Title
FY 1985 ADP LONG-RANGE SITE PLAN FOR THE LAWRENCE BERKELEY LABORATORY

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FY 1985 ADP LONG-RANGE SITE PLAN

for the

LAWRENCE BERKELEY LABORATORY

March 1983

Lawrence Berkeley Laboratory
University of California
Berkeley, California

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February 28, 1983

Ms. Sharon A. Ball
Director, MIS&T Division
Department of Energy
San Francisco Operations Office
1333 Broadway
Oakland, CA 94612

SUBJECT: 1985 ADP Long-Range Site Plan

Dear Ms. Ball:

Enclosed is the Long-Range Site Plan for computing at the Lawrence Berkeley Laboratory. This year's Plan has three components:

1) A proposal to set up a National Center for Energy Research Computing,
2) The acquisition of a replacement for the CDC 7600 and,
3) A Class III computer for administrative data processing.

Your comments and questions are welcomed and may be directed to Ken Wiley or to me.

Sincerely,

Robert J. Harvey, Head
Office of Computing Resources

RJH/ls
Enclosure

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SECTION A. SITE OVERVIEW

The Lawrence Berkeley Laboratory was founded by Ernest Orlando Lawrence. As a young physics professor at the University of California in Berkeley, he invented the cyclotron in 1929, and on January 2, 1931, he and his graduate student Stanley Livingston proved the concept of cyclotron resonance experimentally. This event marked the beginning of a new style of physics research.

To probe the structures and properties of atomic nuclei ever more deeply, Lawrence and his collaborators built successively larger, more powerful accelerators. In addition to the cyclotron, two other basic kinds of "atom smasher" were invented here: the Alvarez-type linear accelerator and the synchrotron. In the ensuing decades, these awesome machines yielded great advances in nuclear and elementary particle physics, nuclear chemistry, and radiation biology. Many of the elementary particles and artificial radioisotopes were discovered at LBL, as were nearly all the transuranium elements. Radioactive substances were synthesized and used in unlocking one of nature's most vital secrets: the mechanism of photosynthesis.

The value of these discoveries is well known. Of equal value--and indispensable to Lawrence's own work--was his emphasis on a mode of research that has come to be called "big science." This is the assembly of highly integrated, multidisciplinary teams of scientists and engineers to attack formidable problems with massive concentrations of brain power and machine power. Such large-scale research has yielded rich dividends in both pure and applied science.

Throughout its first five decades, LBL has given the nation scientific and technological leadership of the highest order. Eight of its researchers have been honored with Nobel Prizes, and countless other awards have been bestowed on the LBL staff.

Today the Lawrence Berkeley Laboratory's major role is to conduct research programs that are appropriate for an energy research laboratory but not suited to the programmatic goals or resources of a university campus. Thus the development and utilization of large experimental facilities are still emphasized, and the interdisciplinary team approach to research is still stressed.

The Laboratory is unique among the National Laboratories in being effectively co-located with the Berkeley Campus of the University of California. The Laboratory serves an important national need by conducting basic research in an environment that combines academic quality and renewal with National Laboratory R&D management experience and facilities. Faculty in scientific and engineering disciplines are carefully selected to augment Laboratory staff in performing research in technology base areas chosen to advance DOE programmatic goals in nuclear and energy research. Lawrence Berkeley Laboratory also supports university-based research nationwide by providing major national facilities--the SuperHILAC, Bevalac, and the National Center for Electron Microscopy--that are readily accessible to qualified investigators.

As a unit of the University of California, Lawrence Berkeley Laboratory has an unmatched role in the training of the next generation of scientists and engineers for careers in advanced energy research and technology. Approximately 500 resident graduate students conduct thesis research at the Laboratory, and many more use LBL facilities or perform collaborative research.

Participation in DOE-supported energy research programs at LBL provides these students with skills in high demand by energy industries. The flow of Berkeley Ph.D.'s to industry is one of many forms of technology transfer that allows Lawrence Berkeley Laboratory to maintain close and supportive relationships with industry. The Laboratory-industry boundaries are defined by LBL's focus on long-term, high-risk generic research particularly suited to the Laboratory's facilities and capabilities, which are not duplicated in industrial laboratories. At the same time, the close contact of LBL with industry ensures the relevance of its generic energy research.

The Laboratory's long-range plan for the period through the year 2000 includes the following components as elements of the LBL role.

In high-energy physics the LBL role has three major components. As a research laboratory, LBL conducts a broad program of experimental and theoretical studies in particle physics. As a detector laboratory, LBL brings resources and skills to bear on developing detectors of the future, such as the highly-successful Time Projection Chamber, in collaboration with consortia of universities. These roles were reaffirmed by a major DOE review in 1982. As a resource laboratory, LBL carries out long-range research and development, as in the 10-Tesla Magnet program, and participates in planning future national high-energy physics facilities.

Nuclear science research at LBL emphasizes the experimental and theoretical investigation of the interaction of heavy ions with target nuclei, both for their intrinsic scientific interest and for their use in the synthesis of new, exotic isotopes and new chemical elements. Complementary research programs in light-ion nuclear science, in the development of advanced instrumentation and in nuclear data evaluation are also carried out. Relativistic heavy-ion physics is rapidly evolving as the major frontier of nuclear science, and is attracting increasing interest from high-energy physicists. This frontier is being explored vigorously at the Bevalac, which can now accelerate heavy ions through uranium for the first time. Continued scientific advances will establish a need for further exploration of this frontier by means of a higher-energy machine such as the Tevalac in the late 1980s.

The intrinsic advantages of heavy-ion radiotherapy and the importance of heavy-ion radiobiology have now been well demonstrated. A major medical accelerator design study is now well along. Coupled with recent successes in treating cancer by heavy-ion radiotherapy, this study establishes the feasibility and urgency for making a major national commitment to build a dedicated heavy-ion medical accelerator in a hospital setting.

The LBL Materials Sciences programs in alloy design, mechanical metallurgy, ceramic science, solid state physics, and materials chemistry, are strengthened by the new National Center for Electron Microscopy. The Materials Sciences and Chemical Sciences programs support LBL's preeminent surface science and catalysis research, while Chemical Sciences supports LBL's unique chemical dynamics research and its new thrust in the use of modern laser techniques to probe temporal aspects of photobiology and photochemistry. The Laboratory's strength in Basic Energy Sciences provides a strong foundation for future growth, as outlined below.

Lawrence Berkeley Laboratory has a uniquely broad range of expertise and interest in the production and use of synchrotron radiation. Several LBL research programs have utilized the facilities at SSRL since 1974. Unique insertion devices (wigglers and undulators), designed and built at LBL, are in use at SSRL, producing superior synchrotron radiation sources. A major collaboration is underway with Exxon Research to build two wiggler-based beam lines at SSRL. Based on the growing importance of synchrotron radiation, LBL is proposing to design and construct the world's first next-generation light source, a dedicated machine based on straight sections and insertion devices, as part of a major new Basic Energy Sciences initiative. Under this initiative, it is proposed to build a National Center for Advanced Materials, consisting of an Advanced Light Source, a Surface Science and Catalysis Laboratory, and an Advanced Materials Synthesis Laboratory/Advanced Device Concepts Laboratory (which will include research on alternative future light sources). This Center will address critical national needs in a technology-base area presently vulnerable to foreign competition, will train many additional graduate students, and will constitute a major redirection for LBL. This initiative will subsume and consolidate several previously proposed construction projects in the energy research program.

In the Magnetic Fusion Energy program, LBL's success in positive-ion neutral beams has led to a long-term program in plasma heating. Now the emphasis is shifting to negative-ion neutral beams.

The Laboratory's expertise in geohydrology addresses national needs in nuclear waste isolation and in geothermal reservoir research. The LBL group is a national resource for solving future nuclear and energy research problems in the geological realm.

The LBL Energy Efficient Buildings program is a national asset, as is the LBL Electrochemistry program. Both of these major programs fill national needs in long-range energy research and fulfill part of LBL's role.

Table LBL-A1 provides a breakdown of the LBL staff by classification; Figure LBL-A1 and Table LBL-A2 summarize LBL research funding estimates for FY1983 by DOE Assistant Secretary.

Table LBL-A1

Total LBL Employment

Classification	Number	Percent
Scientists and Engineers	967	30
Professional Administrators and Managers	91	3
Technicians	1204	38
Administrative/Clerical Personnel	357	11
Service	107	3
Graduate Student Research Assistants	491	15
TOTAL	3217	100

Figure LBL-A1

Estimated Percentage Distribution of LBL Funding for FY 1983, by DOE Assistant Secretary

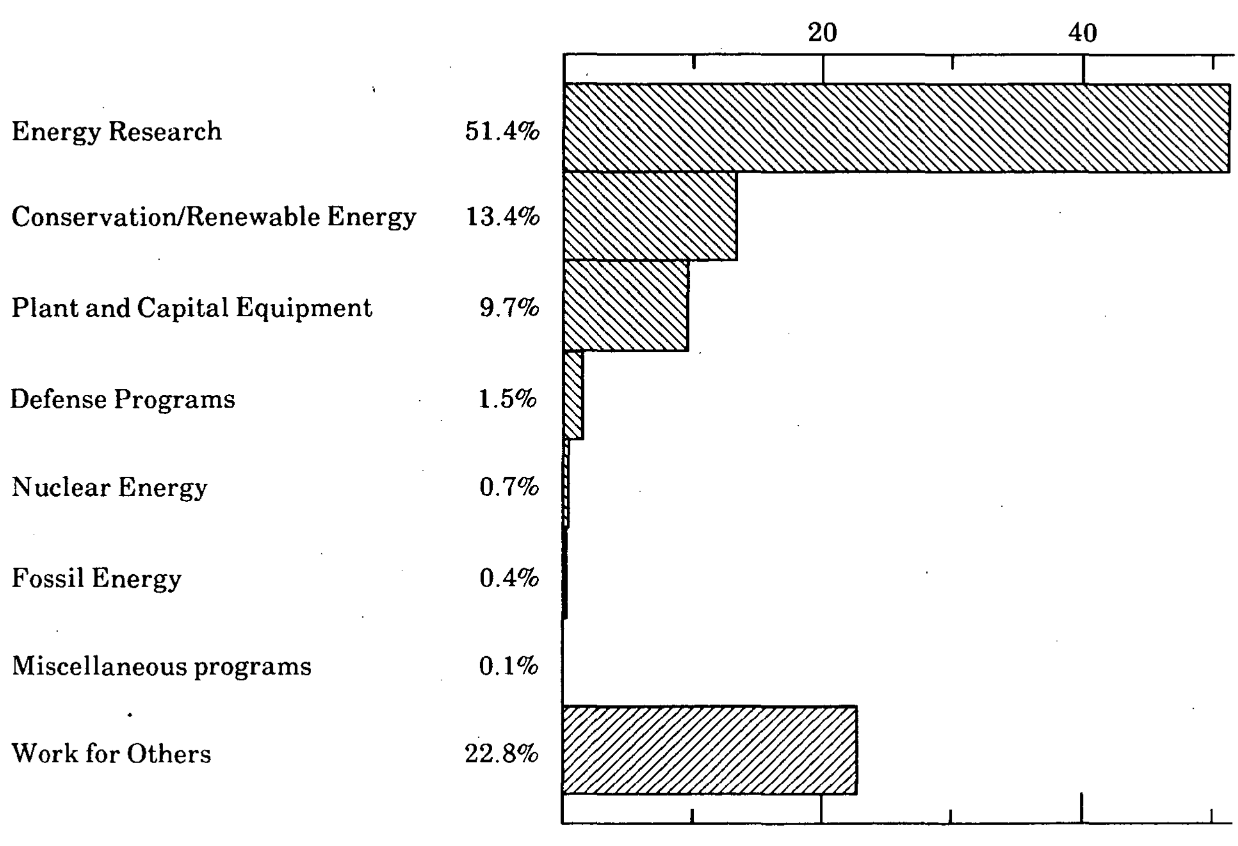


Table LBL-A2

Estimated Laboratory Funding for FY 1983

DOE Assistant Secretary	FY 1983 ($ millions)	Percent
Energy Research	69.6	51.4
Conservation and Renewable Energy	18.1	13.4
Fossil Energy	0.6	0.4
Nuclear Energy	0.9	0.7
Defense Programs	2.0	1.5
Miscellaneous Programs	0.2	0.1
Plant and Capital Equipment	13.2	9.7
Total DOE	104.6	77.2
Work for Others	30.9	22.8
TOTAL LABORATORY FUNDING	135.5	100.0

SECTION B. INSTALLED SYSTEMS

For LBL this section includes only General Management Networks/Systems. To present a more complete picture, all systems of theoretical capacity greater than 1000 NSU's are included even though General Management usage is less than 1000 NSU's in some cases.

1. Central Facility

The principal computer of the LBL Central Facility is a CDC 7600. Support for batch and interactive computing is provided through CDC 6600 and 6400 computers and newer satellite machines configured to support specialized interactive functions. These include two DEC PDP-11/70 systems supporting text-processing, and three DEC VAX-11/780 systems supporting interactive access for program development, numerical computations involving large arrays that exceed the 7600 memory capacity, and interactive graphics. These computers are linked by a Hyperchannel network having relatively high capacity. A DEC PDP-11/44 (DGATE) and an IBM 4331 (BGATE) serve as network gateway machines, allowing access to all machines of the central facility by other LBL computers.

A variety of on-line storage is currently available to all CDC machines, and is being made accessible to all machines in the central facility through the Hyperchannel. This on-line storage includes disks and a Braegen Automated Tape Library (ATL) holding about 2600 reels of magnetic tape. Additional local disk storage is available on the DEC satellite machines. (See Figure LBL-B1). The operating systems in use on the large computers were developed by LBL from early Control Data systems. They provide access to LBL's mass storage systems, on-line documentation, a selection of compilers, cross-compilers, and libraries. Details may be found in SECTION D.

The PDP-11/70 machines are dedicated to text processing, and utilize the UNIX† operating system. The three VAX systems run under the DEC VMS operating system.

2. Distributed Facilities

Computer Science Research System

The Laboratory operates computing research facilities as part of its basic computer science research into information systems, data management, software engineering and networks. First acquired in late FY 1978, this computing system now includes three DEC VAX-11/780 computers and their associated peripheral equipment. The configuration is shown in Figure LBL-B2.

Biology and Biophysics Support System

A distributed system has been developed by the Laboratory to support research programs in biology and biophysics experimentation. This system contains a DEC VAX-11/780, a DEC PDP-11/34, associated storage and I/O equipment and microprocessor based data acquisition front-ends. The configuration is shown in Figure LBL-B3.

Physics Support System

A system to support data reduction and data simulation for the Time Projection Chamber (TPC) detector at PEP utilizes a VAX-11/780 at LBL. This system connects to the Central Facility through the DGATE computer and the Hyperchannel. It also connects to the on-line data acquisition and control systems at SLAC. See Figure LBL-B4.

---

† UNIX is a registered trademark of the Western Electric Company.

Heavy-Ion Spectrometer System

The data acquisition and control function for this large detector utilizes most of the capacity of a DEC VAX-11/780 system. The remaining sixth of its capacity is utilized by the Nuclear Science Division to satisfy a portion of its total computing requirement. See Figure LBL-B5.

Biomedical Research System

This VAX-11/780 based system is used primarily in support of the cancer radiotherapy research program. The balance of its capacity provides a computing resource to other programs in the Biology and Medicine Division. See Figure LBL-B6.

Technical Support System

The Real Time Systems Group (RTSG) maintains a VAX-11/780 mainly as a support system for all other such systems. It is used for the in-house hardware maintenance and the software distribution functions. It is also used by other laboratory groups, on a temporary basis, and by RTSG to support their projects. See Figure LBL-B7.

Molecular Interactions Computation System

The Molecular Interactions Group of the Materials and Molecular Research Division utilizes a VAX-11/780 for the calculation of molecular interactions and potential energy surfaces. See Figure LBL-B8.

