	11
Seminars.....	12
Final Project Summaries of Research Supported by the NRCC.....	13
Manuscripts Received--Research Partially Supported by the NRCC.....	14
Order Form for NRCC Workshop Proceedings.....	17
NRCC Questionnaire.....	19

Prepared for the U.S. Department of Energy under Contract W-7405-ENG-48 and
for the National Science Foundation under interagency Agreement CHE-7721305.

FAB
3470

LAWRENCE BERKELEY LABORATORY
UNIVERSITY OF CALIFORNIA
NATIONAL RESOURCE FOR COMPUTATION
IN CHEMISTRY



NRCC STAFF TELEPHONE NUMBERS

Commercial (415) 486-(Extension)
FTS 451-(Extension)
(800) 227-0198 (Toll free outside California)

Ms. Carolyn Bryant	6722
Dr. David M. Ceperley	6990
Mr. Tim R. Clark	6168
Dr. Michel Dupuis	6073
Dr. Stanley A. Hagstrom	6722
Mr. Larry Johnson	6168
Ms. JoAnn Kim	6722
Dr. William A. Lester, Jr.	6722
Ms. Maudie Noyd	6722
Dr. Arthur J. Olson	6316
Dr. Dale P. Spangler	6993
Dr. Lowell D. Thomas	6991
Mr. George E. Towns	6722
Dr. John J. Wendoloski	6997
Dr. George Zahr	6996

Messages may be left at Extension 6722.

Bulletin Editor:
John J. Wendoloski

NRCC BULLETIN SCHEDULE

The combined impact of changes in the administrative staff (see PERSONNEL CHANGES) and the relocation of the NRCC from its previous home in Building 50 to a new modular building (50D) necessitated the omission of the fall issue of the NRCC BULLETIN. The BULLETIN will resume its quarterly publication schedule with the next issue. Dr. John Wendoloski of the scientific staff has been appointed editor.

NEW HOME FOR THE NRCC

The NRCC is now housed in a newly constructed one-story building situated a few hundred feet from its previous quarters. The new location greatly facilitates communication and access among all functions of the organization. There are 18 offices, a meeting room, and a small computer hardware room into which the NRCC's recently acquired VAX 11/780 will be moved.

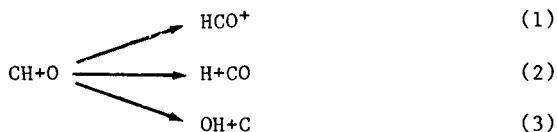
NATIONAL THEORETICAL EFFORT ON COMBUSTION

A collaborative research effort on the chemistry of combustion has been launched by an association of scientists at some of the nation's leading national laboratories and universities. The participants have agreed to pursue a course of research to elucidate the electronic structure and collision dynamics of a system of reactions involving carbon, hydrogen, and oxygen. This extensive and intensive theoretical examination of a process which is basic to the production of energy will be coordinated by the NRCC.

The scientists have met twice--first on June 28, 1979 at Argonne National Laboratory, and then on October 9, 1979 at Brookhaven National Laboratory. The issues discussed at these meetings included:

- . What reactions, or classes of reactions, are of general importance in combustion systems?
- . What can theoretical studies contribute to the understanding of these reactions?
- . How can the participants organize their research programs to ensure that these problems are properly addressed?

As a result of the first meeting the participating scientists resolved to study reaction prototypes, such as $\text{CH}_n + \text{O}$, in their search for general principles of importance in all hydrocarbon processes. The initial project chosen was



The $\text{CH} + \text{O}$ reaction is of unusual importance because channel (1) is presumed to be a dominant pathway for information in hydrocarbon flames, and channel (2) is postulated to be source of highly vibrationally excited CO in acetylene flames.

Collaborating in the program are fourteen quantum chemists and collision theorists supported by the Office of Basic Energy Sciences of the U.S. Department of Energy at Argonne, Brookhaven, Ames, Sandia Livermore and Lawrence Berkeley Laboratories, Princeton University, and the University of California, Berkeley.

Names and affiliations of the participants in the national theoretical effort on combustion follow:

Thom. H. Dunning
Argonne National Laboratory

Michel Dupuis
NRCC, Lawrence Berkeley
Laboratory

Michael L. Gusinow
Sandia Laboratories, Livermore

Michael L. Koszykowski
Sandia Laboratories, Livermore

William A. Lester, Jr.
NRCC, Lawrence Berkeley
Laboratory

Carl Melius
Sandia Laboratories, Livermore

William H. Miller
University of California,
Berkeley

James Muckerman
Brookhaven National
Laboratory

Marshall D. Newton
Brookhaven National Laboratory

Herschel Rabitz
Princeton University

Klaus Ruedenberg
Iowa State University

Lowell D. Thomas
NRCC, Lawrence Berkeley
Laboratory

Al Wagner
Argonne National Laboratory

Stephen Walch
Argonne National Laboratory

NEW SOFTWARE ANNOUNCEMENT POLICY

The practice of announcing programs in the BULLETIN as they become available for general use is being discontinued with this issue. In the future, programs will be announced in an annual catalog that will describe the NRCC's entire software holdings. Between appearances of the catalog special software updates will be issued at irregular intervals as the need arises.

The BULLETIN announcements have served the valuable function of making known the software holdings and our software development efforts. Software projects and plans will continue to be reported in the BULLETIN, but the usual software descriptions will be confined to the catalog.