Figure LBL-B1
LBL Central Computing Facility

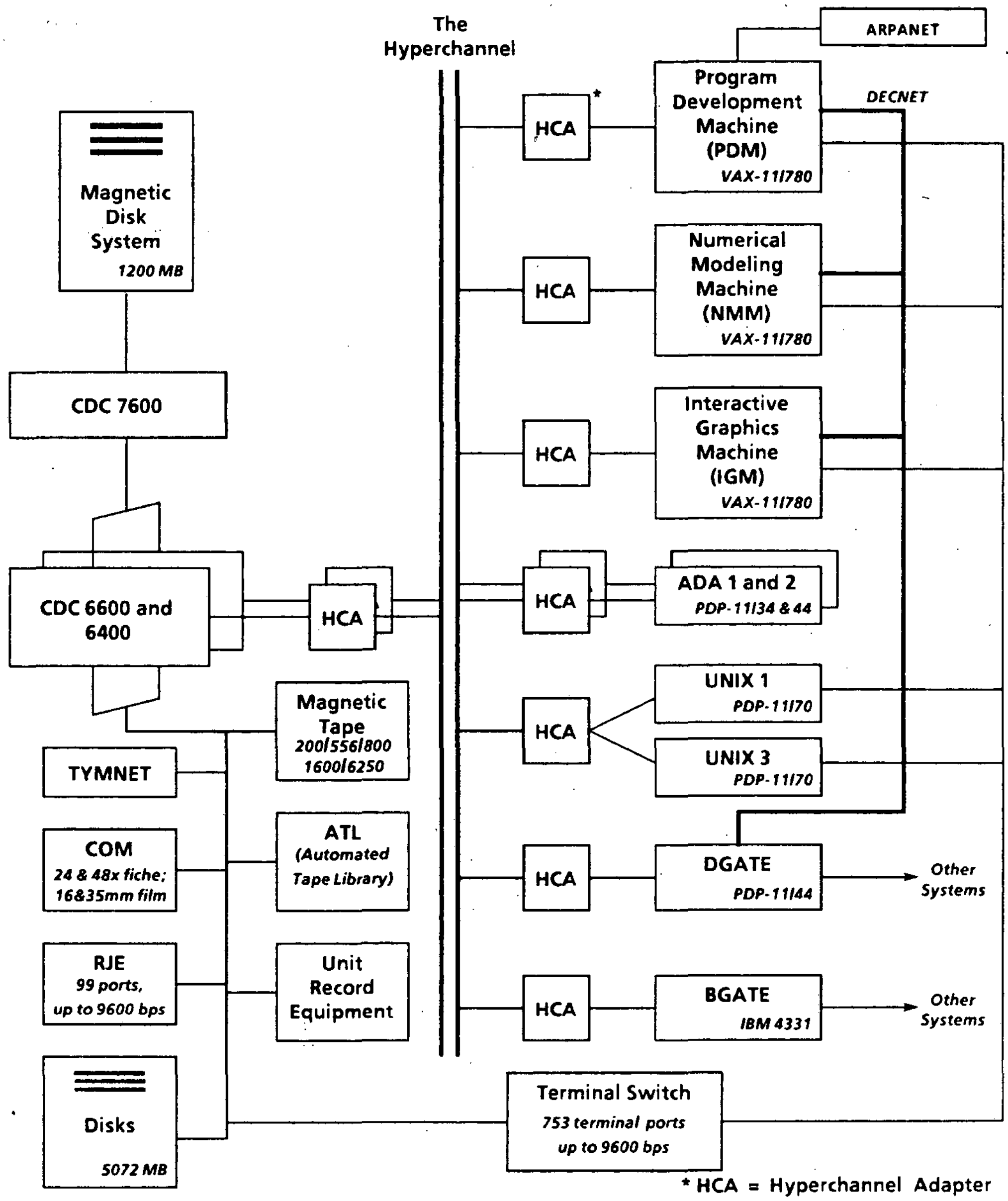


Figure LBL-B2

Computer Science and Mathematics Research Facility

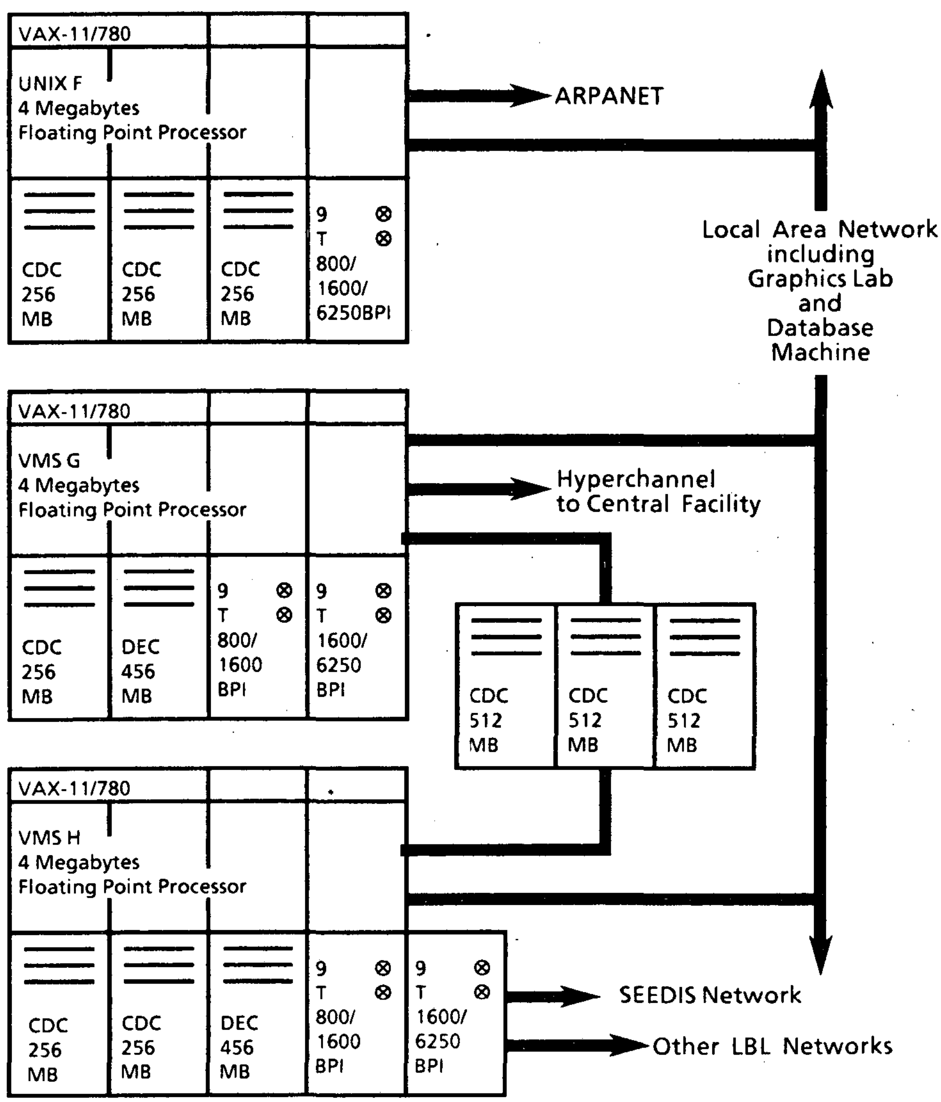


Figure LBL-B3

Biology and Biophysics Support System

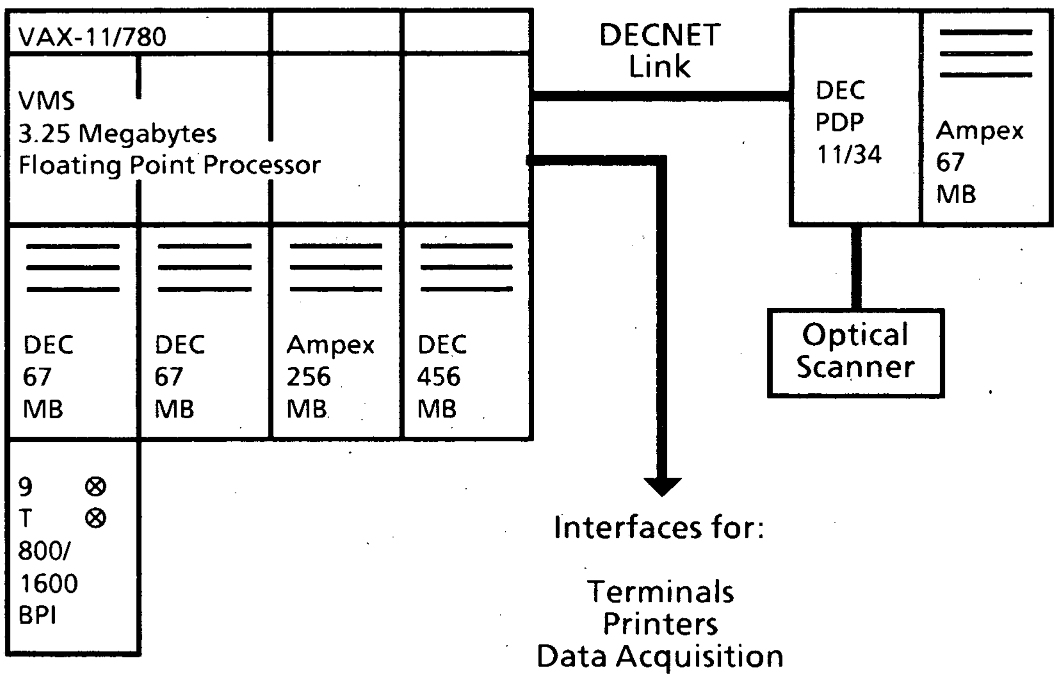


Figure LBL-B4

Physics Support System

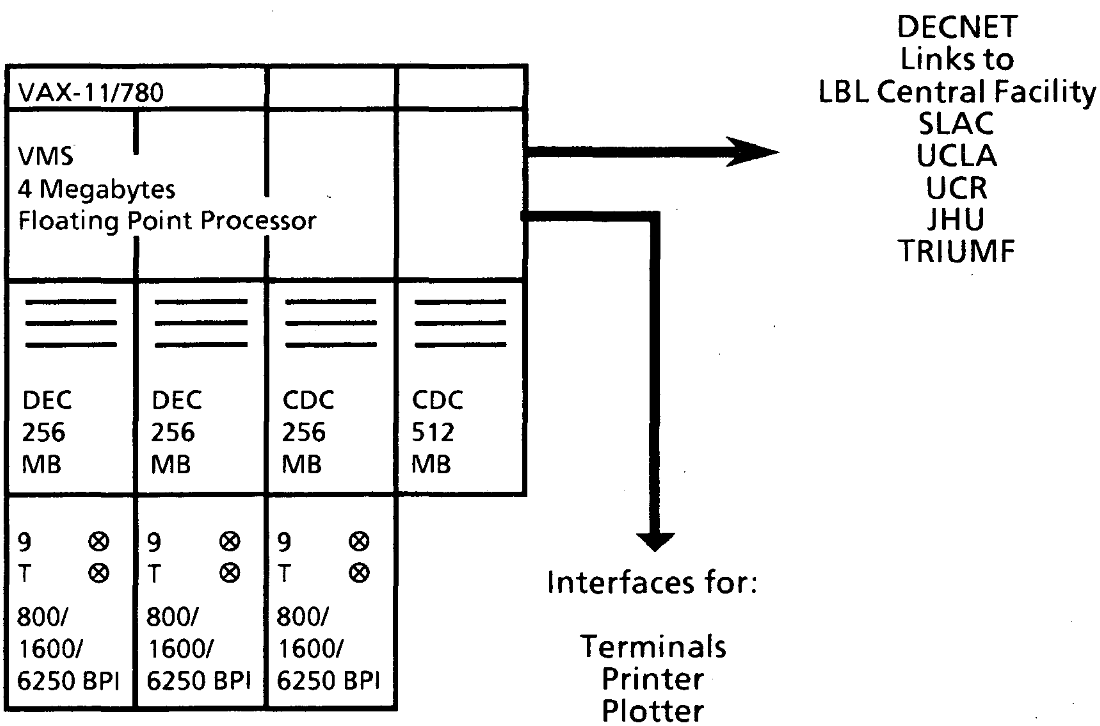


Figure LBL-B5

Heavy-Ion Spectrometer System

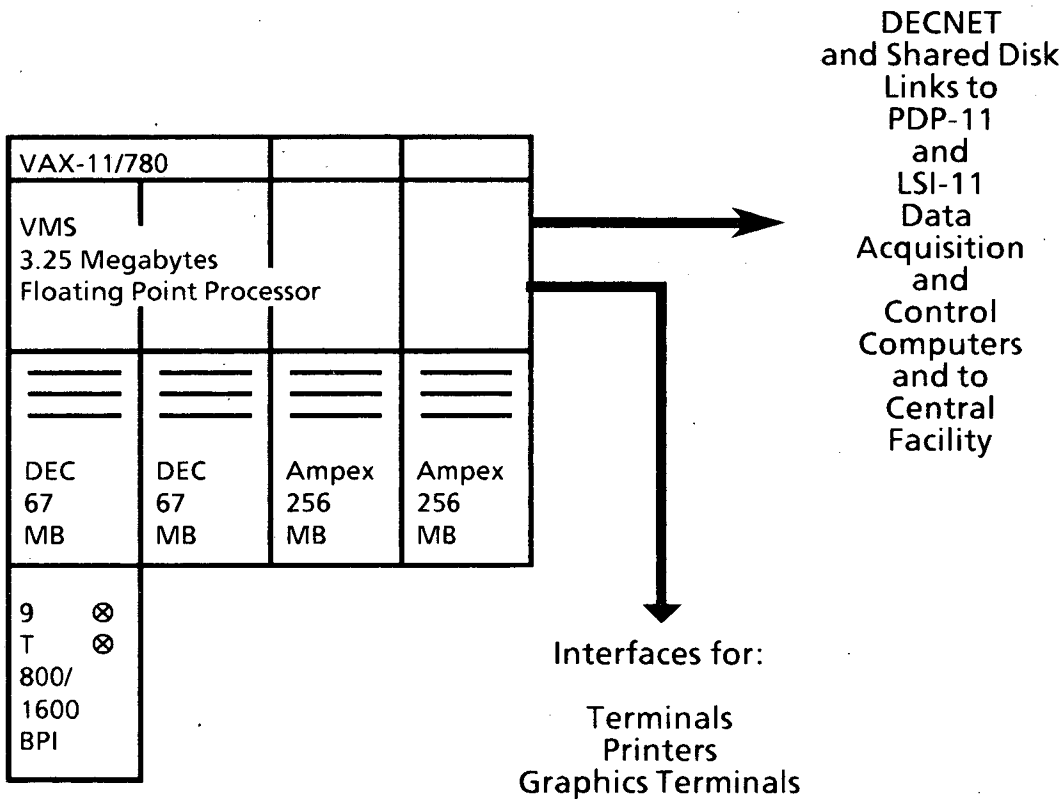


Figure LBL-B6

Biomedical Research System

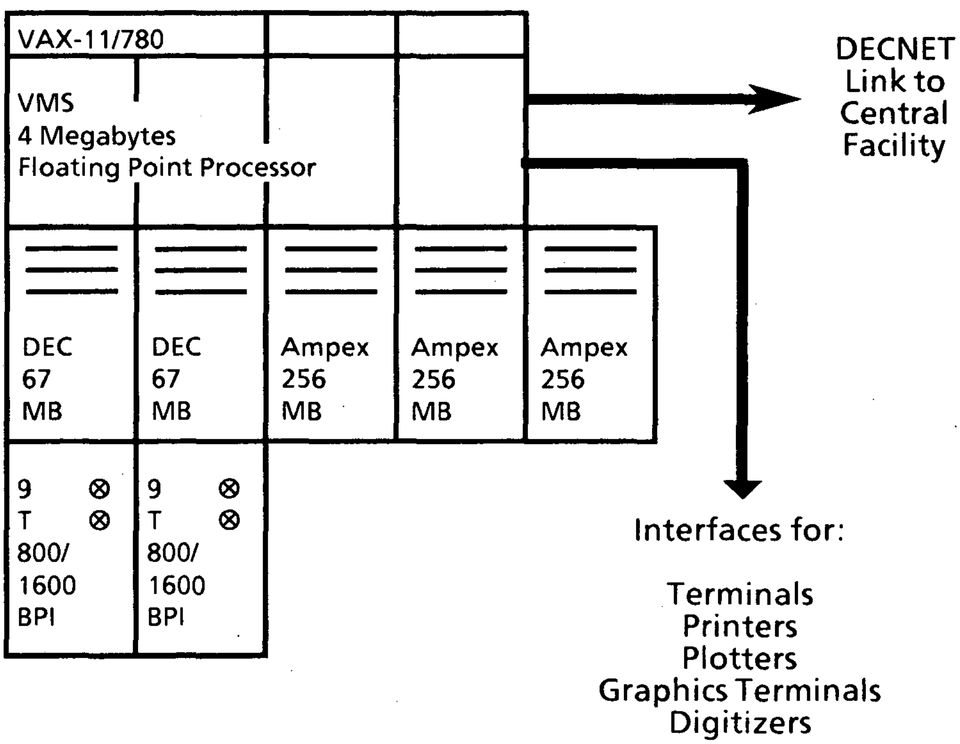


Figure LBL-B7

Technical Support System

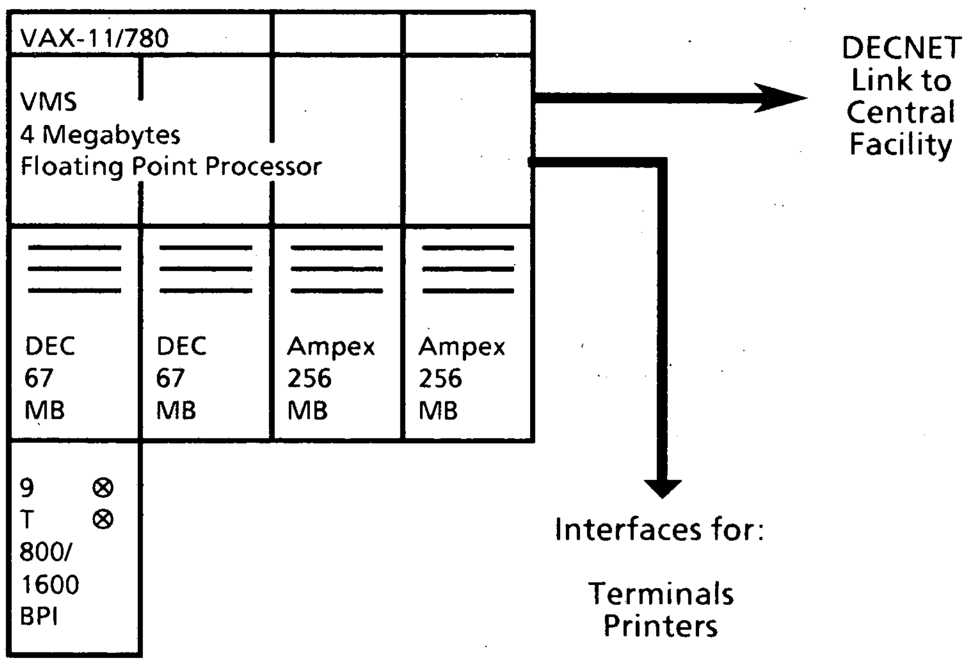
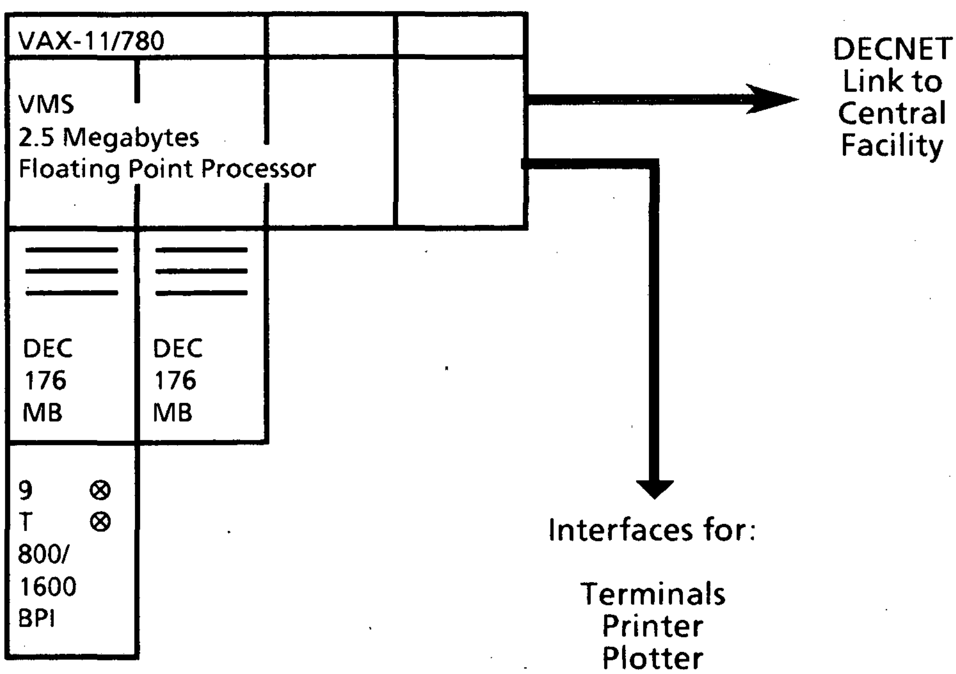


Figure LBL-B8

Molecular Interactions Computation System



SECTION D. COMPUTING ENVIRONMENT

Over the past two years, the Laboratory has reviewed the present computing environment and adopted plans for its future development (See Sections E1 and G1). The environment presented here is expected to change noticeably in the future. In particular, a greater degree of integration between the central and distributed facilities will be exhibited.

The Laboratory is continuously developing its capability to efficiently manage and support the central and distributed facilities. Many of the following descriptions refer to in-house hardware maintenance. This capability has been developed over the past six years so that now the Laboratory has a well-trained and effective group that can provide a more comprehensive, more timely and more economical service than would be otherwise available. Also, commonly used, vendor supplied software is managed globally in terms of acquisition and distribution within the Laboratory. This results in greater economy and efficiency in an area of increasing significance.

1. The Central Facility

The workload at the Central Facility consists of about 1600 batch jobs and about 1300 interactive sessions each day. These result from a broad spectrum of DOE and related users at the Laboratory and in the university and contractor communities across the nation.

The workload is mainly scientific computation. Although some jobs are quite small, others require more than an hour of CDC 7600 CPU time; jobs in the largest 10% by resource usage account for half of the total work, while those in the smallest 50% by resource usage account for less than 10% of the total work. The GSS file storage access and control system, residing in the

CDC 6000 machines, has become the chief means of tape access, and has exclusive use of the Automated Tape Library resource. Applications programming is entirely open shop, with assistance provided by consultants. Documentation describing how to use the computer systems, and a library of mathematical packages, are maintained by the staff of the Central Facility.

The facility is in continuous operation. During FY 1982, the principal computer was available to users 95.4% of the time. Availability of at least one of the 6000 front-end machines was more than 99%. Availability of the UNIX and VAX VMS satellite machines ranged from 93.2% to 97.6% for individual machines, with an average availability of 95.5%

Maintenance of the CDC and IBM computers and the major storage components is by vendor service engineers; Laboratory personnel maintain most of the communications interface equipment and the minicomputers.

The Central Facility uses a locally-developed operating system, BKY, for the CDC machines. This was required initially by the advanced requirements for scientific computation support, a field in which LBL has been at the forefront since the earliest years of computing. Continued use of the BKY system has been required by the diversity of storage devices and communications interfaces incorporated into the system.

Intermixed batch and interactive processing are supported on the CDC 6000 machines, which also handle I/O staging for the CDC 7600. Only batch processing is performed by the 7600 computer. An environment intended for text processing is provided by two PDP-11/70 machines using the UNIX operating system. The VAX-11/780 computers operate under the VMS operating system, primarily supporting programs written in Fortran. The three VAX systems provide specialized environments for three segments of the Laboratory workload: one is optimized for program development, one for numerical modeling and seismic processing, and the third provides interactive graphics support for a range of devices.

About one-fifth of the total batch work of the Central Facility is submitted by means of remote batch facilities. CDC 200UT, Harris COPE, BISYNC, and DECNET standard protocols are currently supported, as well as a locally-developed UNIX/Hyperchannel protocol. In addition to the network gateway machines, there are 35 RJE ports in active use, serving 90 sites, with an average of 18 simultaneously connected during workday hours.

Interactive processing accounts for about 10% of the total workload (25% of jobs) in the CDC machines, in addition to almost the entire workload of the satellite machines. A significant fraction of the batch work is interactively submitted. Access is provided by means of ARPANET and TYMNET, and by direct dial facilities. Automatic switches allow dedicated lines to be selectively connected by the user to any of the interactive computers. During workday hours the average number of simultaneous interactive users connected to the CDC, VAX, and UNIX machines is 100.

The major software systems used by the LBL Computer Center are tabulated in Table LBL-D1. Because of the open-shop environment, applications programs fall within the purview of the users, and are not included. (See SECTION E4).

Performance Measurement

Two areas of performance measurement have been developed in past years at LBL. A continuing activity provides basic reporting of usage details by device. This usage reporting provides the tool for measurement of growth and change in computing demand. Measurements of parameters characterizing specific system components have been used to optimize performance of these sub-systems as the need has arisen.

Historically the usage data were extracted from the operating system dayfiles. Before 1979, all peripherals were attached to the CDC 6000 and 7600 computers, so that dayfiles were a compact and comprehensive source for these data. The installation of DEC and IBM machines running under VMS, RSX, UNIX and VM/CMS operating systems, together with a local area network (based on the Hyperchannel) interconnecting all machines, made desirable the change to real-time collection of usage data via the network using a dedicated Accounting/Data Annalist machine (ADA). Such collection became possible for all computers and most peripherals during 1982, as did accounting reporting from computers. Reporting and collection extensions are planned for the future to allow the complete transfer of the usage reporting system from the obsolete CDC system.

An example of measurements to optimize performance is the installation of software counters to gather statistics of network performance and UNIX system overhead. No hardware monitors have been used. In each case system performance was significantly improved as a result of the increased understanding. Similar studies will be undertakenas the occasion requires.

2. Distributed Facilities

Computer Science Research Facility

This facility runs mostly interactive jobs during prime hours for program development, testing and documentation. Batch processing and experimentation requiring dedicated facilities are done at night and on weekends. Large CPU-bound jobs are used for combustion modeling studies while the information analysis systems (SEEDIS) are large data base codes that involve heavy I/O and CPU processing.

The system is operated by computer technicians and is available 24 hours a day including weekends. Vendor supplied operating system software, VAX VMS and Western Electric UNIX are used. LISP, C, Basic, Cobol and Fortran programming languages are available. Maintenance is performed by DEC and Systems Industries.

Biology and Biophysics Support System

This system, located in the Laboratory of Chemical Biodynamics, is used as a laboratory utility for on-line support of research and experimentation. It is devoted approximately equally to data acquisition and control, and to interactive processing and display of data from on-line or simulated experiments. Batch streams are also utilized for more lengthy analyses.

Applications software is devoted to data acquisition and control, archiving, analysis and simulation in support of Laboratory experiments. Operating systems are VAX VMS and RSX-11M for PDP-11's. The languages used are Fortran and MACRO assembly language. Microprocessor based data acquisition interface software is developed on the VAX and down-loaded to a PROM programmer.

Maintenance and operational support are provided by LBL personnel. The system is available 24 hours per day.

Physics Support Systems

Experimental high energy physics research is supported by three DEC systems, a PDP-11/70 at SLAC and VAX-11/780's at LBL and SLAC. The 11/70 at SLAC runs under the RSX-11M operating system and is used for data acquisition codes. The SLAC VAX is used in an interactive mode to monitor and control data quality; this interaction takes place on line while the experiment is in progress. The LBL VAX is used for production data analysis and Monte Carlo simulations. Both VAX computers use vendor-supplied VMS operating software. Fortran language is used throughout for application programming.

The computers at SLAC are operated by the experimenters, whereas the VAX at LBL is operated by computer operators. All three systems are available for use 24 hours per day.

The PDP-11/70 and LBL VAX are maintained by LBL personnel; the SLAC VAX is maintained under an agreement with DEC.

Heavy-Ion Spectrometer System

The HISS data acquisition and control system contains a VAX-11/780, a PDP-11/45 and an LSI-11/23. VAX VMS, RSX-11M and RSX-11S operating systems and DECNET are utilized. Programming is done in Fortran and MACRO assembly langage.

Applications software is directed toward data acquisition and control for HISS. About one sixth of the capacity of the VAX is available for general computing. Hardware maintenance of all computers is performed by LBL personnel. The system is available 24 hours per day.

Biomedical Research Systems

The Biomedical computer complex involves four distinct systems used in data acquisition, control, reconstructive graphics display and analysis for patient treatment, radiotherapy studies, and biophysics experiments. The patient treatment system is linked to the Bevatron control computer for coordination of operations and archiving.

All systems belong to the same DEC PDP-11 computer family (including one VAX-11/780), have a common technical computer staff, and utilize common systems software.

Applications software consists mainly of a large number of interrelated programs for on-line control and data acquisition, and for patient treatment planning. Operating systems are RSX-11M for PDP-11 systems and VMS for the VAX-11/780. Programming is done in Fortran and MACRO assembly language.

Maintenance is by LBL personnel. The systems are available 24 hours per day, and are operated by 70 users.

Molecular Interactions Computation System

This VAX-11/780 provides interactive computing and batch processing for research into molecular interactions. The VAX VMS operating system and Fortran are utilized. The system is available 24 hours per day and is maintained by LBL personnel.

Bevalac Control Systems

The Bevatron and SuperHILAC (Bevalac) accelerator complex is controlled and monitored by a group of interconnected Modcomp computers. Hardware and software are planned, developed, operated and maintained as a coordinated system. The Bevatron complex consists of a star-network of five computers; the SuperHILAC has another star-network of four computers.

Workloads at each accelerator are primarily on-line data acquisition and control with interactive operator control, some interactive program development and analysis, and almost no batch work. Applications software primarily consists of interrelated programs for on-line control and data acquisition. Operating systems are Modcomp MAX III and MAX IV; programming is done in Ratfor, Fortran, and MACRO assembly language.

The system is linked for data transfer to the Biomedical Research Control and Data Acquisition system and the HISS Data Acquisition System.

Maintenance is done by LBL personnel on a 24 hour per day basis. The systems are used by 20 accelerator operators and are available 24 hours per day.

Magnetic Fusion Energy System

A networked Modcomp II and Modcomp IV are used by physicists at the Neutral Beam Development facility to develop and test on-line data acquisition and analysis codes. A single Modcomp Classic at the Neutral Beam Engineering Test Facility is used to integrate these codes into a prototype "production" system to be used by engineers and trained operators. Versions of this prototype system have already been successfully applied to control of Neutral Beams on the Doublet-III Tokamak experiment at General Atomic and are currently being exported to the TFTR Neutral Beam contol systems at the Princeton Plasma Physics Laboratory.

Maintenance is by LBL personnel and the systems are available 24 hours per day.

Other Real Time Systems

There are a number of other minicomputer systems devoted to on-line data acquisition, control, and analysis, and interactive computation supporting experimental research at LBL. A large portion of these are DEC PDP-11 and LSI-11 series utilizing RSX-11M and RT-11 operating systems and are programmed in Fortran and MACRO assembly language.

Systems used to support physics and nuclear science include a dozen DEC PDP-11's, and share a common set of applications software utilizing the MULTI data acquisition system. MULTI is a set of applications software used at a number of laboratories and universities. Others include Modcomp machines under MAX III and MAX IV operating systems, and Hewlett Packard 1000, 9845 and 85 series machines using the HP operating systems, with programming primarily in Fortran, Extended Basic, and assembly language. Hardware and software maintenance is performed almost entirely by LBL personnel.

3. Business Systems

The responsibility for the Laboratory's administrative computing is shared between LLNL and LBL. The central accounting and personnel systems are maintained on common files processed on the Univac 1100/81 computer located at LLNL. Input to the central systems is prepared at LBL and sent to Livermore where it is processed along with the LLNL data. Administrative reports are produced at the central LLNL location and transmitted to LBL by courier or through telecommunications links to a remote job entry work station and to CRT terminals located at the Berkeley site.

Files that have been processed at the LLNL site are then made available to LBL either in the form of magnetic tapes containing the updated master files and detailed transaction data, or as on-line data base files that can be accessed from remote terminal devices located at LBL.

About half of the administrative computing workload is accomplished in this manner. The remainder is processed at LBL by a variety of methods. That portion of the total workload that is processed at LBL is increasing and present plans call for the LBL site to be essentially self-sufficient in both the accounting and administrative computing functions within five years.

Several administrative computing applications already are processed independently at LBL with necessary data being sent to the LLNL computer center to update the central financial, personnel and equipment files. These applications are processed on the LBL CDC 7600 computer, on a dedicated minicomputer, on an IBM 4341 computer located on the University of California Berkeley Campus, or by use of the NOMAD data base management services obtained commercially.

Data drawn from the LLNL computer are further manipulated at the LBL site and form the basis for the Laboratory's management information systems. These include a comprehensive accounting-report distribution system, an effort-reporting system, a purchase-order commitment report, and a central job-order control system, as well as cost planning and cost projection models.

Certain applications, such as the purchasing of stores inventory, inventory management and the preparation of "work for others" invoices, are performed at Berkeley in support of both sites. Work is currently under way at the Livermore site to develop systems to meet specific needs in these areas, and when completed, these functions will be separated with each site operating independently.

This Plan provides for the installation of a computer system to be dedicated to administrative data processing. In furtherance of this plan, program conversion work has already been initiated to transfer certain COBOL programs now run at Livermore to Berkeley. See Section E7, Justification for LBL-85-2 for a detailed discussion of this plan.

4. Overview of ADP Security Management

The Laboratory computer protection plan implements the provisions of DOE Order 1360.2. This plan is now approximately 75% complete. The computer protection plan is concerned with the physical security of all the Laboratory's ADP resources and with the protection of sensitive, non-classified ADP applications.

A Laboratory Computer Protection Manager is in charge of the overall implementation and supervision of the Laboratory's computer protection plan. He is assisted in these tasks by a number of Assistant Protection Managers associated with various functional areas of computer use in the Laboratory.

The following sensitive, unclassified computer applications are currently in place at the Laboratory:

1. Personnel data base
2. Budget management system
3. Supply applications
4. Proprietary software
5. Password files
6. Medical patient records.

A second version of the Laboratory's contingency plan for the protection of physical computer resources has now been completed An audit of sensitive supply applications at the Laboratory has been completed and its recommendations have been implemented.

Computer protection aspects of software and hardware procurement at the Laboratory have been centralized in the Office of Computing Resources.

Risk analyses of two sensitive computer applications have now been completed. Recommendations associated with these analyses are now in the process of implementation.

Table LBL-Dl

Software at the LBL Central Facility

1. Operating systems:	Two locally-developed multi-programming systems (named BKY), one for the 6000 machines, one for the 7600. Both systems feature automatic job-recovery procedures and sophisticated pre-emptive scheduling. The 6000 system also supports shared files on several devices, shared access to the remote subsystems, and several forms of interactive computing.
	A nearly standard UNIX system (level 7) for the PDP-11/70's. RSX-11M (version 4.0) for the PDP-11/34 and 11/44. VMS (version 3.1) for the VAX-11/780 machines. VM/SP 1.1 for the IBM-4331
2. Assemblers:	COMPASS MACRO-11 VAX-11-MACRO IBM ASSEMBLER
3. Languages:	Fortran: FTN version 4 (ANSI66 extended); VAX-11 FORTRAN (ANSI77) COBOL (version 3) BLIMP (a systems programming language) SNOBOL (an interpreter) PASCAL BASIC C

Table LBL-D1 (continued)

4. Cross-assemblers for:	HIS 516; PDP 8 and 9; MODCOMP I, II, III; NOVA; INTEL 8080; ALPHA LSI 5/2; Motorola 6800; Motorola 68000
5. Editors:	UPDATE (the standard CDC source-library editing facility) MODIFY (similar to UPDATE) NETED (ARPANET interactive editor); POE (an extension) LIBEDIT (the standard CDC object-library editing facility) ex (UNIX line editor); vi (UNIX screen editor); EDT (VAX screen editor)
6. Subroutine libraries and packages:	NPL Optimization Library Sandia Mathematical Library IMSL, SPSS, BMDP, EISPACK, NAG, FISHPAK, LINPACK, FUNPACK (math and statistics packages) MINDS (large, sparse optimization) MIMIC (continuous system simulation) GRAFPAC, IDDS, DI-3000, CONTOUR (graphics packages) CAM, CARTE (cartography packages) CHART, Graphmaker, Tell-a-Graph(display and analysisof tabular data) nroff, troff, and vtroff (text format preparation packages) Software Tools for VAX-VMS and 6000 BKY

Table LBL-D1 (continued)

7. File storage systems:	PSS (disk program storage system) GSS (tape file st orage manager)
8. Data-base management systems:	SYSTEM 2000 (a proprietary data base system) BDMS (a semi-experimental local product) DATATRIEVE for VAX SPIRES (available through a link to the UCB Campus)
9. Seismic Imaging Package:	DISCO (Digicon Interactive Seismic Computer System)

SECTION E. ADP PLAN

E1. ADP Planning Process

Organization

Computing activities at the Lawrence Berkeley Laboratory are managed under a single organization: the "Office of Computing Resources." This Office resides administratively in the Engineering and Technical Services Division and is the operational arm of a Laboratory-wide policy making body, the Computer Policy Board, which reports to the Director of the Laboratory.

The Computer Policy Board is made up of scientists and managers providing a Laboratory-wide perspective on the computing needs of the scientific and administrative programs of LBL. The Charter of the Board is to:

* Advise the Director on major policy matters relating to computing at the Laboratory.

* Seek information and advice from the scientific and technical community on matters relating to computing.

* Consider the scientific and administrative goals and requirements of the Laboratory in its deliberations, including short- and long-range institutional objectives.

* Direct the Office of Computing Resources. This includes setting priorities based on Laboratory scientific program needs, and detailed budget approval.

The Office of Computing Resources has general management responsibility and authority for all Laboratory computing and information processing activities. These duties include:

* Implementation of Laboratory, University and DOE policy and procedures for computing and information processing.

* Maintenance of a close working relationship with the Computer Policy Board, including the periodic development of detailed budgets to be submitted to the Board.

* Direction and development of Laboratory plans for computing and information processing system resources based upon short-term and long-range requirements and strategies.

* Periodic review of computing and information-processing activities to ensure implementation of the plans and to provide a mechanism for making adjustments.

All Divisions of the Laboratory contain computing and information processing functions. Three departments, in two Divisions, that are primarily concerned with computing activities are briefly described here.

* The Computation Department, in the Engineering and Technical Services Division, maintains and operates the Central Facility and the LBL communications network. This activity includes software product installation, systems programming development, consulting, performance analysis and accounting. The department also provides applications programming development and support for a wide range of Laboratory research activities.

* The Computer Science and Mathematics (CSAM) Department, in the Physics, Computer Science and Mathematics Division is a research and development group. In the course of these activities CSAM utilizes

minicomputer-based hardware for the purpose of experimental research in hardware and software systems. In conjunction with the Computation Department, CSAM offers consulting and performs development and maintenance support for the Laboratory's mathematical software library.

* The Real Time Systems Group (RTSG), in the Engineering and Technical Services Division, provides computing services in the areas of data acquisition and real-time control to Laboratory research programs and engineering projects. RTSG also provides the Laboratory with in-house maintenance for ADP equipment.

There are smaller computing functions within the Laboratory's research organizations. These components typically consist of a few people dedicated to computer applications work in a particular research discipline. Examples of such organizations can be found throughout the Laboratory.

An organization chart for the Laboratory is shown in Figure LBL-E1 and the matrix structure of computing management at LBL is shown in Figure LBL-E2.

Development of the Plan

During FY 1981 a major planning effort was undertaken by the Computer Policy Board to consider computing needs at LBL over the following decade. In this endeavor the Board held a series of hearings with divisional representatives who presented their expectations for future requirements. In addition, to aid the Board in their deliberations, three ad hoc subcommittees were formed. The first subcommittee investigated the characteristics, availability and suitability of modern main-frames. The second subcommittee broadly assessed ways to satisfy the near-term (5 years) computing needs of the LBL scientific community. The third subcommittee studied the characteristics and availability of commercially available text processing and electronic mail systems.

Furthermore, an ADP Requirements Team was organized by the Office of Computing Resources. The Team visited each Laboratory Division with the express purpose of exploring its future computing requirements. Finally, workload projections were solicited from individual researchers in support of particular programmatic requirements. Last year's plan was based upon the results of all these efforts. This year's plan represents an update of the previous plan with respect to requirements and contains additional information with respect to strategy.

The Laboratory's Institutional Plan provides the foundation and the general directional guide for the development of this plan for future computational resources.

Plan Review

Since Laboratory research scientists and program managers are the source of the data used in the development of this plan, they are also the first reviewers. Also, the plan has been thoroughly reviewed by the Director's Executive Committee, the Laboratory's Associate Directors, the Computer Policy Board and the Director's Office. The Office of Computing Resources has reviewed the technical aspects of the plan. Finally, the plan has been subsequently reviewed by various components of the San Francisco Operations Office.

Implementation

Implementation of the plan is the responsibility of the Office of Computing Resources. Laboratory research programs that initiated the requirements used in the formulation of the plan play an active role in the various phases of implementation. Periodic reviews and progress assessments are made by the Computer Policy Board.

LBL FY 1985 ADP LONG-RANGE SITE PLAN

Figure LBL-E1
LAWRENCE BERKELEY LABORATORY
UNIVERSITY OF CALIFORNIA

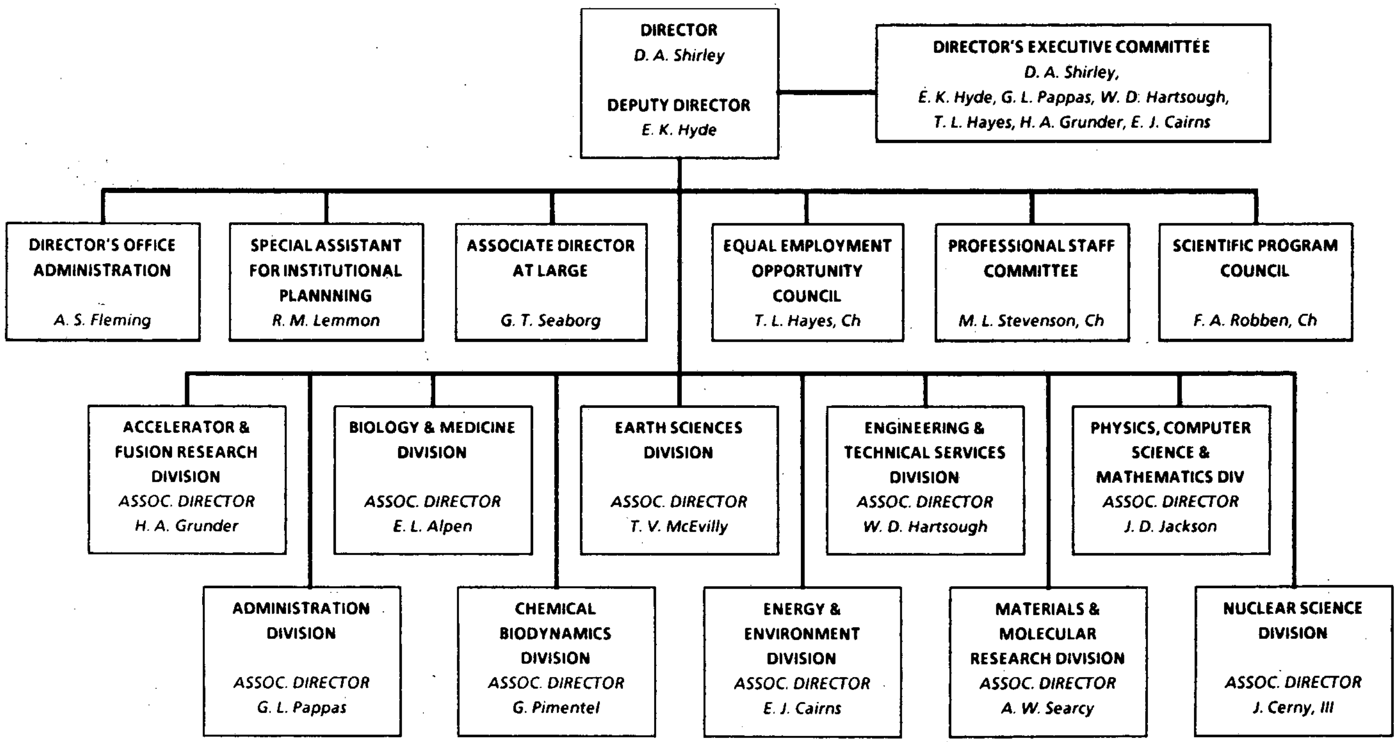
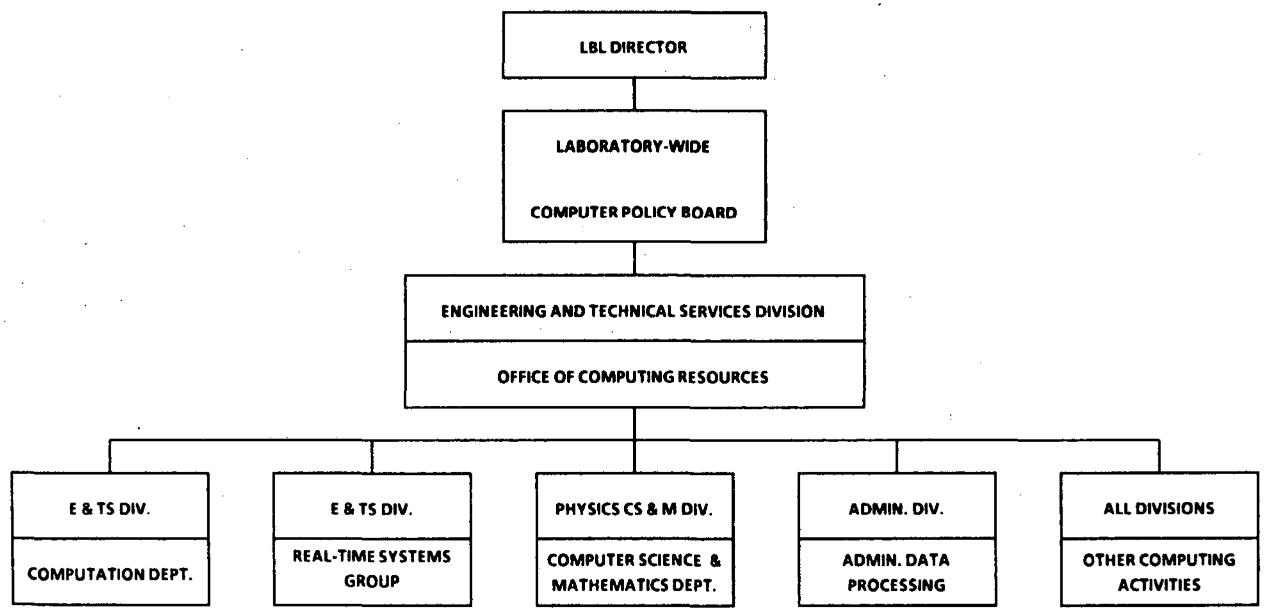


Figure LBL-E2

LBL Management Structure for Computing



LBL FY 1985 ADP LONG-RANGE SITE PLAN

ADP CAPACITY (NSU'S)