As part of the effort to prepare a master catalog, a program and subroutine naming and classification scheme is being developed. Routines are being classified in groups and subgroups corresponding to the major areas of computational chemistry identified by the National Research Council's Planning Committee for an NRCC: the groups include chemical kinetics, crystallography, macromolecular science, non-numerical methods, physical organic chemistry, quantum chemistry, and statistical mechanics. In addition, the catalog will give much more information about each program than could be conveniently included in the BULLETIN descriptions. It is planned that the catalog will also provide extensive descriptions of other software libraries available at LBL that may be of interest to computational chemists. The new catalog is scheduled to appear in the Spring.

NRCC TO PUBLISH COMPUTERS IN CRYSTALLOGRAPHY NEWSLETTER

A quarterly newsletter entitled COMPUTERS IN CRYSTALLOGRAPHY has made its first appearance this Winter. The newsletter is intended to provide a channel of communication among crystallographers concerned with hardware and software developments affecting their field. Topics within the purview of the newsletter include: reports of new crystallographic software; clearinghouse information for software access; background and descriptive articles on both software and hardware tools relevant to crystallographic computing; reports on molecular graphics; announcement of pertinent activities and events. Contributions to the newsletter are welcomed and should be sent to:

COMPUTERS IN CRYSTALLOGRAPHY NEWSLETTER
c/o Dr. Arthur J. Olson
NRCC, 50D, Room 141
Lawrence Berkeley Laboratory
Berkeley, CA 94720

Requests to receive the newsletter should also be addressed to Dr. Olson.

CALL FOR PROPOSALS

The deadlines for receipt of proposals for the next round is July 15, 1980. Proposals are sought of the highest scientific quality and therefore fundable by the criteria of federal agencies such as the NSF and the DOE. In addition, however, it should be remembered that because of its mission, size, and budget, the NRCC is not another federal funding agency. It is an organization created to assist research in chemistry using computational methods in ways not presently possible under federal agency practices. An example worth noting is the support of joint proposals involving researchers across (i) areas (e.g., crystallography and quantum chemistry), (ii) subdisciplines (e.g., analytical and physical chemistry, (iii) departments (e.g., chemistry and biochemistry), (iv) disciplines (e.g., chemistry and physics), and (v) institutions (e.g., corporation x and university y). Clearly there are other possibilities. Do not hesitate to contact the NRCC Director to discuss alternatives of interest.

Besides serving as an information resource, the NRCC scientific staff can participate in collaborative research efforts. There may be problems of appropriate scope for support by the NRCC that need additional computational expertise for implementation. The NRCC staff is a possible resource for filling such gaps. Inquiries concerning collaborative projects with NRCC staff should be directed to the NRCC Director.

Under present NRCC policy, awards are made to cover the cost of computer time at the LBL Computer Center and at other institutions. In the latter case approval of both the NRCC Program Committee and the NRCC Policy Board is required. Proposal may be from any field of chemistry and should promote the development of chemistry through: the advancement of computational methods; the innovative application of existing methods to problems in some frontier areas of chemistry; the study of problems of significant scientific merit that cannot be carried out in the proposer's institution due to lack of large-scale computational facilities; the resolution of intradisciplinary computational methodology issues; and the development of interdisciplinary approaches to forefront problems in chemistry.

Awards from past rounds might lead to the impression that only proposals requiring modest amounts of computer time will be funded. On the contrary the NRCC has increased the funds available for awards, but the NRCC Program Committee has stated that the majority of proposals reviewed to date were for the most part only modest departures from proposals normally received by federal funding agencies. Thus the NRCC Program Committee repeats its request presented in Vol. II, No. 1 of the NRCC BULLETIN that we receive proposals of broad scope and effort.

Directions for proposal preparation follow. The LBL computer system is a complex consisting of a CDC-7600, CDC-6600, and CDC-6400. Further information on the LBL computer system, its rate structure, and details on using it may be obtained by writing to the NRCC.

Directions for Proposal Preparation

The NRCC has established the following guidelines for the submission of proposals. These guidelines supersede those previously provided.

General

1. One-inch left margin on all pages.
2. Pagination on all sheets.
3. Ten copies required.

Cover Page

The following information must appear on the cover page:

1. Name of principal investigator(s) submitting proposal.
2. Name of submitting organization (including department).
3. Address (including building and room where appropriate).
4. Telephone number.
5. Title of proposed research.
6. Computing time on (model of computer); desired level: ____ hours; estimated cost ____; threshold level: ____ hours; estimated cost ____; method of estimating cost.
7. Proposed starting date.
8. Proposed duration of the research.
9. Previous anniversary date and account number (for renewal or continuing award request).

Abstract

A brief summary of the proposed research, including significance to science and impact for the NRCC.

Proposal Narrative

The narrative should be no more than ten double-spaced typewritten pages and include the following information:

1. A description of the work being proposed, including the objectives, significance, and nature of the calculations.
2. A general plan for achieving these objectives, including an explanation of the methods to be used.
3. Relation of the proposed work to the current status of the topic addressed.
4. Outline (with pertinent references) of what has been done on the topic to date.
5. Explanation of how this research will advance understanding in the subject area of chemistry.
6. Justification of requested hours of computer time.
7. A bibliography of pertinent literature.

Budget

The financial statement section should include the following information:

1. Detailed line item budget for the grant monies required, including computer time and communication costs (if any).
2. Other agencies, if any, to which the proposal will be submitted.
3. All current support: title of project, funding period of awards(s), agency and annual budget levels.
4. Other proposals (including renewal applications) which are currently pending (including DOE and NSF).