SITE Lawrence Berkeley Laboratory - LBL

SCHEDULE E2
Page 1 of 4

UNIT/ SYSTEM OR MIE NUMBER	ADP SYSTEM	PAST	CURRENT	BUDGET	PLAN	OUT-YEARS			
		FY 1982	FY 1983	FY 1984	FY 1985	FY 1986	FY 1987	FY 1988	FY 1989
1701-04	Central Facility								
	CDC 7600 (Nominal = 10,000)								
	Theoretical	10,000	10,000	10,000					
	Practical	10,000	10,000	8,000					
	CDC 6600 (Nominal = 2,200)								
	Theoretical	2,200	2,200	2,200					
	Practical	2,200	2,200	1,800					
	CDC 6400 (Nominal = 1,100)								
	Theoretical	1,100	825						
	Practical	1,100	660						
	NMM VAX-11/780 (Nominal = 1,200)								
	Theoretical	1,200	1,200	1,200	1,200	1,200	1,200	1,200	1,200
	Practical	1,200	1,200	1,200	1,200	1,200	1,200	1,200	1,200
	PDM VAX-11/780 (Nominal = 1,200)								
	Theoretical	1,200	1,200	1,200	1,200	1,200	1,200	1,200	1,200
	Practical	1,200	1,200	1,200	1,200	1,200	1,200	1,200	1,200
	IGM VAX-11/780 (Nominal = 1,200)								
	Theoretical	1,200	1,200	1,200	1,200	1,200	1,200	1,200	1,200
	Practical	1,200	1,200	1,200	1,200	1,200	1,200	1,200	1,200

LBL FY 1985 ADP LONG-RANGE SITE PLAN

ADP CAPACITY (NSU'S)

SITE Lawrence Berkeley Laboratory - LBL

SCHEDULE E2
Page 2 of 4

UNIT/ SYSTEM OR MIE NUMBER	ADP SYSTEM	PAST	CURRENT	BUDGET	PLAN	OUT-YEARS			
		FY 1982	FY 1983	FY 1984	FY 1985	FY 1986	FY 1987	FY 1988	FY 1989
LBL-85-3	Central Facility								
	Class IV (Nominal = 8,000)								
	Theoretical				7,000	8,000	8,000	8,000	8,000
	Practical				6,000	8,000	8,000	8,000	8,000
LBL-85-2	Administrative Data Processing								
	Class III (Nominal = 4,000)								
	Theoretical				2,000	4,000	4,000	4,000	4,000
	Practical				1,000	4,000	4,000	4,000	4,000

ADP CAPACITY (NSU'S)

SITE Lawrence Berkeley Laboratory - LBL

SCHEDULE E2

UNIT/ SYSTEM OR MIE NUMBER	ADP SYSTEM	PAST	CURRENT	BUDGET	PLAN	OUT-YEARS			
		FY 1982	FY 1983	FY 1984	FY 1985	FY 1986	FY 1987	FY 1988	FY 1989
1701-C9	Computer Science Research								
	F VAX-11/780 (Nominal = 1,200)								
	Theoretical	1,200	1,200	1,200	1,200	1,200	1,200	1,200	1,200
	Practical	1,200	1,200	1,200	1,200	1,200	1,200	1,200	1,200
	G VAX-11/780 (Nominal = 1,200)								
	Theoretical	1,200	1,200	1,200	1,200	1,200	1,200	1,200	1,200
	Practical	1,200	1,200	1,200	1,200	1,200	1,200	1,200	1,200
	H VAX-11/780 (Nominal = 1,200)								
	Theoretical	1,200	1,200	1,200	1,200	1,200	1,200	1,200	1,200
	Practical	1,200	1,200	1,200	1,200	1,200	1,200	1,200	1,200
1701-D1	Biology/Biophysics Support								
	VAX-11/780 (Nominal = 1,200)								
	Theoretical	1,200	1,200	1,200	1,200	1,200	1,200	1,200	1,200
	Practical	600	600	600	600	600	600	600	600
	Physics Support								
	VAX-11/780 (Nominal = 1,200)								
	Theoretical	1,200	1,200	1,600	2,000	2,000	2,000	2,000	2,000
	Practical	1,200	1,200	1,400	2,000	2,000	2,000	2,000	2,000

LBL FY 1985 ADP LONG-RANGE SITE PLAN

ADP CAPACITY (NSU'S)

SITE Lawrence Berkeley Laboratory - LBL

UNIT/ SYSTEM OR MIE NUMBER	ADP SYSTEM	PAST	CURRENT	BUDGET	PLAN	OUT-YEARS			
		FY 1982	FY 1983	FY 1984	FY 1985	FY 1986	FY 1987	FY 1988	FY 1989
1701-B3	Heavy-Ion Spectrometer System								
	VAX-11/780 (Nominal = 1,200)								
	Theoretical	1,200	1,200	1,200	1,200	1,200	1,200	1,200	1,200
	Practical	400	200	200	200	200	200	200	200
	Bevalac Support								
	VAX-11/780 (Nominal = 1,200)								
	Theoretical		400	1,200	1,200	1,200	1,200	1,200	1,200
	Practical		50	200	200	200	200	200	200
1701-D8	Biomedical Research								
	VAX-11/780 (Nominal = 1,200)								
	Theoretical	1,200	1,200	1,200	1,200	1,200	1,200	1,200	1,200
	Practical	1,200	1,200	1,200	1,200	1,200	1,200	1,200	1,200
1701-D2	Technical Support								
	VAX-11/780 (Nominal = 1,200)								
	Theoretical	1,200	1,200	1,200	1,200	1,200	1,200	1,200	1,200
	Practical	600	600	600	600	600	600	600	600
1701-C7	Molecular Interactions								
	VAX-11/780 (Nominal = 1,200)								
	Theoretical	1,200	1,200	1,200	1,200	1,200	1,200	1,200	1,200
	Practical	1,200	1,200	1,200	1,200	1,200	1,200	1,200	1,200
	TOTAL CAPACITY								
	Theoretical	27,700	27,825	28,200	25,400	28,400	28,400	28,400	28,400
	Practical	25,700	25,110	22,400	20,200	25,200	25,200	25,200	25,200

E2. ADP Capacity

Explanation of deviations in Theoretical and Practical Capacity from Nominal:

CENTRAL FACILITY

CDC 7600:	Will be replaced by the Class IV system.
CDC 6600:	Will be replaced by the Class IV system.
CDC 6400:	Will be replaced by the Class IV system.
Class IV System:	To be installed at beginning of FY 1985. Will have reduced capacity due to initial system orientation and until fully integrated into the Central Facility.

ADMINISTRATIVE DATA PROCESSING

Class III System:	To be installed in mid-FY 1985. Will have reduced capacity due to initial system orientation.

BIOLOGY/BIOPHYSICS SUPPORT

VAX-11/780:	Reduced practical capacity due to about 50% utilization for data collection and real time-experiment control.

PHYSICS SUPPORT

VAX-11/780: It is intended to upgrade this system, possibly to an 11/782 in FY 1984. Initial capacity will be reduced due to partial year availability.

HEAVY-ION SPECTROMETER SYSTEM

VAX-11/780: Reduced practical capacity due to principal use for data collection and real-time control. Although this capacity has decreased, some capacity will continue to be available during accelerator shutdown periods.

BEVALAC SUPPORT

VAX-11/780: Reduced practical capacity due to principal use for data collection and real-time control. Some capacity will be available during accelerator shutdown periods. Initial capacities reduced due to installation late in FY 1983.

TECHNICAL SUPPORT

VAX-11/780: Has reduced practical capacity because of usage to support the in-house hardware maintenance program.

CAD/CAM RESOURCES
NUMBER OF DESIGN/MANUFACTURING STATIONS SUPPORTED

SITE Lawrence Berkeley Laboratory - LBL SCHEDULE E2.1

UNIT/ SYSTEM OR MIE NUMBER	ADP SYSTEM		PAST	CURRENT	BUDGET	PLAN	OUT-YEARS			
	Hardware	Software	FY 1982	FY 1983	FY 1984	FY 1985	FY 1986	FY 1987	FY 1988	FY 1989
Instrument Science and Engineering	HP9845C	EGS45; DP1	2	2	2	3	3	3	3	3
Mechanical Engineering	*To Be Determined*		0	4	8	10	14	18	18	18
Electronic Engineering	*To Be Determined*		0	0	1	2	7	10	10	10
TOTAL NUMBER OF STATIONS			2	6	11	15	24	31	31	31

E2.1 CAD/CAM Resources

CAD/CAM Resources presently consist of two HP9845C based systems (see Figure LBL-E3), each with one workstation. These systems support the Instrument Science and Engineering Department in the Engineering and Technical Services Division. They are used to aid electronics drafting in the following ways:

a) Schematic drawing

b) Printed circuit board design

c) Generation of material lists

d) Artwork generation either on the system plotter or on off-site photoplotters

e) Computer-aided production of printed circuit boards through the generation of drill tapes compatible with numerically controlled machines

f) Full or partial list of equipotentials directly from any schematic for wire wrap tapes to be generated

g) Overall filing and archiving system

These systems came into use just before the end of fiscal year 1982. They share resources such as magnetic tape and a plotter. The acquisition of one or two additional workstations within two years is anticipated.

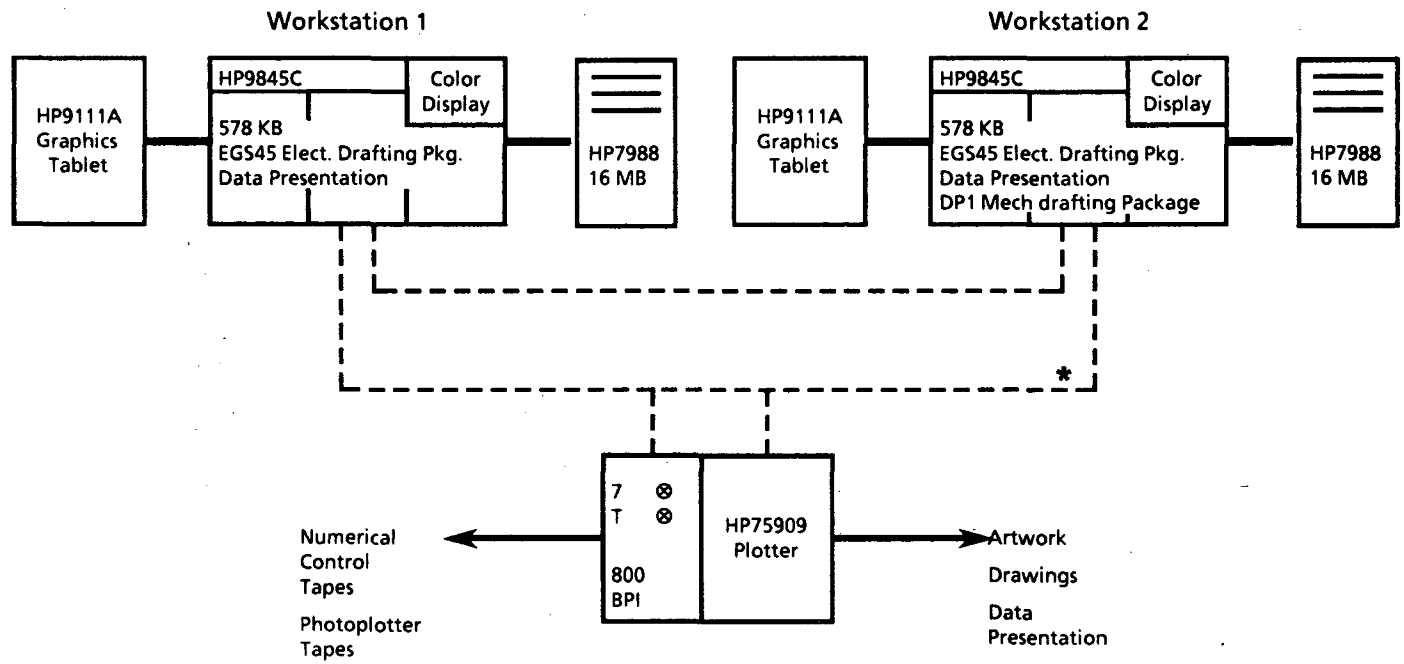
The Electronics Engineering Department, also in the Engineering and Technical Services Division, has similiar requirements, but has not yet obtained any workstations. First workstation installation is anticipated early in FY 1984 with additional workstations added over the following three years to a total of ten.

The Mechanical Engineering Department in the Engineering and Technical Services Division intends to install CAD workstations to gain increased productivity in design. The rapid rate at which CAD workstations are being adopted by industry is a good measure of their cost effectiveness. An initial goal is to achieve more rapid response to the needs of research programs for designs and graphics for proposals. In support of mechanical projects, revision and documentation of schedules, layouts and schematics will be automated and managed by CAD systems. This makes possible the timely distribution of accurate materials to all project members which in turn eliminates errors. Less expensive 2D systems will produce increases in productivity over manual drafting while more expensive 3D systems will increase the speed of design and engineering and provide numerical control capability for manufacturing. The Mechanical Department plans to obtain 4 workstations during FY 1983 and to increase the number, as their experience grows, to 18 workstations over a five year period.

LBL FY 1985 ADP LONG-RANGE SITE PLAN

Figure LBL-E3

Instrument Science and Engineering CAD/CAM Configuration



* These connections are switchable

LBL FY 1985 ADP LONG-RANGE SITE PLAN

ADP REQUIREMENTS (NSU'S)

SITE Lawrence Berkeley Laboratory - LBL **SCHEDULE E3**

B&R CODE	PROGRAM	PAST	CURRENT	BUDGET	PLAN	OUT-YEARS			
		FY 1982	FY 1983	FY 1984	FY 1985	FY 1986	FY 1987	FY 1988	FY 1989
AM	Geothermal	802	800	800	800	800	800	800	800
EB	Solar Applications	271	300	300	300	300	300	300	300
EC	Buildings & Community Systems	693 *	1,000	1,100	1,300	1,500	1,700	1,900	2,100
HA	Biological & Environmental Res.	681	700	700	700	700	700	700	700
HB	Life Sciences & Nuclear Medicine	792	1,000	1,200	1,400	1,600	1,800	2,000	2,200
KA	High Energy Physics	7,139 *	8,000	9,000	10,000	11,000	12,000	13,000	14,000
KB	Nuclear Physics	1,635 *	2,000	2,300	2,600	2,900	3,200	3,500	3,800
KC	Basic Energy Sciences	7,056 *	9,000 *	11,000 *	15,000 *	17,000	19,000	21,000	23,000
	Other Programs (AL, AP, AT, GB, LA)	699	800	900	1,000	1,100	1,200	1,300	1,400
	General Support	1,888 *	2,100	2,300	3,000 *	4,000 *	4,900 *	4,900	4,900
	Reimbursables -- DOE	2,263 *	2,200	1,800	1,600	1,600	1,800	1,800	1,800
	Reimbursables -- NRC External	35	0	0	0	0	0	0	0
	Reimbursables -- DOD Internal	360	400	400	400	400	400	400	400
	Reimbursables -- DOD External	1,082	500 *	250	50	0	0	0	0
	Reimbursables -- Other Internal	2,230	2,400	2,600	2,800	3,100	3,300	3,600	3,900
	Reimbursables -- Other External	2,116	2,000	1,000 *	500 *	100	0	0	0
	DOE Program Requirements	19,768	23,600	27,300	33,100	36,900	40,700	44,500	48,300
	General Support	1,888 *	2,100	2,300	3,000	4,000	4,900	4,900	4,900
	Reimbursables	8,086	7,500	6,050	5,350	5,200	5,500	5,800	6,100
	TOTAL REQUIREMENTS	29,742	33,200	35,650	41,450	46,100	51,100	55,200	59,300

*REQUIREMENTS FOR THIS PROGRAM INCREASE OR DECREASE BY 20% OR MORE AND BY 500 NSU'S OR MORE OVER THE PREVIOUS YEAR'S PROGRAM REQUIREMENTS OR FOR THE SAME YEAR OF LAST YEAR'S PLAN (A BRIEF EXPLANATION OF THE REASON FOR THE INCREASE/DECREASE MUST BE PROVIDED ON A SEPARATE PAGE).

E3. ADP Requirements

Reasons for increases or decreases of more than 20% and 500 NSU's in computing requirements in certain fiscal years:

EC Building and Community Systems

The decrease in actual usage between FY 1981 and FY 1982 stems from the completion of projects which had utilized substantial amounts of purchased time on a DEC PDP-10. Usage of this system was mostly phased out during FY 1982 and the system will be retired by mid-FY 1983.

KA High Energy Physics

Actual usage in FY 1982 increased over both FY 1981 actual usage and the FY 1982 prediction in last year's plan. During FY 1982 two new experimental programs began to analyze data. These are the TPC project and the TRIUMF muon experiment. At the same time the analysis effort for the Fermilab muon experiment continued at a high rate. Projected requirements for this year and beyond have been adjusted to reflect the increased analysis requirements of current and future experiments.

KB Nuclear Physics

Increases in computing requirements in the heavy ion nuclear physics program are associated with enhancements of experimental facilities. At the SuperHILAC and Bevalac, a project to provide high intensity beams of very heavy ions (up to U-238) was completed during FY 1982, and opened up new experimental vistas with an attendant increase in analysis requirements. Also, a new high-charge-state ion source is presently being developed for the 88-Inch Cyclotron; its successful completion will allow new classes of experiments to be performed. To take advantage of these accelerator enhancements, several major detection systems have been (or are being) developed, including the Plastic Ball, the HISS spectrometer, and a 4π gamma-ray counter. These devices will push the number of parameters measured per event into the hundreds, or even the thousands, thus substantially increasing the complexity of the data analysis.

The construction of a modern high-energy accelerator, such as the 10 GeV/nucleon Tevalac, will require computing for design calculations. Included will be such aspects as beam dynamics, magnet design and shielding. This requirement will cover a four-to-five-year period.

KC Basic Energy Sciences

The following principal sources account for the increased demand for computation by workers in the Basic Energy Sciences during the coming five years.

Theoretical Physics and Theoretical Chemistry

Pseudo-Potentials

At the present time, effective or pseudo-potential applications for the solid state are limited to elemental systems. Access to more powerful computational resources will make possible the extension to compound semiconductors, transition metals, more complex crystal types, and will permit more atoms per unit cell. In addition, the computation of surface states will become realizable and with it, the prospect of providing detailed information on catalysts of chemical interest. Such work would represent a considerable advance over computational studies of systems currently the subject of investigation in ultra high vacuum apparatus.

Monte Carlo Simulations

Many areas of chemistry and physics are being advanced by the use of Monte Carlo techniques, which are providing benchmarks against which to test approximations and new information in cases where experiments cannot provide accurate data. Simulation studies have played a crucial role in the elucidation of phase transitions and are also beginning to be used for the study of molecular electronic structure and the forces between atoms and molecules. LBL researchers are pioneers in this effort.

Ab Initio Electronic Structure Determination and Potential Energy Surfaces

Molecular theorists have been in the forefront of the use of powerful computers to determine the electronic structure and properties of atoms and molecules. New methods for describing electron correlations in large systems and excited states, including the graphical unitary group approach for reducing the difficulties associated with configuration interaction calculations and multi-configuration Hartree-Fock methods, are being spearheaded by LBL researchers. Furthermore, older methods are being applied to larger and more complex molecules and interacting systems with useful benefits. In addition, LBL scientists have been successful in developing new automated methods for finding reaction barriers, transition states, and equilibrium geometries of molecules. All these developments require increasing usage of computational resources.

Collision Dynamics

Advances in quantum, semi-classical, and classical methods for determination of inelastic collision events have reached the stage where theory is an essential adjunct to experimental verification of models. Theory further serves as a source of new information not obtainable by experimental methods for those atom-diatom systems for which accurate potential energy surfaces can be computed. For molecule-molecule energy transfer studies, important milestones depend upon computational power as well as new theoretical advances. For reactive scattering studies of large systems that may proceed through collison complexes, transition state theory can lead to undesirable uncertaintities in rates and cross sections. Quasiclassical trajectory calculations can provide better results in such cases when sufficient computing resources are made available.

Combustion Research

Laboratory activities in the DOE combustion research program account for a large portion of the increase. Experimental verification of two dimensional numerical models of turbulent combustion in simple geometries has now been achieved. It is planned to expand these models to three dimensions and to much more intricate and realistic geometries. This will require approximately thirty times more computational capacity by FY 1988 than is currently being used.

In addition, advances in theoretical and computational methods have enabled the confirmation of the postulated initial chemical steps in the combustion of ethylene. Studies of larger systems of combustion interest cannot be performed to comparable accuracy because of their large CPU speed requirements and because of the memory limitations of the CDC 7600. Both the capability and capacity of a Class VI computer are necessary for this research.

Geosciences

The Laboratory's Earth Sciences Division is engaged in an ambitious program of research to understand certain fundamental geological processes. These processes include the flow of fluids and gases through fractured and porous media, and the chemistry associated with this flow.

This research involves developing sophisticated mathematical models of geological and geochemical systems and the implementation of these models in computer programs. During the period covered by this Plan some of these models will reach sufficient refinement to deliver new insights into real geological processes. Computing requirements for certain types of numerical modeling could increase very rapidly by factors up to ten or more given adequate capacity and capabilities. Analysis and graphical display of geological and geophysical data could result in an annual doubling in required capacity given adequate interactive computing and graphics capabilities.

Until a more powerful computing system is made available, the Earth Sciences Division will be constrained by the paucity of real memory, the slowness, the inaccessibility, and the expense of the existing Laboratory central facility. For example, most Earth Sciences numerical modeling programs are written for three dimensions but executed for only one or two in the majority of cases. When these constraints are removed it will be possible to reap the benefits of the current Earth Sciences research program.