Staffing

The statement of staffing should include the following documentation:

1. List of all collaborators who will be computing on the research outlined in the proposals (include names, titles, and telephone numbers).
2. Curriculum vitae of the principal investigator(s).
3. Principal publications of other senior personnel during the past five years on the subject matter covered by the proposal.

Computer Information

1. Briefly describe the available equipment, policies, and capabilities of the computer center at your home institution. If the computations proposed are not to be carried out at LBL or your home institution computer center, provide the above information for the system to be used.
2. Do you wish to compute at LBL or elsewhere? If elsewhere, skip 3-7 and answer 8-9.
3. Have you ever computed at LBL before? If not, skip 4-5, and answer 6-7.
4. If so, are you currently connected to the LBL computer system?
5. What is your access code (account number)?
6. What type of equipment is currently available to you for connection with the LBL Computer Center?
 - (a) REC Terminal (make _____ model _____)
 - (b) RJE (make _____ model _____)
 - (c) Other (make _____ model _____)

7. Briefly describe the hardware and communications software available, if any, for remote access to the LBL Computer Center.

Go to Next Section

8. Give institution at which computations will be done and reasons for carrying out computations at institutions.
9. Briefly indicate how computer codes extended or developed under an NRCC award would be made available to the chemistry community through the NRCC.

Communication Availability (for Computing at LBL)

1. LBL has provided communication systems (TYMNET, ARPANET and FTS) for toll-free access to the LBL computers for interactive (RECC) calculations. If you are planning to compute via the Remote Batch Entry System (RJE), have you made provisions, either in the proposal or elsewhere, for communication costs? If so, please explain in detail.
2. Is your computer terminal connected to any other leased phone line system? If so, what kind?
3. Do you have a teletype (TWX) machine available to you? If so, what is the phone number of the machine?
4. Do you have a telecopier available to you? If so, list the make, speeds, type (automatic or manual), machine telephone number, and confirmation telephone number.

NRCC MINICOMPUTER DELIVERED

NRCC's Digital Equipment Corporation VAX-11/780 minicomputer arrived at LBL during the first week in June. After some minor startup problems, the system was officially turned over to NRCC on July 3. The system has virtual memory architecture and is configured with 512K bytes of error correcting MOS memory, a Floating Point Accelerator Unit, one single access 176M byte disk drive, a 45 ips 9-track 1600 bpi magnetic tape drive, a Versatec 1000 lpm, 200 dots/inch electrostatic printer/plotter, and eight asynchronous EIA terminal lines operating at up to 9600 baud. An additional eight terminal lines will be added shortly. Four VADIC VA-317S/P direct connect 300 BPS modems are available for remote access over the dial-up telephone networks. Terminal access to the VAX is by means of a computerized digital switch (called GANDALF) that also allows access to the 6000's and the 11/70 UNIX text editing system.

The standard VAX/VMS Operating System, Version 1.5, is being used. This system features multiuser timesharing concurrent with background batch. Languages available are FORTRAN, BLISS, and assembly language. Dr. John Wendoloski and Dr. Dale Spangler are acting as the installation managers.

Initially the VAX is being used primarily for software development in such areas as chemical kinetics, crystallography, quantum chemistry, and statistical mechanics. Many of the major packages currently running on the CDC7600 are in the process of conversion to the VAX. Already converted are the programs MULTAN (crystallography), CLAMPS (macromolecular science and statistical mechanics), ALIS (quantum chemistry), and a general Slater integrals package for molecules (DERIC, ERIC) while a number of other programs are nearing completion. In the area of systems support software, a Fortran NAMELIST processor has been written for the VAX, since VAX Fortran does not provide this useful feature. This will enable the user interface for NAMELIST directed codes to be preserved when moving programs to the VAX.

Researchers involved in developing minicomputer-based codes for computational chemistry applications are encouraged to discuss their plans with the NRCC since we are seeking opportunities for collaborative efforts. Two such efforts are currently underway. One is an experiment in networking involving a DECNET link (4800 baud dial-up) between NRCC's VAX and a VAX in Prof. John Pople's group at Carnegie-Mellon University. The second involves an adaptation by Dr. David Ceperley of his CLAMPS (Classical Many Particle Simulation program) program to a Floating Point System Array Processor connected to a VAX-11/780 in Prof. Bruce Berne's group at Columbia University.

A substantial hardware upgrade of the NRCC's VAX is planned for the Spring of 1980. This will involve an additional 2M bytes of memory, a second disk drive, a conventional 600

lpm printer, and a state-of-the-art real-time interactive graphics system. A high-speed DECNET connection from the VAX to the LBL CDC 7600/6600/6400 complex of machines should also be a reality sometime early in 1980. This should largely eliminate the present need to carry tapes back and forth between the VAX and the CDC 6600.

ARRAY PROCESSORS

As part of its educational function the NRCC has initiated a study of the use of attached scientific processors ("array processors") for chemical computations. Although each commercially available array processor has its own architectural features, in most cases the array processor is a special purpose "box" which is attached to an existing minicomputer (or mainframe computer) to provide high speed processing of floating point operations in vector- or matrix-oriented applications. For certain restricted classes of calculations, array processors appear to have the possibility of providing very cost-effective computation. The use and programming of current products presents, however, difficulties beyond those normally encountered by computational chemists. Initially, this project of the NRCC involves an investigation of the state-of-the-art in array processing and the preparation of a corresponding report.

Prof. Neil Ostlund, Department of Chemistry, University of Arkansas, is serving as a consultant to the NRCC on the project. Prof. Ostlund is on leave-of-absence in the Computer Science Department of Carnegie-Mellon University where he is doing research into parallel algorithms and parallel computer architectures for scientific calculations. He spent the month of July 1979 at the NRCC preparing a report on array processors which will be distributed by the NRCC to interested members of the chemistry community. A future newsletter will announce the availability of this report which provides a pedagogical introduction to array processors, describes selected commercially available array processors, and presents the experiences of a number of researchers now using array processors for applications related to computational chemistry.

In conjunction with this report and the NRCC's investigation into array processors, a small one-and-one-half day meeting was held July 19-20, 1979 at the NRCC. This meeting, with the title "Array Processors for Chemical Computations," brought together a small number of invited speakers to describe their direct experience with array processors to the NRCC staff and interested local scientists. A considerable amount of open discussion was generated concerning the advantages and disadvantages of using an array processor. The possible role of the NRCC in advancing this mode of computation was also discussed. Prof. Ostlund's report will contain the agenda of this meeting and will abstract the main results brought forward at that time.

The NRCC is considering a continuing assessment of array processors, and interested members of the community are invited to contribute their ideas on this subject to the NRCC Director, Dr. William A. Lester, Jr. It appears that more general purpose 64-bit array processors will be appearing in the near future and one possibility that has been raised is that the NRCC consider acquiring an array processor to attach to its VAX-11/780.

SCATTERING THEORY WORKSHOP

On June 25-27, 1979 the NRCC sponsored a workshop on "Algorithms and Computer Codes for Atomic and Molecular Quantum Scattering Theory," organized by Prof. John C. Light, University of Chicago and Dr. Lowell D. Thomas, NRCC, held at Argonne National Laboratory. The goals of the workshop were to identify which of the existing computer codes for solving the coupled equations of quantum inelastic scattering theory perform most efficiently, and to make those codes available to the chemistry community through the NRCC software library.

Included among the 20 participants were most of the developers of the commonly used algorithms and codes. Somewhat surprising, in view of the stated goals, was the amount of new material presented. For example, a promising new hybrid method, which attempts to combine the best features of many methods, was presented there for the first time.

Besides presentations and discussions of the methods, a set of test problems was proposed, discussed, and agreed upon as a common basis for comparing the speed and accuracy of the various computer codes. Representatives of most of the more popular methods agreed to solve these problems on the same LBL computer so that an unbiased comparison could be made. At a second meeting held at the NRCC on October 26-27, the participants in the earlier meeting reconvened to compare performance of the various algorithms on the test problems. The proceedings of this workshop will appear in two parts. The first part, containing the lecture summaries from the first meeting, is now available. The second part will include the results of the comparisons presented and discussed in the October meeting.

STOCHASTIC MOLECULAR DYNAMICS WORKSHOP

On July 9-11, 1979 at Woods Hole, Massachusetts, the NRCC held a workshop, organized by Dr. John Tully of Bell Laboratories, on the topic of "Stochastic Molecular Dynamics." Twenty-five scientists, most of whom are involved in computer simulations of stochastic systems, attended the workshop and reported on their work. The problem addressed by the workshop was that of the simulation of a single molecule surrounded by a solvent. In such problems one would like to ignore the solvent atoms in the simulation in order to simplify the computation; however, they are continually exchanging energy and momentum with the molecule of interest. The simplest approach is to treat the solvent as an idealized heat bath which leads to the Langevin equation. This model leaves out important memory and hydrodynamical effects. The workshop focused on practical ways to generalize the Langevin equation and on such applications as: the dynamics of chain molecules, vibrational relaxation in condensed phases, gas phase collisions, and atom-surface scattering. The proceedings of the workshop are scheduled to be available for distribution shortly.

CONFERENCE ON SOFTWARE STANDARDS IN CHEMISTRY

In late July, the NRCC sponsored a three-day conference on "Software Standards for Chemical Computation." The meeting was organized by Prof. Frank Harris and was held at the University of Utah, Salt Lake City. Of the 30 invited participants, there were 12 quantum chemists, 13 crystallographers and 5 computer scientists and applied mathematicians. The objective of the conference was to discuss and recommend standards for machine-independent, modular, and well-documented software suitable for use on the larger minicomputers that are rapidly becoming available to chemists.

The conference began with a plenary session comprising talks of general interest on various aspects of portability and standardization. There was general agreement among the speakers as to the virtues of structured programming and the value of software tools in attaining good programming practice and portability. Fortran preprocessors were recommended both as an aid to producing structured programs and as a means of attaining machine independent code. Verification programs, such as PFORT, were suggested as tools for testing existing code for portability. Two talks in this session dealt with examples of applications in the two main areas of interest. Dr. G. Diercksen of the Max-Planck Institute for Physics and Astrophysics (Munich) reported on his system of data interfaces and data bases for quantum chemistry, and Prof. James Stewart of the University of Maryland talked about his efforts in the area of portable crystallographic software.