General Support

Decrease in FY 1982 actual usage from FY 1981 is primarily due to reduction in force in the Computation Department. This decrease reflects a large reduction in development for existing systems in the Central Facility. Increasing requirements in FY 1985 through FY 1987 reflect the planned transition from a batch processing environment to an interactive one. See Justification for LBL-85-2 for a detailed discussion of these requirements.

Reimbursables--DOE

Usage was predicted to decrease due to the planned release of the present Central Facility CDC 6000/7000 machines. Since LBL-84-1 was not approved, no steps were taken to begin phase out of these systems during FY 1982. Actual usage in FY 1982 was equal to that in FY 1981.

Reimbursables--DOD External

The planned release of the present central facility CDC 6000/7000 machines will result in the phasing out of this external usage.

Reimbursables--Other External

The planned release of the present central facility CDC 6000/7000 machines will result in the phasing out of this external usage.

LBL FY 1985 ADP LONG-RANGE SITE PLAN

CAD/CAM REQUIREMENTS

NUMBER OF DESIGN/MANUFACTURING STATIONS NEEDED

SITE Lawrence Berkeley Laboratory - LBL

SCHEDULE E3.1

UNIT/ SYSTEM OR MIE NUMBER	ADP SYSTEM	PAST	CURRENT	BUDGET	PLAN	OUT-YEARS			
		FY 1982	FY 1983	FY 1984	FY 1985	FY 1986	FY 1987	FY 1988	FY 1989
KA	High Energy Physics	1	2	3	4	5	6	6	6
KB	Nuclear Physics	1	3	6	7	12	15	15	15
	Other Programs (AL,GB,HA)	0	0	0	3	5	7	7	7
	General Support	0	1	2	2	3	4	4	4
	TOTAL NUMBER OF STATIONS	2	6	11	16	25	32	32	32

E3.1 CAD/CAM Requirements

LBL is just beginning to integrate CAD/CAM systems into its Engineering Departments. Section E2.1, CAD/CAM Resources, contains a short discussion of future goals and requirements for CAD/CAM systems.

E4. Narrative

AM Geothermal

The Earth Sciences Division is engaged in numerous projects connected with geothermal energy research and development. These projects include research in geophysical exploration techniques and analysis, theoretical investigation of geothermal reservoir dynamics, geological and reservoir engineering work at several present and potential geothermal reservoirs (for both geothermal electric and direct thermal applications), and numerical modeling of geothermal power plant performance. Computer usage by these projects generally falls into one of three categories. These are: mathematical modeling of hydrothermal, geophysical, and other phenomena; collection, storage and manipulation of geological and geophysical data; and analysis, comparison and display of data and results.

Numerical Modeling

Numerical modeling accounts for more than half of the total geothermal-related computer usage. The four groups most heavily engaged in modeling are Reservoir Engineering, Cerro Prieto, Geophysical Exploration Technology, and Energy Utilization Technology. The cost of computing is the principal constraint for all four of these programs. Due to funding limitations, one group--Geophysical Exploration Technology--is not able to apply the models they have developed to the solution of realistic three-dimensional problems. The amount of computing that could constructively be done on these projects is at least ten times the present usage.

The memory size on the CDC 7600 is a major constraint on the reservoir engineering and geophysical models. To model adequately some interesting problems a substantially larger memory than that on the 7600 is needed. The virtual memory system on the VAX-11/780 addresses this constraint, but the VAX is significantly slower than the CDC 7600 and hence results are delayed.

Data Storage and Manipulation

Geological, hydrothermal, and geophysical research frequently involves handling large quantities of information. These data are normally stored on magnetic tape and processed using the LBL central facility. Since much of this work must be done interactively, the poor interactive response on the present computer system is a major problem. The Automatic Tape Library has helped data storage requirements somewhat, but further improvement is still needed.

Analysis and Display

The analysis and display of geological and geophysical data through computer graphics and other methods are essential tools in this research. Computer graphics is especially useful in the earth sciences because of the very large quantities of data involved, which make understanding and analysis almost impossible without graphic visualization.

Interactive computing for data analysis, especially with graphics is immensely useful to research in the earth sciences. Interactive methods allow a researcher to change or add to a planned course of action, to follow up interesting leads or to modify a display in minutes rather than in hours or days. The added flexibility and "friendliness" possible with interactive software make it easier for a researcher to deal directly with the data and bring the computer closer to its ideal role as a "mind amplifier". The Earth Sciences Division has begun to move into this area with the recent purchase of the PETROS interactive well-log analysis software package.

A very great improvement in interactive response time is needed, especially during the normal working hours. It does very little good to enable a researcher to interact with an executing program if the time between interactions is 20 minutes. In addition, better interactive graphics hardware and software, fast hard-copy graphics, much more disk capacity, and a good interactive data base management system are needed. Given a system that satisfied these requirements, a very large increase in this category of computing, on the order of threefold, could be expected. At present, poor interactive response and lack of good interactive graphics systems have a very strong negative effect on the amount and type of computing done.

EB Solar Applications

Energy and Environment Division projects in this area include Passive and Active Solar Systems.

Research in passive systems involves the development, maintenance, and application of several large, complex Fortran programs that simulate the thermal performance of either whole buildings, or some particular aspect in great detail. These programs are run in batch mode on either the CDC 7600 or CDC 6600. Interactive time on the CDC 6600/6400 is used primarily for maintenance and development projects related to the simulation codes. These activities account for approximately two-thirds of passive research computer usage.

The remaining third of passive research computer usage is on the PDP-11/70 UNIX systems, and consists of word processing, document preparation, and input preparation for applications use of the simulation codes. At present, almost all applications batch jobs are submitted to the 7600 from the ll/70's via the Hyperchannel. Some interactive programs have been written and implemented on the ll/70's for the analysis of small amounts of output data from the simulation codes.

There is presently only a small amount of use of the VAX systems; it is expected to increase with the planned development of more sophisticated interactive data analysis programs, including graphics. In the future, significantly increased use of graphics capabilities for presentation and analysis of simulation data generated by the codes described above is anticipated. Requirements for computing are expected to grow slowly for passive research projects.

The Active Systems project investigates active solar systems, such as those containing solar driven air conditioners. Computer utilization is similar to that of the passive projects and is expected to remain roughly constant in future years. Graphics output is a requirement of this project, as well as a document-preparation utility.

EC Buildings and Community Systems

Research in this area covers heat transfer in residential and commercial buildings, ventilation and air infiltration, and windows and lighting; a second research area includes residential energy demand, including appliance energy consumption.

The largest demand on computing facilities comes from the DOE-2 building energy analysis program. This is a public-domain computer program, devised at LBL, which simulates energy usage in buildings. It is developed and maintained by the Building Energy Simulation (BES) group at LBL on the CDC 7600 and on the Numerical Modeling VAX-11/780. It is run by both the BES and the Building Energy Analysis groups on these machines. Further development of the program is severely hindered by lack of adequate memory capacity on the 7600. VAX machines avoid the memory limitation but have proved to be too slow and to have inadequate secondary storage for DOE-2 development. Application of DOE-2 on the 7600 is also limited by the small memory size. Although designed to simulate a building with up to 64 thermal zones, at most 20 zones can be run on the 7600. Again the VAX systems are too slow to make the simulation of large buildings practical. Provision of the memory capacity, along with the CPU speed, of a large modern machine will be immediately beneficial to the users and developers of DOE-2 and will result in a doubling of usage.

LBL research on windows and lighting utilizes computers for engineering analysis of window systems, for analysis of data from demonstration buildings, and for studying the economics of various window and lighting systems. Both batch and interactive modes are used.

Tracer gas experiments are utilized to study air infiltration through building envelopes. Presently, computer facilities are used to provide background data processing for an experimental house in a nearby suburb. Equal use is made of batch and interactive processing. Long turnaround times for interactive users at the central facility are a major restraint to researchers involved in these studies.

Researchers studying ventilation use computing facilities for data analysis and ventilation data base development and implementation. Both batch and interactive modes are used.

Development work has begun on a finite element indoor air quality model. As the model developes, it is expected that the increased computing speed (and therefore reduced cost) of a modern machine will provide an improvement over the CDC 7600.

Research is also undertaken on educational facilities and hospitals. Computing is done to evaluate the effects of modifications on the facilities.

The LBL UNIX system is used a great deal for both document and job preparation. More capable facilities for these purposes are urgently needed. The ability to connect to other computer installations via ARPANET is also important to these projects.

In the Energy Analysis Program appliance energy demand is modeled using the BERD/RES Residential Energy Demand Model, a public-domain program for use at the national and regional levels. The Residential Hourly and Peak Load Model developed at LBL uses the results of the BERD/RES Model. These models run on the VAX-11/780 because of the modern Fortran 77 compiler, virtual memory capability and interactive graphics facilities. The peak load model takes 1 to 2 hours to run on the VAX depending on overall system load. The running performance of these models will benefit greatly from a modern system. Model development and data base acquisition are handicapped by limited storage space and inadequate communications with other machines.

HA Biological/Environmental Research

Environmental Pollution and Human Health.

Relationships between disease and environmental quality are under investigation utilizing an integrated data base and sophisticated analytical tools and methodologies. In addition to specific studies of the relationships between disease (especially cancer), mortality, environmental quality and socio-economic data, this research encompasses development and evaluation of analytical methods applicable to questions about the health effects of environmental pollution.

The Populations at Risk to Environmental Pollution (PAREP) project is a continuation and expansion of research initially begun in collaboration with the Environmental Protection Agency.

Computational resources to support this work include the central facility at LBL, the SEEDIS VAX-11/780 system, and systems at Brookhaven National Laboratory and the EPA. Computer system capabilities critical to the environmental health effects research program include archival mass storage, rapid access storage, analytical software including powerful statistical routines, and color mapping in both batch and interactive modes.

Mutagenesis, Carcinogenesis and Plant Biochemistry

This research will reveal how environmental factors influence the normal functions of cells. Mutations produced by environmental chemicals are a rapidly increasing cause of cancer. To learn how chemicals cause mutation and what role this process has in the neoplastic transformation of mammalian cells is the goal of this research. Data acquisition and graphical analysis for these studies are performed on the Biology and Biophysics Support VAX.

Biological Effects of Magnetic Fields

Physiological performance in mammals exposed to magnetic fields is being evaluated from measurements of metabolic parameters, core body temperature, activity and neurobehavioral parameters, and specific functions associated with the cardiac, neural, visual, immunological, and hematopoietic systems. Circadian variations are being monitored as an index of stress imposed by magnetic field exposure.

The assessment of physiological functions in animals exposed to magnetic fields is being carried out primarily by means of noninvasive techniques that utilize special transducer systems, e.g., biotelemeters for monitoring deep-body temperature for periods of weeks, thereby providing information on the amplitude and phase of circadian rhythms in physiological parameters as an index of stress associated with chronic magnetic field exposure.

An extensive set of computer codes is used at the central facility for the analysis of circadian rhythms in core body temperature, activity, respiration, body mass, food intake and excreta. The acrophase, amplitude and period of the circadian variation are determined by a time series analysis.

Epidemiology of Magnetic Effects

The health effects of static and slowly varying magnetic fields are being evaluated through a retrospective epidemiology survey of cyclotron and bubble chamber workers at the national laboratories. The data collection is complete and the analysis will be carried out using general purpose computers. The data base involves approximately 1500 by 100 parameters (750 exposed and 750 controls with 100 attributes per individual).

Computer codes for statistical analyses have been developed and will be used on these data during the next few years.

Combustion Research

The combustion research group carries out the statistical analysis of large quantities of experimental data on the CDC 7600, as well as calculations of some complex chemical kinetics and fluid mechanics problems. This work uses the file handling, data storage and computational capabilities of the CDC 7600. The level of computing is expected to remain constant over the next several years. Improvement in the cost-effectiveness and speed of the Central Facility would lead to increased utilization through the initiation of new projects.

HB Life Sciences Research and Nuclear Medicine Applications

Structural Biophysics and Biophysical Chemistry

This research is composed of many projects in the areas of molecular and cellular biology, organic and photochemistry, and biophysical chemistry. Major examples are the mechanisms of chemical and viral transformations of living cells, chemical evolution, the role of biological structure in the energy conversion processes of green-plant photosynthesis, and the applications of the newest biophysical techniques (such as NMR, x-ray spectroscopy and x-ray diffraction) to study fundamental processes in nucleic acids, proteins, membranes and nerves.

New methods and models have been developed for computing the structure of nucleic acids whose base sequences are known. These projects utilize experimenal data acquisition and analysis resources of the LCB Biology and Biophysics Support VAX System.

Electron Diffraction/Structure

The objective of the Electron Diffraction/Structure program is to determine the three-dimensional structure of unfixed and unstained biological materials at near-atomic resolution. The electron microscope is used to collect both image data and diffraction data from crystalline arrays. Three-dimensional reconstruction algorithms utilizing Fourier transform methods are used to determine the 3-D electron density from the series of resulting 2-D projection data sets.

Currently, methods are being developed which will extend the attainable resolution from the present 7Å range to 3.5Å. These methods include advances in specimen preparation techniques that maintain hydration and preserve flatness.

A variety of membrane proteins are under active investigation. Their structure is being determined using presently available techniques. In addition, they are being studied with new methods presently under development.

This work involves the following major computational tasks:

1. Fourier transformation of images up to 2048 x 2048 in size.

2. Image processing and interactive display for both data selection and evaluation and for analysis and interpretation of 3-D results.

3. Extraction and reduction of electron diffraction information from arrays up to 6000 x 1000 in size.

4. Algorithm development for the automation of a significant portion of the data processing required.

Effects of Heavy Particle Radiation

Because of their physical and biological characteristics, heavy-ion beams show special promise for the treatment of vascular abnormalities. The depth-dose characteristics of heavy ions allow a more effective dose of radiation to be delivered locally to the vascular abnormality rather than the skin and normal tissues that surround it.

The objective in charged particle dose delivery is to shape a three-dimensional high-dose region around a defined target volume. Using a series of CT scans through the region of interest, computer programs generate a treatment plan and both physical and isoeffect isodose distributions.

Experimental Clinical Medicine

The objective of the Clinical Experimental Medicine program is to perfect and apply noninvasive methods of assessing the biological function of brain, heart, lung, and other organs in man. Positron emitting isotopes attached to naturally metabolized compounds are used for the quantitative assessment of the three-dimensional distribution of metabolites. Radiation doses are very small, so that studies can be perfomed to delineate physiology and health effects in man without risk. Methodological approaches include use of positron tomography, autoradiography, and stable isotope analytical instruments and multidimensional kinetic analysis.

The specific goal is to perfect a method for noninvasive three-dimensional assessment of biochemistry and physiology in health and disease with emphasis on brain disorders, coronary heart disease, pulmonary biochemistry, and radiation effects. Specific health effects being investigated are the influence of magnetic fields, heat, and carbon monoxide on metabolism and blood flow in the brain and heart of man.

Specific tasks requiring the use of a general purpose computer are:

1. Monte Carlo simulation of physical processes for the purpose of evaluation of medical instrument design (geometry, detector materials and configurations, etc.).

2. Monte Carlo simulation of the operation of electronic circuits for the purpose of evaluating dead time as a function of event rate in data acquisition systems.

3. Four-dimensional reconstruction algorithm development using maximum entropy, pseudo-inverse, and iterative techniques.

4. Kinetic analysis of four-dimensional biological data involving non-linear fitting programs using compartmental modeling techniques.

5. Image processing and display of physiological functions and metabolic activity.

KA High Energy Physics

Physics Research

The high energy physics program at LBL is a comprehensive research effort in both experimental and theoretical particle physics. Much of the high energy physics computation is devoted to experimental design, data reduction and analysis, and the development of programs.

The experimental program utilizes accelerator facilities at a number of laboratories. At SLAC, a number of groups are working at PEP and are planning to utilize a new facility, the Stanford Linear Collider (SLC), which may be built there by 1986. There is a program of colliding beam and fixed target experiments at Fermilab. There is an experiment underway at TRIUMF in Vancouver, Canada. It is expected that by the late 1980's there will be an active program using a colliding beam facility at Brookhaven. Each of these research activities has different computing requirements.

An LBL-SLAC collaboration is using the magnetic detector, Mark II, for the study of electron-positron collisions at PEP. The experiment has an on-line SLAC VAX-11/780 computer for data-taking and monitoring. All data reduction and analysis, as well as program development, are done on the computer systems at SLAC. Program libraries are maintained at SLAC. LBL physicists make extensive use of the LBL Dataswitch and microwave facilities to compute interactively on the SLAC system. In 1986, the MKII will be moved to the SLC. This future work will also use the SLAC computer facilities.

The Time Projection Chamber (TPC) is an innovative detector which has been installed at PEP. LBL is collaborating with groups from UCLA, UCR, Yale, Johns Hopkins University and University of Tokyo. The experiment uses a SLAC VAX-11/780 on-line computer for analysis of a data sample. The same analysis programs are used offline for data reduction and for data simulation. Program libraries are maintained on the Physics Support VAX within the LBL Central Facilty.

Analysis is done there and on other VAX systems at LBL, UCLA, UCR, and Johns Hopkins. Physicists working on the remote systems can access the library using DECNET.

The TPC group makes use of all LBL network facilities. The Dataswitch and microwave link are used for terminal communication, and a microwave DECNET link between the TPC on-line computer and the Physics Support VAX is used to transfer programs and data files. The high speed Hyperchannel network is used to connect the Physics VAX to the central facility in order to use printers and microfiche. The Hyperchannel will also be used to provide access to mass storage facilities within the Central Facility.

The Colliding Detector Facility (CDF) is a large detector designed to study high energy proton-antiproton collisions at Fermilab. The large collaboration of institutions who are constructing this facility is centered at Fermilab, and much of the data reduction and analysis will be done there, when the apparatus begins taking data in 1986. LBL physicists will use DECNET to link the LBL VAX system with VAX computers at Fermilab.

The Fermilab muon program has used the LBL CDC 7600 extensively. Approximately half the data reduction was carried out at LBL; the remainder used the same programs on the Fermilab CYBER 175's. Most data analysis was done at LBL. The muon program will be continued at the Fermilab Tevatron beginning in 1985. It is expected that some of the data reduction will be done at Fermilab but that a significant fraction will be done on the Physics Support VAX at LBL.

The muon decay experiment at TRIUMF is an effort comparable in size to that of the Fermilab muon program. Data taking in 1982 resulted in approximately 300 tapes that were processed on the Physics Support VAX and on the VAX computers in the Central Facility. Data taken in 1983 will also be processed on these computers.

Work in theoretical physics uses the VAX systems and other computers. Future work will use either a Class VI machine or a large array processor.

In addition to the major projects described above, there are continuing programs of experiment design, analysis of data from smaller experiments, software development, and word processing.

Accelerator Design: Superconducting Magnets

This is a study of the design of superconducting magnets required for particle accelerators in high energy physics. The physics of quench phenomena and techniques of quench protection are included. Techniques resulting from this study can be used in other laboratories such as the Cornell Electron Storage Ring as well as in private-sector laboratories.

Accelerator Theory

Theoretical work on accelerators encompasses a broad range of activities, from direct contributions to design and development of operating and proposed accelerator facilities at LBL, to collaboration with other laboratories on projects of mutual interest.

KB Nuclear Physics

Nuclear Science

The principal objective of Nuclear Science research is the experimental and theoretical investigation of heavy ion induced nuclear reactions. Experimental research utilizes three of LBL's major accelerators: the 88-Inch Cyclotron, the SuperHILAC, and the Bevalac. At all three accelerators the trend is toward measuring more and more parameters per event, using local minicomputers for data acquisition. For example, the low energy experimental groups, using heavy ion beams from the 88-Inch Cyclotron and SuperHILAC, are now measuring data with more than 16 parameters per event. New detection systems now being designed for these groups, such as a 4π gamma-ray counter system, are expected to double or triple the number of parameters per event within the next 2-3 years. At the Bevalac, experiments utilize unique relativistic heavy ion beams, and take on more of the character (and complexity) of high energy physics work, with perhaps as many as 1000 parameters per event expected for the newly designed detection systems such as the Plastic Ball and HISS spectrometer--both of which are now on-line.

The main ADP requirement for the experimental groups is for the reduction and analysis of large amounts of data from on-line experiments, typified by the transformation and sorting of multiparameter incremental data. Currently, much of this work is accomplished by the same minicomputers, varying in size from the PDP-11/34 to the VAX-11/780 and the MODCOMP CLASSIC 7870, that are incorporated into experimental configurations. These computers are utilized to the extent possible to develop and run experimental data analysis programs in the most economical fashion. In addition to the increasing complexity of data reduction and analysis, which requires progressively more processing capability, solutions to these problems are often also limited by I/O and memory restrictions. A single experiment may produce up to 200 magnetic tapes of data to scan and may require the ability to manipulate several multi-megaword arrays. Anticipated growth necessitates the continuing addition of computing capacity geared toward the analysis of multiparameter data. It is expected that the MIDAS system (See Appendix A.) will provide a facility dedicated to this type of analysis.

The Nuclear Science theory group's computing consists mostly of program development. At present, only a few medium-size programs are in use at any one time; these concern nuclear-matter calculations and calculations related to the statistical breakup of nuclei in heavy ion collisions. The major limitation on computer usage for this group is cost. For example, due to budgetary constraints, cascade or time-dependent Hartree-Fock calculations are only carried out on the HISS VAX or at other sites (such as LLNL) by collaborating scientists.

Any improvements that would facilitate the editing, debugging, and storage of programs would be of direct benefit here, as would improved interactive capabilities and more easily accessible graphics programs.