After the general session, the participants divided into several smaller working groups in order to discuss topics and formulate recommendations relevant to their own interests. The topics of the working groups were:

1. Portability considerations and standards
2. Documentation and coding standards
3. Machine specification: what is a minimal computer configuration
4. Quantum chemistry software base
5. Quantum chemistry data interfaces
6. Small molecule crystallography
7. Large molecule crystallography

Each working group formulated a preliminary report, presented it to a general session for discussion and then reconvened to draft a final report. These reports will be included in a published proceedings of the conference and will be distributed by the NRCC upon request.

A notable aspect of the conference was the confluence of quantum chemists and crystallographers. Prof. George Jeffery of the University of Pittsburgh expressed the hope of growing exchange between the two groups. In his recollection, this was the first such joint gathering to take place in over 20 years. It was felt that such exchanges could lead to agreement on common formats for related chemical structural data bases, and could be of substantial benefit to both fields.

The crystallographers, who initially divided into small- and large-molecule working groups, reconvened as a single working group to draft their final report. There was

widespread agreement among them on the steps that both the NRCC and the crystallographic community should take in attaining software standardization and machine-independent portability. Several of their recommendations focused on the demonstration of the feasibility of standardized programming systems and data formats through the NRCC sponsorship of workshops to produce useful crystallographic code. They settled upon a specific preprocessor language and a set of program conventions and data file formats to be used in such pilot demonstrations.

In the area of quantum chemistry, the working group on the quantum chemistry software base drafted a list of program types and program capabilities which should be included in a software base. The working group on standard data interfaces prepared a preliminary draft of a standard data interface for this software base. A committee was then established to develop a detailed standard data interface. This committee, which consists of authors and users of major quantum chemistry systems such as GAUSSIAN 70, ALIS, and MUNICH, will make final recommendations within a year.

Both the crystallographers and quantum chemists felt that a standard set of bit primitives should be defined, and a committee was established to accomplish this. They also agreed on the need for upward compatibility of new versions of ANSI Fortran. They recommended that NRCC communicate this position to the ANSI Standards Committee X3J3, and also sponsor a member on this committee who would lobby for the interests of computational chemists.

COMPUTATIONAL METHODS FOR MOLECULAR STRUCTURE DETERMINATION: THEORY AND TECHNIQUES

On August 13-24, 1979, the NRCC, in conjunction with the Quantum Chemistry Program Exchange, held a workshop at the Chemistry Department of Indiana University. The workshop provided an introduction to the use of state-of-the-art computer software for the semiempirical and ab initio computation of electronic structure and for the determination of the geometry of small and large molecules.

Forty-five participants from the academic, industrial, and governmental sectors attended the lectures on the theoretical foundation of molecular structure determination, presented by Profs. N. L. Allinger, E. R. Davidson, W. A. Goddard, J. A. Pople, M. Zerner, and Dr. B. Liu.

Remote interactive access to the Lawrence Berkeley Laboratory CDC7600 was provided in order to give the participants "hands-on" experience with the NRCC-QCPE software. Fifteen terminals as well as a remote job-entry station were effectively utilized by the participants both to familiarize themselves with the software and to examine molecular system of chemical interest.

NRCC HOLDS WORKSHOP TO DEVELOP PORTABLE CRYSTALLOGRAPHIC CODE

As a direct result of the workshop on software standards held in Salt Lake City in late July, the NRCC has initiated a pilot project to develop portable crystallographic software. The crystallographers present at the Utah conference recommended that the NRCC should sponsor the development of a code that has a standard data format and is portable from computer to computer. In order to demonstrate the feasibility of the idea, the NRCC held a workshop November 10-17, at which ten invited scientists came together for one week in order to develop and code a multiple isomorphous replacement (MIR) program for distribution among crystallographers. The MIR code, which is used for the phasing of macromolecular structures, was developed on the NRCC's VAX 11/780 and will be tested on other computers to insure its portability. The success of such a project could signal the beginning of a new era in program exchange among computational chemists.

NRCC SCIENTIFIC STAFF ACTIVITIES

In addition to the other functions performed by the NRCC scientific staff, they also serve as consultants to the chemistry community at large on a wide range of subjects. The most common request is to provide answers to questions dealing with the NRCC software library, ranging from communicating which programs are available, to detailed explanations of program capabilities and limitations. When a chemist presents a problem he or she wishes to solve, the NRCC staff indicates which program is best suited, and can often provide rough estimates of the computer resources required. In several recent instances, when such estimates were not readily available, exploratory calculations were performed in order to

obtain them. Once the chemist is actively using the program, the staff provides assistance in dealing with any technical difficulties encountered in using the program.

Based on their broad experience with various computers, the staff can provide insight on the adaptability of most NRCC programs to the chemist's local computer. Answers to these questions are made possible through a detailed knowledge of the program's machine dependencies and conversion problems--a knowledge which the NRCC staff is in a unique position to provide, having previously converted most of these codes to the LBL system.

If a chemist decides to compute remotely at NRCC, the staff makes available upon request information on how to do it. Once the chemist begins computing, the NRCC staff answers questions on the operating system of the LBL computer--particularly on how to most effectively compute at LBL.

PERSONNEL CHANGES

Dr. George Zahr joined the NRCC scientific staff on a short-term appointment to pursue collaborative studies on inelastic atom-molecule scattering theory with Dr. Lowell Thomas. Dr. Zahr is no stranger to the University of California, Berkeley, having received his doctorate under Prof. William H. Miller of the UCB Chemistry Department in 1976.