Accelerator Research

The Bevatron/Bevalac and the SuperHILAC utilize the central computing facility, primarily in an interactive mode, for such functions as beam optics calculations, statistical management and analysis of accelerator operations and calculations of parameters for advanced accelerator devices. Computing requirements for both on-line and batch work are expected to increase 10-15% per year. Some of this increase, however, can be handled on micro- or minicomputers.

In addition, research and development efforts in the design of superconducting magnets for the Tevalac will require some computer time for field calculations and stress analyses. Most of these calculations can be handled on an existing small computer, but there will remain a need for some large scale capability.

KC Basic Energy Sciences

Materials Sciences

The bulk of Materials Science computer usage is concentrated in four research groups. The first of these is concerned with the computation of the fundamental physical properties of metals and semiconductors and their surfaces, largely through the use of pseudopotential models.

The second concentrates upon the direct simulation of phase transformations and mechanical behavior in idealized solids, and particularly addresses the kinetics of those processes at finite temperature. The other two most computationally-oriented groups are concerned with the structural analysis of crystals, defects and surfaces, through the analysis of electron diffraction data. The remaining Materials Science computer usage is spread over a large number of smaller efforts and principally involves data analysis and routine computation.

The level of computer usage in Materials Science will continue to increase substantially if low-cost computation is available. Moreover, the trend in metallurgy and ceramics is toward an increasing recognition of the value of numerical computation and simulation as a theoretical tool. A new computer user is the National Center for Electron Microscopy. NCEM usage is expected to grow over the next 3 years, drawing on both graphics capabilities and the handling of large arrays via remote terminals with direct lines. Such computation will provide theoretical support for the Atomic Resolution Microscope by performing image simulation and image processing.

Chemical Sciences

The principal computer usage by Chemical Sciences groups includes computation of (1) the electronic structure and properties of novel ground and excited-state molecules, (2) regions of potential energy surfaces for characterization of reaction pathways, (3) isolated molecule properties and characteristics of interacting systems for collisional energy transfer studies, (4) force constant matrices and anharmonic corrections for excited states of polyatomic molecules needed for theories of polyatomic photodissociation and chemical reaction.

Also included are the synthesis and measurement of the physical and chemical properties of compounds of the actinide and lanthanide elements, and the development of sequestering agents for plutonium. In the latter program, the computer facilities are used in crystal structure determinations from x-ray diffraction methods, calculating formation constants from potentiometric titration data in the Pu sequestering project, atomic structure analyses of optical spectra using Hartree-Fock calculations, and parametric analysis of optical data.

Computer usage for quantum chemistry in FY 1981 was doubled compared with FY 1980, and it doubled again in FY 1982. This trend will probably continue if low-cost computing is made available. In order to remain competitive in this computationally oriented field, substantial computing capacity must be available. Moreover, significantly increased computing capability must be obtained at costs low enough to be met by the various groups needing these resources.

Low Energy Nuclear Science

The Isotopes Project compiles and evaluates nuclear structure and decay data and develops compilation methodology; its efforts are coordinated with those of other domestic and foreign data centers. The mass chain evaluations are published in Nuclear Data Sheets and the data are maintained in the international Evaluated Nuclear Structure Data File (ENSDF). This computer file is available for data retrievals and serves as the basis for specialized publications. In particular, the Isotopes Project will use data in ENSDF to produce a Radioactivity Handbook for applied users of nuclear data.

The Isotopes Project uses the LBL Computer Center to assist with the evaluation of published data, for the preparation of input to ENSDF, and for the production of publications such as the Radioactivity Handbook. It requires both batch and interactive processing to assist in handling and storing large quantities of data. DATATRIEVE, a DEC data base management system now in use, is a great asset. Other requirements are a highly reliable mass storage system and publication-quality text and graphics output devices. Work required for the publication of the Radioactivity Handbook is expected to double the modest computing requirement for this project in FY 1984.

Geosciences

Computational Center for Seismology

The Computational Center for Seismology conducts research into earthquakes, earth structure, wave propagation, and the mathematical bases of, and applications for inverse theory and acoustic imaging. The present computational resources of the Center were achieved by augmenting an existing Central Facility VAX-11/780 with specialized hardware and software. The hardware includes magnetic tape drives and controller suitable for tapes formatted according to the conventions of the Society of Exploration Geophysicists, a floating point array processor, a 36-inch-wide electrostatic plotter, and graphics terminals. The Digicon Interactive Seismic Computer System software package has been obtained to provide a base for current research and for further software development.

The Center is designed to provide a focused environment for research into modern computational seismology. Emphasis will be on increasing access to state-of-the-art numerical algorithms for seismology research, and on supporting an active computer science research effort addressing problems in seismology.

Other Programs

The Geosciences Group in the Earth Sciences Division is presently using the CDC 7600 to develop and run large numerical models of geochemical processes. These models are being applied to investigations of chemical migration in ground-water and to simulation of chemical processes in hydrothermal systems.

The comparatively small memory capacity of the CDC 7600 is a limiting factor in the development of the very large combination heat and fluid flow and geochemical codes which are presently being contemplated. When they are developed, these codes will require a very large address space (on the order of 30 megabytes) and a great deal of processor time. It is expected that the virtual memory system on the Numerical Modeling VAX will help in development, however, its slow speed will limit is usefulness for calculation of numerical models.

The Reservoir Engineering and Exploration Group performs research in geophysical exploration techniques and analyses, theoretical investigations of isothermal and non-isothermal reservoir dynamics, and numerical modeling of ground water flows. All these efforts require substantial computer usage for modeling, data analysis, data storage and graphics display.

Applied Mathematics Research

Research programs in applied analysis, computation mathematics, and numerical methods for partial differential equations emphasize numerical studies and techniques applicable to computational fluid dynamics, in particular combustion modeling. The combustion studies are directed towards the construction of realistic models that are suitable for comparison with experiments and are capable of being used for design purposes. Large-scale scientific computing capabilities are clearly required by research of this type.

Anticipated growth of these research programs will require continued and expanding use of large-scale computational resources.

The CRAY-1 computer at the Lawrence Livermore National Laboratory is currently being utilized via ARPANET to develop numerical methods based on explicit local wave tracking for computing compressible fluid flows. Vector computers such as the CRAY-1 have the capacity to perform realistic calculations because the numerical methods used interact strongly with the computer architecture. Furthermore, as the physics being modeled becomes more complicated, the amount of computer time required to explore the range of design options for these methods will increase substantially. For the methods currently being investigated, one hour on the CRAY-1 is about equivalent to 10 hours on the LBL CDC 7600.

Computer Science Research

This program involves basic research to advance the state-of-the-art in computer science and information systems. The major areas of development include data management, information display and analysis, distributed systems and software engineering. Data management research provides methods for organizing, accessing and manipulating large, complex data collections. Emphasis is on statistical data bases, such as socio-economic data, energy production and consumption and experimental data. Techniques being developed are in the areas of data modeling, user interfaces, data base compression and efficient data access. Research into information display and analysis addresses methods for unifying graphics, data management and analysis tools and for making them easier to use.

Distributed computing research centers on integrated approaches to inter-site and intra-site linking of computer systems and the role of "personalized resources" (local minicomputers oriented to the needs of small groups but with access to remote large-scale facilities). Software engineering provides techniques for the synthesis of reliable software systems from standard, quality modules, and the creation of tools to increase the productivity of software systems designers, implementors, and users.

SEEDIS

The Socio-Economic Environmental Demographic Information System (SEEDIS) is a development and demonstration component of basic research in information analysis techniques. The objective of the SEEDIS project is to establish a comprehensive, computer-based information system for energy policy analysis, environmental impact studies and other socio-economic analysis applications. The information system is a tool for the investigation of analytical technology and display techniques, the investigation of user interfaces and the application of data management to very large, complex data bases.

Seismic Data Center

As an extension of the basic research program in Computer Science, the Computer Science and Mathematics Department is funded by the Office of Geophysical Research of the Defense Advanced Research Projects Agency for development of a Seismic Data Center. This effort supports DOD-directed efforts, agreed upon in a Memorandum of Understanding between DOE and DOD, on the development of Comprehensive Test Ban Seismic Monitoring Stations and attendant systems. The research effort at LBL focuses on data management architectures within distributed systems, local network interconnections, analytical work stations and data display.

Plant Biochemistry

Plant biochemistry research is concerned with the biochemistry of photosynthesis and biosynthesis in green plants, and ranges from biochemical structures of the membrane responsible for light conversion to the elucidation of biosynthetic pathways leading to end products such as sugars, proteins, alkaloids, hydrocarbons and toxins formed in plants. Bacterial conversion of plant organic compounds to H_2 and other useful substances is being investigated.

Solar Energy Utilization Based on Photosynthesis

This research is directed towards developing methods, based on research in green plant photosynthesis, for the economic utilization of solar energy. It involves the study of photo-induced electron transfer reactions with the ultimate goal of producing hydrogen and oxygen from water. Synthetic systems are prepared involving sensitizer, electron acceptor, and electron donor, and their behavior is studied under the influence of visible light. The kinetics of individual steps in the reaction are of primary interest.

A flash photolysis apparatus has recently come on-line, which sends data to the Biology and Biophysics Support VAX for computation. Modeling, kinetics analysis, and deconvolution of absorption and emission spectra are expected to be the principal applications of the computer to the research effort. These analysis programs are being developed on the VAX and will require an increasing level of service as this research progresses.

Other Programs

AL Energy Storage Systems

The Electrochemistry group in the Energy and Environment Division is presently using the central facility for modeling of battery electrodes. The group also uses UNIX for documentation. Modest growth is anticipated in both activities.

AP Waste Isolation

The safe isolation of toxic and radioactive wastes is the focal point of a number of research projects in the Earth Sciences Division. These projects are primarily concerned with characterizing the natural geologic and hydrologic environments at disposal sites, and with predicting the ways inwhich the natural environments are disturbed by introduction of the waste. Computers are used in all stags of this work, including design and analysis of field test programs, modeling of predisposal *in situ* conditions, prediction of environmental changes produced by excavations and waste introduction, and prediction of rates and directions of waste transport. These efforts involve both basic investigations of the fundamental behavior of heterogeneous rock and soil, and applied investigations of specific sites.

Computer applications to basic research in waste isolation have primarily addressed the hydrologic behavior of fractured rock masses. Codes have been prepared to study the narture of fluid movement through networks of discrete, interconnected fractures. The objective of this work is to determine the conditions under which the discontinuous fracture system can be macroscopically treated as a continuum for regional groundwater flow analysis. Studies are being carried out for both mass fluid flux and contaminant transport. The VAX systems are being used to run the codes, and the CDC 7600 is being used for plotting output. The capabilities of these systems are sometimes exceeded by realistic two-dimensional approaches to these problems, and operational costs are very high. A three-dimensional code is being developed which will better simulate the natural conditions, but its application will probably be restricted due to present limitations in funding and equipment.

Computer applications to applied research have concerned field sites where test facilities are located (e.g., Stripa, Sweden) and field sites at existing or proposed waste isolation facilities (e.g., Hanford Reservation, Washington; Weldon Spring, Missouri). These applications have involved studies of the thermomechanical behavior of rock, prediction of contaminant transport, and analysis of vertical hydraulic conductivity. The CDC 7600 has been used for most of this work, although conversion to the VAX is in progress to permit larger problems to be treated. A significant limitation in this work is the lack of good computer graphics systems at LBL.

AT Magnetic Fusion

The Technical Support VAX is used to support and develop pieces of the Neutral Beam Data Acquisition and Control System. Although the Neutral Beam System runs on a Modcomp Classic, the fact that most of the Neutral Beam software is written in Fortran and rests on the portable "Software Tools" virtual operating system allows significant development to be done in the richer interactive environment of the VAX and later transported to the Classic. Also, the large virtual address space of the VAX allows physicists and computer scientists to do analyses that are too large for the Modcomp Classic address space.

GB Inertial Confinement Fusion

The Heavy Ion Fusion research program carried out by the Accelerator and Fusion Research Division could easily double computer usage if computing costs were significantly less. The simulation computations involved in this research are well suited for very large scale machines. These programs solve systems of nonlinear partial differential equations by some discretization process, which simulates the continuous problem with many discrete ones. The number of discrete points used to simulate a continuous problem is limited by the size of the computer memory available and the cost per computed point. In this category of problems, a Class VI machine can provide tremendous computational benefits.

LA Data Retrieval

The Information Methodology Research Project is developing a system to provide computer assisted aids to document indexing for the DOE Technical Information Center Energy Information Data Base (RECON). The goal is to provide more efficient processing of documents and document surrogates through the use of interactive computing techniques.

LBL FY 1985 ADP LONG-RANGE SITE PLAN

ADP SYSTEM RESOURCE SHARING (NSU'S AND COSTS)
(Dollars in Thousands)

SCHEDULE E5
Page 1 of 2

SITE Lawrence Berkeley Laboratory - LBL

PROGRAM B & R CODE	IDENTIFICATION OF SHARING PARTNER/ NATURE OF SERVICE/ ADP SYSTEM	PAST FY 1982	CURRENT FY 1983	BUDGET FY 1984	PLAN FY 1985
	Resource Sharing Requirements				
KA	SLAC	3500 ( )	3500 ( )	3500 ( )	3500 ( )
KA	Fermi	500 ( )	500 ( )	500 ( )	500 ( )
LA	DOE-TIC	0 ( )	200 ( )	200 ( )	200 ( )
General Support	LLNL	297 (413)	390 (500)	430 (550)	390 (500)
	Resource Sharing Commitments				
	Argonne	32 (30)	28 (30)	28 (30)	28 (30)
	Richland	590 (355)	430 (300)	430 (300)	430 (300)
	GE	298 (216)	210 (175)	210 (175)	210 (175)
	Ames	89 (35)	0 (0)	0 (0)	0 (0)

LBL FY 1985 ADP LONG-RANGE SITE PLAN

ADP SYSTEM RESOURCE SHARING (NSU'S AND COSTS)
(Dollars in Thousands)

SCHEDULE E5

SITE Lawrence Berkeley Laboratory - LBL

PROGRAM B & R CODE	IDENTIFICATION OF SHARING PARTNER/ NATURE OF SERVICE/ ADP SYSTEM	PAST FY 1982	CURRENT FY 1983	BUDGET FY 1984	PLAN FY 1985
	Resource Sharing Commitments, Continued				
	LLNL	82 (71)	0 (0)	0 (0)	0 (0)
	Other DOE	78 (66)	0 (0)	0 (0)	0 (0)
	UC DOE-Related	273 (201)	172 (200)	172 (200)	172 (200)
	Other Universities DOE-Related	85 (44)	0 (0)	0 (0)	0 (0)
	EPRI	189 (128)	130 (100)	65 (50)	30 (25)

POINT OF CONTACT: Eric Beals (415) 486-5351
FTS 451-5351

LBL FY 1985 ADP LONG-RANGE SITE PLAN

ADP COMMERCIAL SERVICES (NSU'S AND COSTS)
(Dollars in Thousands)

SITE Lawrence Berkeley Laboratory - LBL

SCHEDULE E6

PROGRAM B & R CODE	IDENTIFICATION OF VENDOR/ NATURE OF SERVICE/ ADP SYSTEM	PAST FY 1982	CURRENT FY 1983	BUDGET FY 1984	PLAN FY 1985
EC	University of California, Berkeley DEC PDP 10	210 (12)	200 (11)	0 (0)	0 (0)
KB	Stanford University Data Base Management System	46 (48)	20 (20)	10 (10)	0 (0)
LA	University of California, Berkeley DEC PDP 10	210 (12)	200 (11)	0 (0)	0 (0)
General Support	National CSS, Inc. Data Base Management System	202 (263)	240 (350)	240 (350)	170 (250)
General Support	University of California, Berkeley IBM 4341, Data Base Management System	40 (49)	60 (60)	75 (75)	70 (70)

E7. Major Planned Acquisitions/Lease Continuations

Introduction

The thrust of the LBL FY 1984 ADP Long-Range Site Plan was directed towards achieving access to very-large-scale (Class VI or above) computational capability. Many LBL research programs are unable to make adequate progress without such a resource. The access mechanism proposed in that plan was the acquisition of a Class VI computer (LBL-84-1) to become LBL's principal computing resource. Provision of Class VI capability to LBL scientists continues to be a major concern, and it is clear that this concern is shared by the Office of Energy Research (OER) and by other DOE research institutions. During the past year the OER has studied the problem of providing such large-scale resources to all of its contractors. One of the solutions that has been proposed is the establishment of a shared, central facility with access available to all Energy Research contractors. LBL supports this option because it would provide high quality service in a cost-effective manner to the entire Energy Research community. The LBL FY 1985 ADP Long-Range Site Plan is based upon the assumption that such an OER central facility will come into being within the next few years, and that it will satisfy LBL's growing requirement for large-scale computing. As a result, LBL-84-1 has been removed from this year's Plan . In its place a complete proposal for the establishment of a National Center for Energy Research Computing (NCERC) to offer large-scale, very-high-speed computing to all Energy Research contractors is included as LBL-85-1.

LBL-84-1 was also intended to replace the existing CDC 7600, 6600 and 6400 computers, which are the principal LBL general management computers. The LBL FY 1985 ADP Long-Range Site Plan includes provision for replacing these obsolete and operationally expensive systems with a modern, interactive and cost-effective mid-scale Class IV system. This replacement system will satisfy those LBL scientific computing requirements that will not need the unique resources of the NCERC. The replacement system is labeled LBL-85-3. Installation of this system in FY 1985, coupled with the establishment of a National Center for Energy Research Computing, will satisfy the LBL programmatic requirements for computing in a cost-effective manner. The benefits of this replacement are given in detail in the Justification for LBL-85-3.

The implementation strategy associated with LBL-84-1 included an initial system (for service front-end development) that was to be subsequently reutilized for administrative data processing once the total LBL-84-1 system was installed. The present Plan provides for administrative data processing requirements as a separate acquisition which is detailed in the Justification for LBL-85-2.

LBL FY 1985 ADP LONG-RANGE SITE PLAN
MAJOR PLANNED ACQUISITIONS/LEASE CONTINUATIONS

SCHEDULE E7

SITE: LAWRENCE BERKELEY LABORATORY **MIE NO.** LBL-85-3 **LAST MIE NO.** LBL-84-2
MIE NAME: Class IV Computer System

PROGRAM B & R CODE: KB† **PROGRAM NAME:** Nuclear Physics

MIE DESCRIPTION: Principal LBL Scientific Computer System.

FUNDING PROFILE ($000) (Direct Costs Only)

	PAST	CURRENT	BUDGET	PLAN	OUT-YEARS			
ACQUISITION	FY82	FY83	FY84	FY85	FY86	FY87	FY88	FY89
CAPITAL								
OPERATING				640	640	640	640	640
CONSTRUCTION								
NON-ACQUISITION								
MAINTENANCE				94	94	94	94	94
OTHER (Specify) ††				109	105	100	100	100
TOTAL †				843	839	834	834	834
OFFSETS †††				(1,488)	(1,529)	(1,570)	(1,611)	(1,611)
NET				(645)	(690)	(736)	(777)	(777)

INSTALLATION DATE (MO/YR) October, 1984

MANAGEMENT CLASSIFICATION: X **GENERAL** __ **SPECIAL**

INITIAL PURCHASE EQUIVALENT COST $2,600 **(ALL LEASED ITEMS)**

ACQUISITION STRATEGY:
__ PURCHASE __ LEASE FOR ____ YEARS
__ LEASE WITH OPTION TO PURCHASE; EXERCISE PURCHASE OPTION (MO/YR) ____
X LEASE TO OWNERSHIP; PAYMENTS TO BE COMPLETED BY FY 1989
__ OTHER (EXPLAIN):

PROCUREMENT STRATEGY:
X FULLY COMPETITIVE __ SOLE SOURCE (Explain)
__ LIMITED COMPETITION (Explain)

EXPLANATION:

MILESTONES: (FOR ITEMS TO BE ACQUIRED IN FY83 THRU FY85)
IMPLEMENTATION PLAN July, 1983
SOLICITATION RELEASE October, 1983
CONTRACT AWARD June, 1984
(JUSTIFICATION MUST BE APPENDED TO THIS SCHEDULE)

† Costs will be distributed to all programs on basis of usage.
†† Training in FY 1985, 86 and Software Maintenance.
††† These offsets are explained in Justification for LBL-85-3.

Justification for LBL-85-3

Access to a large-scale, high-speed computing resource is a major computing concern for LBL. However, this Plan is based on the assumption that such access will be provided as an OER-wide shared resource. With large-scale requirements satisfied in this manner, the scientific computing capacity dedicated to LBL program needs may be reduced accordingly. To match internal capacity and requirements properly and to provide a more effective computing environment for LBL scientists, the Laboratory intends to retire its obsolete CDC 7600, 6600 and 6400 systems and install a state-of-the-art Class IV system. This replacement will remove a large number of severe limitations imposed by the old CDC systems, reduce operating costs; it will, however also reduce the internal LBL scientific computing capacity by approximately 5,300 NSU's. Each aspect of this replacement program is discussed in the following paragraphs.

Removing Limitations.

There are six areas where the existing CDC complex seriously limits computational support to LBL programs. All of these limitations will be removed by the installation of LBL-85-3.