Ms. Jane Greer of the administrative staff left the NRCC on September 14, 1979, to return to fulltime studies at California State University at Hayward. On October 15, Ms. Carolyn Bryant and Ms. JoAnn Kim joined the administrative staff. Ms. Bryant will have primary responsibility for all departmental typing and Ms. Kim will coordinate all workshop arrangements and activities related to NRCC Boards and Committees.

DARESBURY LABORATORY INTERACTIONS

During June and the first part of July 1979, Dr. Victor Saunders visited NRCC as part of a staff and software exchange program between the NRCC and the Theory and Computational Science Division of Daresbury Laboratory, England. This Division of the Daresbury Laboratory has a mandate similar to the NRCC's in a number of areas. Dr. Stanley Hagstrom, NRCC, spent six weeks in May and June of last year under this same program installing selected NRCC software. During his visit Dr. Saunders installed the ATLMOL3 system of programs on the LBL CDC7600. ATLMOL is a sophisticated system for carrying out molecular Hartree-Fock calculations of various types using s, p, and d-type Gaussian and Slater basis orbitals. The systems is laboratory documented. ATMOL also runs on IBM systems, for which a CI extension (called SPLICE) based on the bonded function approach of Sutcliffe also exists.

Dr. Brian Buckley, Daresbury Laboratory, visited the NRCC for two weeks in September. During this period he adapted the R-matrix program, RMATOM, of Berrington, Burke, LeDourneuf, Robb, Taylor and VoKylan to the LBL CDC7600. RMATOM is a suite of three programs for performing electron-atom, electron-atomic ion and atomic photoionization cross section calculations and atomic frequency-dependent polarizability calculations using the R-matrix methods. Extensive modifications were necessary to implement the software here. We are grateful to Dr. Buckley for carrying out this task.

VISITORS

Dr. Sheldon Green, NASA Institute for Space Studies, New York, visited the NRCC October 30 through November 9. During this period he made several improvements to his molecular scattering program, MOLSCAT. He added atom-asymmetric rotor collisions to its capabilities and created a second version which utilizes the large core memory of the CDC 7600. This version permits the solution of much larger sets of coupled equations than the small core version. We are grateful to Dr. Green for his effort and contribution to our software library.

Dr. Frank Rebentrost, Project Group for Laser Research, Max Planck Society for the Advancement of Science, Garching, West Germany, June 1-July 31, 1979.

Dr. Glen T. Evans, Department of Chemistry, University of Oregon, June 11-15, 1979.

Dr. Victor R. Saunders, Daresbury Laboratory, England, June 12-July 6, 1979.

Dr. Chiakao Kawabuta, Okuyama University, Japan, June 14, 1979.

Dr. Clair Cheer, Department of Chemistry, University of Rhode Island, June 15, 1979.

Dr. Russell Pitzer, Department of Chemistry, Ohio State University, June 19-July 17, 1979.

Prof. DeLos DeTar, Department of Chemistry, Florida State University, June 26-July 10, 1979.

Prof. Marvin Bishop, Department of Chemistry, Fordham University at Lincoln Center, June 27-July 30, 1979.

Prof. Neil S. Ostlund, Computer Department, Carnegie-Mellon University, July 3-31, 1979.

Dr. Stephen T. Elbert, Ames Laboratory, Iowa State University, July 16-24, 1979.

Prof. Reed A. Howald, Department of Chemistry, Montana State University, July 27-August 7, and September 24-26, 1979.

Dr. Larry McMurchie, Department of Chemistry, University of Washington, Seattle, Washington, August 6-8, 1979.

Prof. William Jorgensen, Department of Chemistry, Purdue University, August 17, 24-26, 1979.

Prof. V. Renugopalakrishnan, Department of Physiology & Biophysics, University of Illinois at the Medical Center, Chicago, Illinois, September 5-26, 1979.

Dr. George F. Adams, U.S. Army Ballistics Research Laboratory, Aberdeen Proving Ground, Maryland, September 6-14, 1979.

Dr. Brian D. Buckley, Daresbury Laboratory, England, September 10-24, 1979.

Prof. George C. Schatz, Department of Chemistry, Northwestern University, October 5-8, 1979.

Prof. Gerald M. Maggiora, Department of Biochemistry, University of Kansas, October 8, 1979.

Dr. Joachim Schaefer, Max-Planck-Institut für Physics und Astrophysics, Munich, West Germany, October 15-16, 1979.

Dr. Sheldon Green, Institute for Space Sciences, NASA, New York, New York, October 30-November 10, 1979.

Dr. Jack Tossell, Department of Chemistry, University of Maryland, November 8-9, 1979.

Dr. John J. C. Mulder, University of Leiden, The Netherlands, November 13, 1979.

SEMINARS

Prof. DeLos DeTar, Florida State University, "Steric Effects on Reactions by Molecular Mechanics," July 5, 1979.

Dr. Marvin Bishop, Fordham University at Lincoln Center, New York, New York, "Computer Simulations of Polymeric Systems," July 17, 1979.

Dr. George Schatz, Northwestern University, Evanston, Illinois, "Classical Trajectory Studies of Polyatomic Molecule Collision Dynamics," October 5, 1979.

Dr. Joachim Schaefer, Max-Planck-Institut für Physics and Astrophysics, "A Discussion of Resonance Structures of Atom-Diatom Systems. Examples: He-H₂/HD, Xe-HD, H-CO," October 15, 1979 and "Tests of Ab Initio Calculated Interaction Potentials," October 16, 1979.

Prof. Clemens C.J. Roothaan, University of Chicago, "Newton-Raphson MCSCF Program Architecture, October 17, 1979.

*Dr. Alan Luntz, IBM Research Laboratory, San Jose, California, "Reaction Dynamics of Oxygen Atoms with Hydrocarbons," October 31, 1979.

Prof. W. Todd Wipke, University of California, Santa Cruz, "Non-Numerical Methods in Chemistry--One Person's View," November 2, 1979.

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

FINAL PROJECT SUMMARIES OF RESEARCH SUPPORTED BY THE NRCC

1. Title of Project: "Classical Trajectory Studies of State to State Energy Transfer in Triatomic Molecules"
2. Duration: April 1978-May 1979
3. Amount of CDC 7600 Time: \$2,000
4. Principal Investigator: George C. Schatz
5. Address: Department of Chemistry, Northwestern University, Evanston, Illinois 60201
6. Co-investigators: Thomas Mulloney, graduate student
Mark Moser, graduate student

Brief Description of Project; Status of Codes

Our primary objective was to apply certain newly developed methods for determining the semiclassical stationary states of polyatomic molecules to classical trajectory studies of state to state collisional energy transfer involving triatomic molecules. Prior to this study, no accurate determination of state resolved cross sections involving molecules other than diatomics had ever been accomplished due to the difficulty associated with determining the good action-angle variables needed to describe the semiclassical states of these molecules in the presence of anharmonic and Coriolis coupling. As will be detailed below, the goals of this research have now been achieved in that we have developed a trajectory program (named ABCD) for determining cross sections for state to state energy transfer in atom plus triatomic molecule collision systems, and we have used this program to study $V \rightarrow V$ and $V \rightarrow T$ transfer in $\text{He} + \text{SO}_2$, $\text{Li}^+ + \text{CO}_2$, and other systems. This program treats nonseparable effects accurately and efficiently enough to enable the determination of state to state cross sections to within a few percent, while requiring only a small fraction of the trajectory computation time to calculate the good action-angle variables. It can be quite easily applied to collisions involving any linear or nonlinear symmetric triatomic molecule for which cubic or quartic force field parameters are available, and it can be used to determine both differential and integral state to state cross sections as well as final translational distributions, and moments of the final state distributions. The program does have a few limitations, including an inability to describe the states of molecules which are in Fermi resonance, an approximate treatment of certain terms in the Coriolis Hamiltonian (which limits the amount of rotational energy a molecule can have if it is to be described accurately), and the use of a rotational sudden approximation to uncouple rotational and other degrees of freedom during the collision. None of these limitations is fundamental to the methods that have been used, and in continuing research on this topic, more general codes are being developed.

The present program development involved several preliminary studies, several of which were by themselves extensive research projects. First, it was necessary to develop accurate and efficient methods for determining good action-angle variables for nonseparable systems. This led to the development of two methods, one based on a Fourier series representation of the generating function for these good variables¹ and one based on classical perturbation theory.² These two methods were then used in a general study of anharmonicity effects in a collinear model of $\text{Kr} + \text{CO}_2$,³ which formed much of the computational basis for the three dimensional trajectory code ABCD. In another study, several different types of classical rotational sudden approximations were used to study rotationally inelastic scattering in $\text{He} + \text{I}_2$ and $\text{He}, \text{Ar}, \text{Xe} + \text{O}_3$,⁴ and on the basis of the results of these applications, the sudden approximation used in ABCD was implemented. Finally, a number of studies of semiclassical eigenvalues were undertaken^{1,2,5} to assess the accuracy of the semiclassical treatments used, including the nature of convergence of classical perturbation theory under a variety of coupling strengths, and frequency ratios. These results were used to assess the accuracy of our later applications to collisional energy transfer in $\text{He} + \text{SO}_2$ ⁵ and $\text{Li} + \text{CO}_2$ ⁶ using ABCD.

References (All are publications stemming from this project.)

1. G. C. Schatz and M. D. Moser, Chem. Phys. 35, 239 (1978). "A Method for Determining "Good" Action-Angle Variables and Semiclassical Eigenvalues in Nonseparable Systems."
2. G. C. Schatz and T. Mulloney, J. Phys. Chem. 83, 989 (1979). "Classical Perturbation Theory of Good Action-Angle Variables: Applications to Semiclassical Eigenvalues and to Collisional Energy Transfer in Polyatomic Molecules."
3. G. C. Schatz and T. Mulloney, J. Chem. Phys., in press. "Collisional Energy Transfer in Polyatomic Molecules: A Study of Anharmonicity Effects in Kr + CO₂."
4. T. Mulloney and G. C. Schatz, Chem. Phys., submitted. "Classical Rotational and Centrifugal Sudden Approximations for Atom-Molecule Collisional Energy Transfer."
5. G. C. Schatz and T. Mulloney, in preparation. "Classical Perturbation Theory Determination of Good Action-Angle Variables in Nonlinear Triatomic Molecules: Application of Collisional Energy Transfer in He + SO₂."
6. G. C. Schatz and T. Mulloney, in preparation. "A Quasiclassical Trajectory Study of Collisional Excitation in Li⁺ + CO₂."