1. Architectural limitations. The CDC systems do not have virtual memory, which means that large problems must be specially structured to utilize complicated overlaying and buffering techniques. The memory architecture of the CDC 7600 compounds the problem by imposing a two-level central memory structure upon its users. Furthermore, the operating systems are not suitable for interactive access. (The maximum effective capacity on the two 6000's is less than 40 simultaneous users each, and the 7600 does not support interactive use at all.)

2. Reliable service. One of the most dramatic improvements in computing hardware in the last ten years has been in *reliability*. The CDC complex could not benefit from this improvement because of its outmoded design. It requires several on-site maintenance personnel and a large store of expensive spare parts. Despite the care lavished upon the 7600 the time between consecutive interruptions averaged just over 16 hours in 1982; modern machines typically run a week or more between service interruptions.

3. Non-availablilty of new software. For historical reasons, these computers are supported by locally developed operating systems. A consequence of this situation is the difficulty of providing industry-standard software packages to the users. This difficulty increases with time, for two reasons:
   i) The locally-developed operating system started out logically, philosphically, and technically close to the standard, vendor-supplied system. With time, the two grew increasingly apart, and it required increasing effort both to understand new software releases and to re-tailor them to fit the LBL environment.
   ii) The difficulty of the integration task increases geometrically with the increase in the number of software packages that have to be integrated.

4. Diminished scientific productivity. This is clearly the most significant problem. The LBL CDC systems do not provide the users with modern computer tools, whether they be languages, libraries, applications packages, or comprehensive interactive job-preparation and debugging facilities *on the target machine.*

5. Lack of support for modern peripherals. These computers were not designed to be coupled to equipment from the mainstream development of peripheral technology. LBL has partially solved this

problem by developing and installing its own channel adapter to provide hardware compatibilitywith IBM-type tape and disc systems. However, each new peripheral required a significant software effort before it could be used. As time passes it becomes more difficult, and more expensive, to fit new peripherals into these old systems.

6. Non-transferability of skills and programs. There is essentially no other installation to which programming developed at LBL can be transferred without a major conversion, and vice versa. In the early days of the CDC complex this was much less of a problem; for several of LBL's kindred institutions had similar hardware and the same compilers as were available at LBL. Today, essentially all of those kindred institutions have converted or are converting to Fortran 77, the new ANSI-standard version of Fortran. LBL cannot convert the existing CDC complex to Fortran 77, so that retention of these systems with their outmoded compilers would have the effect of further isolating LBL users from their peers in other institutions.

Because all these limitations will be removed with the installation of a modern system, the acquisition and installation of a Class IV system in FY 1985 best serves the programmatic needs of the Laboratory.

Reducing Operating Costs

Schedule E7 shows that replacement of the present CDC complex with LBL-85-3 reduces the operating costs of the Central Facility by $645 K in FY 1985 and by more in subsequent years. The incremental cost on the Other line of Schedule E7 consists of software license and maintenance expenses and some additional training expenses in the first two years. The $1,488 K offset which produces this savings is the sum of reduced personnel, internal and vendor maintenance, supplies and power costs made possible by the change from an old batch oriented system to a modern interactive environment.

During FY 1984 and FY 1985 there will be two sources of one-time expenses. The first, in FY 1984, is the possible purchase of commercial time on the type of Class IV system selected to allow the conversion process to begin before the actual installation of LBL-85-3. The second one-time cost is borne by each individual user of the systems being replaced. Many staff members will invest time in moving essential programs and data files to LBL-85-3. Installation of a more standard computing environment will both ease the conversion and increase its value.

Matching Capacity with Requirements

Table LBL-E1 derives LBL internal scientific computing requirements from Schedule E3 requirements under the assumptions discussed above. The net internal requirements are then compared to LBL internal scientific capacity derived from Schedule E2. This comparison shows that a reduction of 5,300 NSU's provides a good match to the projected internal requirements. The figures for Class VI requirements for FY 1985 and beyond are taken from the LBL FY 1984 ADP Long-Range Site Plan. They are based on the survey that was detailed in that Plan and have been subjected to exactly the same adjustments and growth rate (20% per year) assumptions.

Schedule E2 reflects the retirement of the CDC complex starting with the CDC 6400 in late FY 1983 and finishing by the end of FY 1984. Schedule E2 also indicates the installation of LBL-85-3 at the beginning of FY 1985 and the administrative computer, LBL-85-2, later in FY 1985. Table LBL-E1 shows only the net internal scientific capacity taking into account all these events. Schedule E3 reflects the phasing out of external reimbursable work which will be almost entirely gone by the end of FY 1985.

The slowly increasing internal scientific requirements represent that portion of the workload described in Section E4, Narrative, that is presently being done on the CDC complex and that will not migrate to the OER-wide, shared resource.

LBL FY 1985 ADP LONG-RANGE SITE PLAN

TABLE LBL-E1

SCIENTIFIC COMPUTING REQUIREMENTS (NSU's) TO BE MET WITH INTERNAL CAPACITY

	CURRENT	BUDGET	PLAN	OUT-YEARS			
	FY 1983	FY 1984	FY 1985	FY 1986	FY 1987	FY 1988	FY 1989
Total LBL requirements (from Schedule E3)	33,200	35,650	41,450	46,100	51,100	55,200	59,300
less Class VI requirements (to be satisfied at an OER Facility)	(2,750)*	(8,000)*	(15,560)	(18,600)	(22,000)	(25,500)	(29,000)
less Administrative ADP requirements (resource sharing, commercial services and LBL-85-2)	(690)	(745)	(1,630)	(2,880)	(4,160)	(4,080)	(4,000)
less other externally supplied computing (resource sharing and commercial sources)	(4,620)	(4,210)	(4,200)	(4,200)	(4,200)	(4,200)	(4,200)
Remainder: LBL computing requirements to be met with *internal scientific capacity*	25,140	22,695	20,060	20,420	20,740	21,420	22,100
Internal scientific capacity (from Schedule E2, with LBL-85-2 subtracted)	25,110	22,400	20,200	21,200	21,200	21,200	21,200

* On the assumption that OER provides an interim source.

Alternatives

Four alternatives for the satisfaction of this requirement were considered; they are:

1. Acquisition of a Class VI machine. In this alternative, LBL would acquire a Class VI computer and use it for all of its mid- and large-scale computing. It has been discarded in favor of directing the Class VI requirements to the proposed OER central facility, where (because that facility will be dedicated to large problems) they will be satisfied more efficiently.

2. Satisfying the demand from commercial sources. This alternative has been rejected on the grounds of cost. A typical cost for commercially supplied Class IV time is $1,620 per hour after taking full advantage of discounts for being a federal contractor, for being an educational institution, for running on off-shifts, and for using large blocks of time. The Offsets (cost avoidances) would be approximately $500 K greater ($2 M total) under this alternative. To achieve the same net ($645K) savings, the Laboratory could spend only $1,355 K per year for commercial time, or less than 1,000 hours. Table LBL-E1 shows that LBL will fully utilize a Class IV system (7,000-8,000 hours per year).

3. Acquisition of a suitable number of smaller machines. This alternative has been rejected because there exists a class of jobs that are too large for a significantly smaller machine and yet do not require the resources of a Class VI or VII facility. Work that is suitable for smaller machines is already being done on smaller machines; the mid-scale work remaining on the CDC 7600 requires a mid-scale machine.

4. Retain the CDC 7600 and release part of the present equipment. Because of the architecture of the present CDC complex, only one of the two CDC 6000 machines could be released. This alternative has been rejected because it does not achieve most of the desired cost reductions and removes none of the service limitations discussed above.

Procurement Strategy

Acquisition of LBL-85-3 will be based upon functional specifications and will be a fully competitive procurement. Schedule F5, Summary of Financial Alternative Analyses, for LBL-85-3 indicates acquisition via the 5 year lease-to-ownership method. This alternative is preferred over straight lease and lease with option to purchase, but is only slightly preferrable to purchase. Since LBL must convert from an obsolete and non-standard environment, there are no significant backward compatibility constraints that will prevent achieving a completely modern environment. Thus this acquisition will be as safe from obsolescence due to technological advance as is possible.

Dependency on Other Acquisitions

This acquisition is independent of other acquisitions. However, it is based on the assumption described above that the LBL large-scale requirements will be satisfied by an OER shared facility.

ADP Security

LBL has a Laboratory Computer Protection Manager, and an implementation plan for DOE Order 1360.2 is in place. LBL-85-3 will be integrated into that plan and satisfy all relevant security requirements.

LBL FY 1985 ADP LONG-RANGE SITE PLAN
MAJOR PLANNED ACQUISITIONS/LEASE CONTINUATIONS

SCHEDULE E7

SITE: LAWRENCE BERKELEY LABORATORY **MIE NO.** LBL-85-1 **LAST MIE NO.** None
MIE NAME: National Center for Energy Research Computing (NCERC)

PROGRAM B & R CODE: ____________ **PROGRAM NAME:** Energy Research

MIE DESCRIPTION: A Class VII computer system, storage , I/O, and communications system.

FUNDING PROFILE ($000)

	PAST	CURRENT	BUDGET	PLAN	OUT-YEARS			
ACQUISITION	FY82	FY83	FY84	FY85	FY86	FY87	FY88	FY89
CAPITAL								
OPERATING				3,300	3,300	3,300	3,300	3,300
CONSTRUCTION								
NON-ACQUISITION								
MAINTENANCE				800	800	800	800	800
OTHER (Specify)*				7,620	7,445	7,445	7,445	7,445
TOTAL				11,720	11,545	11,545	11,545	11,545
OFFSETS				NA	NA	NA	NA	NA
NET				11,720	11,545	11,545	11,545	11,545

INSTALLATION DATE (MO/YR) October, 1984

MANAGEMENT CLASSIFICATION: X **GENERAL** ___ **SPECIAL**

INITIAL PURCHASE EQUIVALENT COST $13,400 **(ALL LEASED ITEMS)**

ACQUISITION STRATEGY:
___PURCHASE ___ LEASE FOR ________ YEARS
___LEASE WITH OPTION TO PURCHASE; EXERCISE PURCHASE OPTION (MO/YR) ________
X LEASE TO OWNERSHIP; PAYMENTS TO BE COMPLETED BY FY 1989
___OTHER (EXPLAIN):

PROCUREMENT STRATEGY:
X FULLY COMPETITIVE ___ SOLE SOURCE (Explain)
___LIMITED COMPETITION (Explain)

EXPLANATION:

MILESTONES: (FOR ITEMS TO BE ACQUIRED IN FY83 THRU FY85)
IMPLEMENTATION PLAN January, 1984
SOLICITATION RELEASE March, 1984
CONTRACT AWARD June, 1984
(JUSTIFICATION MUST BE APPENDED TO THIS SCHEDULE)

* These costs are detailed in Table LBL-E3.

Justification for LBL-85-1

Introduction

In order to serve the very high-speed computing requirements of Office of Energy Research contractors, the Lawrence Berkeley Laboratory proposes to establish the *National Center for Energy Research Computing* (NCERC). The NCERC is designed to satisfy the large-scale computing requirements of that portion of the Energy Research community not served by the NMFECC.

The Center will be equipped with a state-of-the-art high-speed computer and appropriate front-end systems to support mass storage, unit record, and communications gateway services. It will also have enough communications equipment, eventually including one or more satellite earth stations, to ensure nation-wide access around the clock. Both batch and interactive services will be available to all users.

Goals

The National Center for Energy Research Computing will have two principal goals:

- to provide the *most powerful computing possible*;
- to provide this service to the *whole spectrum* of OER contractors.

It will address the situation spotlighted by Alvin W. Trivelpiece, Director of Energy Research,* when he noted "...that there are scientific problems that cannot be addressed because some ER scientists do not have

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* In *Study of ER Program Needs for Class VI Computers*, a DOE memorandum dated January 17, 1983

adequate access to Class VI computers. The present total suppressed demand for this type of large-scale scientific computing is estimated to exceed one Class VI system."

The problems addressed by the Office of Energy Research grow in number, size, and complexity faster than industry's ability to design and construct computers powerful enough to cope with them. (The LBL workload includes several examples of large computational problems. A description of some of those that require Class VI or VII resources will be found at the end of this proposal, and in Section E 13, Examples of Programmatic Use.) The NCERC as proposed here will relieve this situation by ensuring that state-of-the-art high-speed computing is always available to the Energy Research community.

State-of-the-art high-speed computing is by its very nature an extremely scarce resource, and it has generally been accessible in the past only to those researchers in residence at very large installations. The NMFECC provides an encouraging exception to this generality, however, demonstrating that it is possible to provide large-scale capability to a nation-wide constituency, including some quite small groups, in a cost-effective manner. The National Center for Energy Research Computing, designed, configured, and organized as outlined here, will provide state-of-the-art high-speed computing power to OER contractors regardless of the size of the group or installation; the only requirement is the availability of at least a dumb terminal and a dial-out capability.

The central feature of the NCERC will be a state-of-the-art high-speed computer. It now appears that Class VII computers will become available in FY1985. Such a computer could satisfy the needs of the OER community for several years, and the cost of computation with such a machine will be about one-third to one-quarter the cost of today's computing on Class VI machines.

Siting at Lawrence Berkeley Laboratory

The National Center for Energy Research Computing is designed to satisfy the high-speed computing requirements of OER users, wherever they are located. It is desirable to place this facility at a site with considerable understanding of large-scale computing, its application to Energy Research problems, and its distribution to a national constituency. LBL is such a site: it has been a center of scientific large-scale computing for more than two decades; approximately 80% of the large-scale computing done by LBL scientists supports Energy Research programs covering nearly the whole range of ER activities; and for the past ten years LBL has been providing large-scale computing services to a widely distributed user community. Furthermore, since LBL can be expected to be one of the major users of the NCERC, the Laboratory has a strong interest in seeing that the facility is run in an efficient and cost-effective manner.

In addition, LBL's location and close ties with the University of California provide the Laboratory with a unique resource: the graduate departments of the University. (The pre-eminence of the Berkeley campus of the University in mathematics and the sciences has just been re-affirmed in a two-year study conducted by four academic groups, including the National Research Council.) The relationship between the Laboratory and the University is of long standing, and has been beneficial to both organizations. That it continues to be a fruitful one was emphasized recently in a speech* by George Keyworth II, in which he said "Lawrence Berkeley Laboratory is the only national laboratory located in such intimate proximity to a university. I think that stimulation and interaction has been partly responsible for their

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* January 14, 1983; Distinguished Lecture Series, Lawrence Livermore National Laboratory

proposal to establish, as a new major mission, the state-of-the-art cooperative research facility for materials science...."

Organization

The National Center for Energy Research Computing will be physically located at the Lawrence Berkeley Laboratory. It will have its own management and staff, and will be operationally independent of the LBL Computation Department and Computer Center.

The resources of the NCERC will be allocated to the various OER contractors. The allocation will be done by the Director, Energy Research or his designee. It is expected that explicit advance allocation will not account for the total effective capacity of the Center, but that a portion will be held in reserve as a cushion to absorb emergency high-priority distortion of normal usage and to accommodate late requests for service.

The Center will also support a national Users' Group, representative of the entire spectrum of the Energy Research community. The Users' Group Executive Committee will meet semi-annually, and will report both to the Director, Energy Research and to the Director of the Lawrence Berkeley Laboratory. The Users' Group is not expected to occupy itself with the day-to-day details of running the Center, but with more general questions such as

- system availability (both overall and site-specific)
- the suite of utility packages and libraries supported
- the usability of the Center and its quality of service
- the timeliness of system upgrades (hardware and software)

Configuration

It is expected that a state-of-the-art Class VII computer with the following characteristics will be available in FY 1985:

- individual processor speed 2-4 times Class VI speeds
- well-developed vector capabilities
- at least 500 megabytes of main memory

The proposed configuration (see Figures LBL-E4 and LBL-E5) is based upon such a computer.

Peripherals to be attached to the central computer will include twelve disk spindles. Each disk spindle will have a capacity of 1.2 gigabytes, two access mechanisms, and a transfer rate approaching 100 megabits per second. Sufficient controllers to support eight simultaneous data transmissions will be included.

A service front-end machine will provide mass storage, tape reading and writing for data interchange, and graphics services. This front-end will include 4.8 gigabytes of local disk storage, four 200-inch-per-second, multi-density tape drives, two tape controllers, and a printing device. In addition it will support a mass storage system, probably implemented on optical disks, capable of storing 500 gigabytes of information.

Finally, the center will include communications concentrators and gateways, as described below.

Communications

Primary access to the National Center for Energy Research Computing will be via existing common carriers. In the initial stages of operation of the Center, there will be heavy reliance upon value-added common carriers such as TYMNET and TELENET, because

- TYMNET and TELENET are widely accessible to the Energy Research community, either directly or by means of a local phone call;
- dumb terminals, personal work stations, and personal computers will be well-served by terminal access and the X.25 services of TYMNET and TELENET;
- DECNET, IBM, and CDC protocols can all utilize the X.25 services of TYMNET and TELENET;
- initial bandwidth requirements from individual users are expected to be relatively low.

The NCERC will, of course, support ARPANET access to take advantage of the existing experience and facilities throughout the Energy Research community.

As usage grows and higher bandwidth is required, the Center will adopt OPMODEL, the DOE satellite standard. (Note that in the pre-satellite stages, communication with the Center will generally require **no** additional equipment at the remote user sites. Dial-up access to a common carrier will have to be provided, if it is not already installed.)

To support the communications load, the Center itself will need several limited-function Network/Communications Gateways (N/CG's) to act as concentrators and system entry points. Multiple N/CG's are required to provide redundancy and reliability; the exact number will depend upon the initial load and upon the availability of candidate servers at the time of implementation. A conceptual view of the communications and network architecture is shown in Figure LBL-E6.

Staffing

A staff of 47 is proposed. This number includes 27 professionals, 12 computer operators or operations technicians, three clerical staff, and 5 engineering technicians. Tentative assignments will be as shown in Table LBL-E2. The adequacy of this staff is strongly dependent upon the following assumptions:

1) Highly qualified full-time systems programmers to support the operating system fully for the life of the installation will be provided by the vendor of the central processor. (Current experience with vendors of Class VI computers indicates that this is a reasonable assumption.)

2) Availability of a mass-storage system (with the characteristics specified here), including software, that is *designed* to work with the service front-end and overall architecture proposed.

3) All N/CG concentrator and gateway machines utilize compatible hardware and operating systems.

4) The purpose of the National Center for Energy Research Computing is to provide *very fast computing for the solution of very large problems*, rather than to provide general-purpose computing.

Departure from any of the first three assumptions would necessitate additional systems programming professionals for system maintenance and development. Departure from the fourth would necessitate additional user support and operations personnel.

Facilities

The Lawrence Berkeley Laboratory maintains 11,375 square feet of computer room space. These rooms are temperature- and humidity-controlled and are false-floored. By relocating existing equipment and offices the Laboratory will make available approximately 4000 square feet of contiguous prime space for the installation of the system proposed here. An additional 3,400 square feet of operations support space (suitable for operations, engineering, supplies, and tape and disk storage) are also available. This space is located in a modern, concrete building that has been reinforced against seismic stress. Furthermore, all computer spaces are protected by a total-flooding Halon™ gas system, in addition to pre-action sprinklers and smoke and heat detectors.

Access to the LBL site is controlled, and access to the machine-room space is further limited by means of a cardkey entry system. Present power sources are adequate to handle the configuration proposed here. Some additional cooling capacity will be required, and some minor plant modifications will be necessary. (Total site preparation costs, including the expansion of the cooling plant, will be approximately $175K.) Adequate telephone capacity exists to handle the traffic that will be generated by the Center.

Office space for the 30 professional and clerical staff proposed will be made available in the building complex that houses the computer room spaces.

Costs

Table LBL-E3 gives the (one-time) installation costs and the (annual) operating and maintenance-level equipment costs. The table is self-explanatory for the most part, but the following comments are important:

1) It is assumed that the principal computing hardware will be acquired on

a lease-to-ownership basis. The numbers given reflect a five-year payout with a 8.5% interest rate.

2) It is assumed that all of the principal computing equipment (down to and including the N/CG concentrators and gateways) will have vendor (or equivalent third-party) maintenance.

3) The "Communications" line item includes *all* communications services for the Center.

4) LBL overhead (currently 45%) applies to all direct costs except power.

5) The annual equipment budget will provide maintenance-level gradual upgrades of computer equipment (additional disks as needed, for example, or an additional N/CG to accommodate a new class of service or increasing traffic), or an occasional large piece of communications equipment (such as a satellite earth station).

An Interim Facility

Although this proposal is aimed at FY 1985, the need for a widely accessible National Center for Energy Research Computing is keenly felt today. The plan to provide some 800 hours of Class VI time at the NMFECC in FY 1983 recognizes the existence of this need and demonstrates the determination of the Office of Energy Research to satisfy it. However, it is understood that this is an interim solution, and it will be effected with minimal impact on the Magnetic Fusion program. A start earlier than FY 1985 for the NCERC would clearly be desirable. One way in which this could be accomplished would be through the establishment of an *interim facility*, offering somewhat less capacity but with full nationwide access.

Such a facility would require the availability of a Class VI machine. This Class VI machine would be a *physical replacement* for the central computer shown in Figures LBL-E4 and LBL-E6, allowing development of the rest of the configuration as shown. By this is meant that network access via the proposed Network/Communications Gateways would be implemented on the Class VI machine rather than installing a different network/communication architecture. This would require re-implementing some of the N/CG access software when the Class VII is installed.

The facility would provide utilities, training, and direct assistance to all users as necessary for converting their work onto both the interim and final configurations.