-
1. Title of Project: XASW: A Program to Calculate Molecular Orbitals in The X Scattered Wave Approximation
 2. Duration: April 1978-September 1979
 3. Principal Investigators: David A. Case, Department of Chemistry, University of California, Davis, and Joe E. Norman, Jr., Department of Chemistry, University of Washington, Seattle

Brief Description

This program performs self-consistent X scattered wave calculations,¹ and is an extensive revision of the MIT programs of K. H. Johnson and F. C. Smith, Jr. It uses less core (especially for large molecules) and is substantially faster than the original programs. New options include: (a) calculation of one-electron properties,² (b) generation of the wavefunction on a grid of points, suitable for input to a contour plotting routine; (c) estimation of oscillator strengths;³ (d) use of quasirelativistic radial functions for heavy atoms.⁴ The auxiliary program IPOT may be used to generate starting potentials for input to the SCF procedures.

XASW was written by Michael Cook (Harvard University) and David A. Case (University of California, Davis). IPOT is a reversion by Dick Hoskins (University of Washington) of the MIT program MOLPOT, originally written by K. H. Johnson and F. C. Smith, Jr. Support from NRCC for the development of these codes is gratefully acknowledged.

References

1. K. H. Johnson, Adv. Quantum Chem., 7, 143, (1973).
2. D. A. Case and M. Karplus, Chem. Phys. Lett., 39, 33 (1976); M. Cook and M. Karplus, submitted to J. Chem. Phys.
3. L. Noodleman, J. Chem. Phys., 64, 2343 (1976).
4. D. D. Koelling and B. N. Harman, J. Phys., C10, 3107 (1977).

MANUSCRIPTS RECEIVED--
RESEARCH PARTIALLY SUPPORTED BY THE NRCC

Arthur E. Stillman, Gary P. Zientara, and Jack H. Freed, Department of Chemistry, Cornell University, "The Variational Method and the Stochastic-Liouville Equation: II. ESR Spectral Simulation via Finite Elements," J. Chem. Phys., July 1, 1979.

Gary P. Zientara and Jack H. Freed, Department of Chemistry, Cornell University, "The Variational Method and the Stochastic-Liouville Equation. III. Infinite Elements for CIDN(E)P," J. Chem. Phys., July 1, 1979.

Gary P. Zientara and Jack H. Freed, Department of Chemistry, Cornell University, "Spin-Echoes for Diffusion in Bounded, Heterogeneous Media: A Numerical Study," J. Chem. Phys., July 1, 1979.

Paul L. DeVries, C. H. Chang, Thomas F. George, Department of Chemistry, University of Rochester, Bernard Laskowski, and James R. Stallcop, NASA-Ames Research Center, "Production of $\text{Na}^*(4s)$ by Collision of $\text{Na}(3s)$ with Xe in the Presence of Two Nonresonant Lasers."

William L. Jorgensen, Department of Chemistry, Purdue University, "The Structure and Properties of Liquid Methanol," submitted to the J. Am. Chem. Soc.

William L. Jorgensen, Department of Chemistry, Purdue University, "Monte Carlo Results for Hydrogen Bond Distributions in Liquid Water."

Zeki C. Kuruoglu and David A. Micha, Departments of Chemistry and Physics, University of Florida, "Diatomic Transition Operators: Results of L^2 Basis Expansions," submitted to J. Chem. Phys.

Robert R. Lucchese and Vincent McKoy, Arthur Amos Noyes Laboratory of Chemical Physics, California Institute of Technology, "Application of the Schwinger Variational Principle to Electron-Molecular Ion Scattering," J. Phys. B: Atom. Molec. Phys., Vol. 12, No. 14.

LEGAL NOTICE

This book was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

This report was done with support from the Department of Energy. Any conclusions or opinions expressed in this report represent solely those of the author(s) and not necessarily those of The Regents of the University of California, the Lawrence Berkeley Laboratory or the Department of Energy.

Reference to a company or product name does not imply approval or recommendation of the product by the University of California or the U.S. Department of Energy to the exclusion of others that may be suitable.

ORDER FORM FOR NRCC WORKSHOP PROCEEDINGS

Please send a copy of the proceedings indicated below:

Crystallographic Methodology	_____
Minicomputers & Computations in Chemistry	_____
Numerical Algorithms in Chemistry	_____
Post-Hartree Fock	_____
Atomic and Molecular Quantum Scattering Theory	_____

Name _____

Organization _____

Mailing Address _____

Detach and return to: NRCC Workshop Proceedings
Lawrence Berkeley Laboratory
Building 50D
Berkeley, CA 94720

NRCC QUESTIONNAIRE

If this is the first NRCC BULLETIN that you have received you may wish to fill out this questionnaire.

1. Would you like to receive future issues of the BULLETIN?

Yes _____ No _____

2. Would you like to receive detailed information on the LBL Computer Center?

Yes _____ No _____

3. Can you suggest specific codes that should be made a part of the NRCC library at the LBL Computer Center? If so, give the names and as many particulars as possible on a separate sheet. Please comment on quality of documentation, if known.

4. Have you developed codes for your own use which might be of interest to NRCC users? If so, supply detailed information about the code and its level of documentation.

5. Do you have suggestions for workshop topics which the NRCC might sponsor in the next two years? If so, send a brief statement.

Name _____

Institution/Company _____

Street address _____

City and State/Country _____

Zip code _____

Telephone
no. _____

Return to: NRCC - Questionnaire
Lawrence Berkeley Laboratory
Building 50D
Berkeley, CA 94720

LAWRENCE BERKELEY LABORATORY
University of California, Berkeley 94720

ADDRESS CORRECTION
REQUESTED

Nonprofit Org.
U.S. Postage
PAID
Berkeley, Calif.
Permit No. 1123