Figure LBL-E4

Proposed Configuration for the National Center for Energy Research Computing

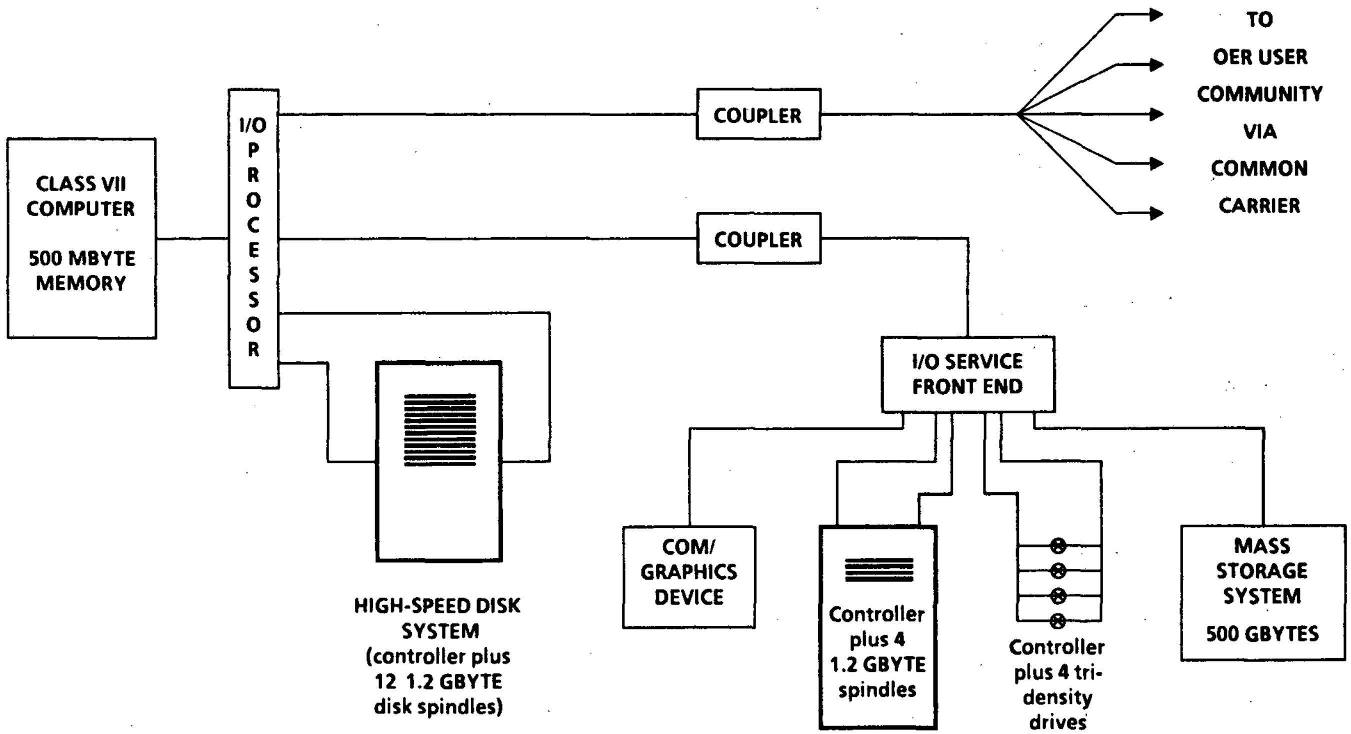


Figure LBL-E5

Sample Configuration for a Mass Storage System for the National Center for Energy Research Computing

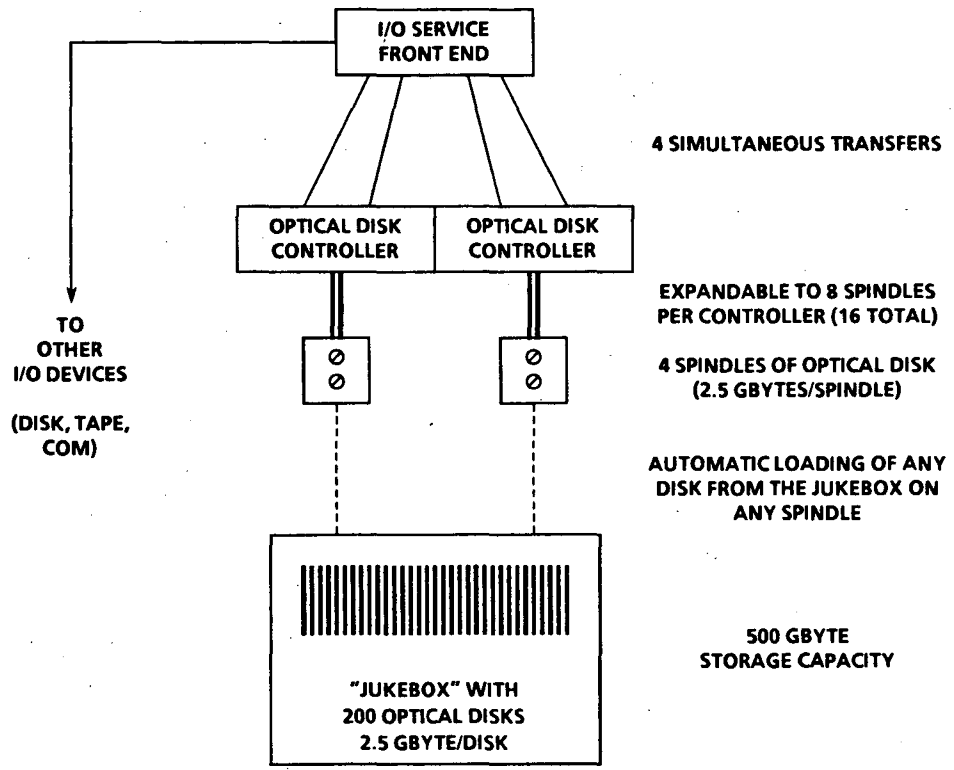


Figure LBL-E6

Conceptual View of User Access to the National Center for Energy Research Computing

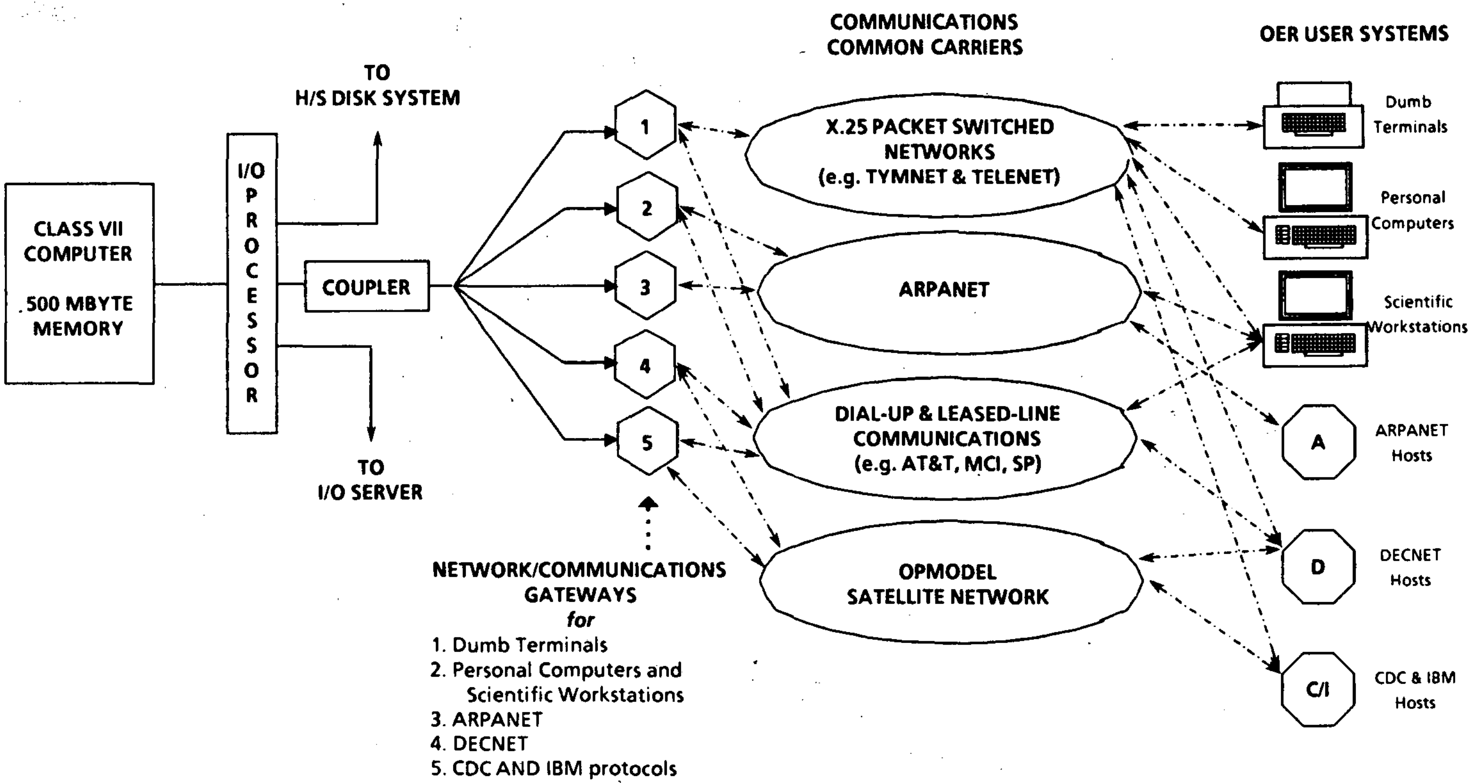


Table LBL-E2

Personnel Requirements for the National Center for Energy Research Computing

(FTE)

	Professional	Computing Technicians	Clerical	Electronics Technicians	Total
Central Processor					3
Operating System	*				
Product Set	3				
Storage Server					8
Operating System	2				
Mass Storage	3			2	
Utilities, COM, Graphics	1				
Communications Server					10
Operating System	1				
Protocols, Interfaces	3				
Network, Telecommunications	1	1	1	3	
User Support Services					10
Consultants	5				
Documentation	2	2			
Training	1				
Operations					11
Accounting	1	1			
Machine Operation	1	8			
Administration	3	—	2	—	5
Total NCERC Personnel	**27**	**12**	**3**	**5**	**47**

* It is assumed that vendor-supplied analysts will fully maintain the operating system of the central processor.

Table LBL-E3
Annual Costs
for the
National Center for Energy Research Computing

(K$)

Operating			**11,545**
Hardware LTO Costs		3,300	
Class VII System (Capital Cost $10.5M)	2,575		
Storage and I/O Server (Capital Cost $1.9M)	475		
Communications Servers (Capital Cost $1.0M)	250		
Personnel Costs		2,000	
Vendor Maintenance		800	
Communications		825	
Software Licenses		100	
Power		200	
Supplies and Services		800	
Total Direct Cost		8,025	
LBL Overhead*		3,520	
Capital Equipment Costs (*Second and Succeeding Years*)			**500**
Site preparation cost of $120K + 45% Overhead (*first year only*)			**175**

* LBL overhead (currently 45%) applies to all operating costs except power.

LBL Requirements for National Center for Energy Research Computing

A major computer requirement is the pressing need to satisfy LBL's present and growing demand for large-scale computing that cannot be satisfied with the installed or planned (LBL-85-3) computational resources. (The FY 1984 Long-Range Plan contained a detailed list of the LBL applications which can *only* be done on a Class VI resource, as well as a supplemental list of applications that could be done most conveniently on a system of that (or larger) capacity.) Indeed, many research programs in progress at LBL are in danger of falling behind the leading-edge of their respective fields without the capability to perform large, CPU-intensive calculations requiring the power and flexibility of a Class VI or VII mainframe.

These research programs are concerned with the modeling and mathematical simulation of complex physical systems found in solid state physics and quantum chemistry, geothermal reservoir and electromagnetic/seismic scattering calculations, and three dimensional turbulence studies. All of these applications require computational capability of a magnitude at least that available from a Class VI machine. In addition, research projects in experimental seismic data analysis, design of biological imaging systems, and multiple shock studies in combustion research have very large scale computing requirements. Finally, it is likely that access to a Class VI or better computer will stimulate additional uses for this capability.

Atomic Structure of Solids: Surface and Bulk

At the new National Center for Advanced Materials (NCAM), expected to begin construction in FY 1984, both experimental and theoretical techniques will be used to characterize the atomic- and subatomic-scale features on the surfaces of solids. All properties of the surface depend critically on these features.

The theoretical aspects of such research will focus on determining atomic arrangements near the surface of a solid, the most probable arrangement being the configuration with the lowest energy. Researchers at Lawrence Berkeley Laboratory have developed techniques for calculating the total energy for given configurations of atoms at the surface. This energy comes from interactions between the ions in the crystal lattice and the electrons, and from interactions among the electrons themselves. By comparing computed energies for different possible configurations of the atoms, researchers can identify the most likely arrangement. Confirmation by experiment is important, however, and is especially crucial when energy considerations alone are not adequate to select between two competing structures.

Initial work will concentrate on silicon, germanium, and carbon surfaces. Other important surfaces include the boundaries between two semiconductors (heterojunctions) and interfaces between semiconductors and metals (Shottky barriers). The atomic arrangements at such interfaces are critical to the behavior of these electronically useful systems.

Subsequent efforts will be directed to the development of techniques to calculate and predict where and how foreign materials, such as adsorbates, attach themselves to a semiconductor surface, as well as the properties of the adsorbate-covered surface.

The calculations require very fast computers with large memories; they approach the limit of the capability of a Class VI system, and would benefit greatly from the availability of a Class VII machine.

In parallel with these theoretical activities, experiments will be performed using advanced Low Energy Electron Diffraction (LEED), surface Extended X-ray Absorption Fine Structure (EXAFS), and photoelectron diffraction. Initially the experiments requiring synchrotron radiation will be carried out at the Stanford Synchrotron Radiation Laboratory. When the Advanced Light Source is available at LBL, they will move to NCAM.

High Pressure Crystal Structures and Phase Transitions

The National Center for Advanced Materials will be a leading facility for studying the structure of crystals and the processes, called phase transitions, whereby crystals change their structure. This research will combine ongoing theoretical studies of crystalline structures and transitions with a new experimental effort to use the Advanced Light Source to obtain time-lapse snapshots of the rearrangements occurring within the crystal during a phase change.

Phase transitions, such as the conversion of carbon from its common graphite form to diamond, tend to occur at high pressure. Like diamond, the high pressure forms of many materials may be stable and marvelously useful. Results from this NCAM project will help guide the search for new and useful crystalline materials that only form under high pressure.

Initially the high-pressure research will focus on predicting theoretically the conditions under which certain semiconductors will change their crystalline structure. In addition, this work will indicate what the properties of the new crystals will be, and whether they will be stable under ordinary conditions.

In addition, similar calculations will be made for metals, such as beryllium, magnesium, zinc, and lead. During FY 1984, a special effort will be devoted to understanding the transitions of bismuth, a semimetal which undergoes fascinating changes in structure. As the pressure increases, bismuth transforms from a semimetal to a semiconductor and finally to a metal.

Ultimately, theoretical techniques will be developed to calculate phase transitions and properties of rare-earth elements and compounds and of unusual but useful materials, such as organic superconductors and magnetic semiconductors.

When the Advanced Light Source starts operating, the optical properties and structure of the high-pressure forms of materials can be studied. Moreover, the high-intensity, short, and frequent bursts of light from the ALS will provide strobe-like glimpses into the crystal while its atoms rearrange into the new phase. These snapshots should provide key information for understanding the process of phase transitions.

Pseudo-Potential Studies

At the present time, effective or pseudo-potential applications for the solid state are limited to elemental systems. The availability of a very high speed computer would make possible the extension to compound semiconductors, to transition metals, and to more complex crystal types, and would permit the study of systems having more atoms per unit cell. In addition, the computation of surface states becomes realizable, and with this the prospect of providing detailed information on catalysts of chemical interest. Such work would represent a considerable advance over computational studies of systems currently the subject of investigation in ultrahigh vacuum apparatus.

Monte Carlo Simulations

Many areas of chemistry and physics are being advanced by the use of Monte Carlo techniques which provide benchmarks against which to test approximations and new information in cases where experiments cannot obtain accurate data. Computations on a high speed computer can make possible studies of many-body systems in condensed phases (liquid, solid, metallic) and at interfaces. Simulation studies have played a crucial role in the elucidation of phase transitions and, with the availability of a Class VI or better machine, the complete fermion system (electrons and nuclei) becomes amenable to treatment, as evidenced in pilot studies by LBL scientists.

Extensions of time-dependent phenomena at the microscopic level, leading to rigorous calculations of electrical and thermal conductivities by means of response functions, become practical with a Class VI or faster computer. In addition, the complicated area of finite temperature many-body systems also becomes accessible. Simulations can significantly benefit from increased CPU capability. Unlike many other areas, improved accuracy and reliability of Monte Carlo calculations are critically dependent on CPU cycles.

Monte Carlo methods are also beginning to be used for the study of electronic structure and interactions of atoms and molecules, utilizing quantum as well as semi-classical and classical theories. LBL researchers are pioneers in this effort. The CPU capability of at least a Class VI computer will allow a thorough testing of this method.

Ab Initio Electronic Structure Determination and Potential Energy Surfaces

Molecular theorists have been in the forefront of the use of powerful computers to determine the electronic structure and properties of atoms and molecules. New methods for describing electron correlations in large systems and in excited states, including the graphical unitary group approach for reducing the difficulties associated with configuration interaction calculations and multi-configuration Hartree-Fock methods, are being spearheaded by LBL researchers. Furthermore, traditional methods are being applied to larger and more complex molecules and interacting systems with useful benefits. In addition, LBL scientists have been successful in developing new automated methods for finding reaction barriers, transition states, and equilibrium geometries of molecules.

These developments presage a period of exciting developments that can have significant practical impact in areas such as combustion and pollution chemistry when the full power (both memory and speed) of a Class VI system is made available.

Collision Dynamics

Advances in quantum, semi-classical, and classical methods for determination of inelastic collision events have reached the stage where theory is an essential adjunct to experimental verification of models. Theory further serves as a source of new information not obtainable by experimental methods for those atom-diatom systems for which accurate potential energy surfaces can be computed. For molecule-molecule energy transfer studies, progress will be governed by the computational power available.

Quantum mechanical reactive scattering calculations (requiring large memory storage as well as raw computing speed) present even more of a challenge to computational facilities. The methodology has progressed to the stage that, with Class VI or better facilities, reliable reactive cross sections for simple atom-diatom systems are possible. There have also been important advances in theoretical methodology for reactive processes in polyatomic molecular systems. These approaches interact closely with the quantum chemistry techniques for generating reaction paths (see previous section) and involve various dynamical approximations, but they are an important first step toward dealing with more complex systems.

Geosciences

Research in the field of earth sciences requiring the capability of a modern, Class VI or VII machine is presently concentrated in two main areas:

(i) numerical modeling of subsurface systems
(ii) processing and analysis of geophysical data

Current research in these areas addresses ever more complex systems, emphasizing a greater degree of realism, completeness, and detail. As a consequence, existing computational software is applied to more difficult problems, while ongoing research develops new large computer programs with greater demand on computational hardware. Typically, the most computationally intensive work involves the solution of very large sets of coupled equations. Computational tasks of a similar nature arise in petroleum engineering (exploration, field development). These kinds of calculations have provided a strong incentive for the development and application of computers with vector processing capability. The so-called "vector-machines" can simultaneously perform a large number of operations which arise in the solution of systems of equations. This capability can improve computational speed by a factor of 10 or more in comparison with scalar computers.

LBL's earth scientists are presently among the leaders in the field of numerical modeling and analysis of subsurface systems. As other research organizations are acquiring higher speed vector machines, it becomes more difficult for LBL groups to remain in the forefront of research. A Class VI or better computer will ensure a world-class posture for future research in the earth sciences.

Additional Computationally Intensive Activities

LBL plays an important role in DOE's combustion research program. This work is carried out in the Energy & Environment Division and in the Computer Science and Mathematics Department. It is estimated that in 1983 the program of research into turbulent combustion under way in the mathematics group could use 7-10% of a Class VI machine if it were available. Additional time will be required by investigators working in the Energy & Environment Division.

In recent years the Laboratory's Accelerator & Fusion Research Division has undertaken a limited study program in heavy ion fusion. Should this very promising avenue of attack on the controlled fusion problem receive additional funding, it would require massive amounts of computation on a Class VI or better machine. LBL participants in this program are currently engaged in a cooperative program with the Naval Research Laboratory in which LBL codes are run on the NRL's ASC computer.

Development of numerical algorithms by the Computer Science and Mathematics Department is an important program of research. This work requires the use of a state-of-the-art computer. Of particular interest is on-going research in fast direct methods for the solution of partial differential equations.

Biological imaging systems currently being developed in the Laboratory's Biology & Medicine Division require the use of a large scale super-computer. These systems produce an enormous amount of data which must undergo computationally intensive transformations before they are presented to the user. The development of three-dimensional imaging systems intensifies this requirement for computation.

The Energy Efficient Buildings Program is a large user of computing power at the Laboratory. It is anticipated that this usage will increase as codes developed under this program are used in the production mode. Furthermore, current codes are limited by the speed and memory size of the present system and can immediately use new capabilities.

Building energy simulations by the Energy & Environment Division requires additional computing power for the development of more detailed and more realistic models.

LBL FY 1985 ADP LONG-RANGE SITE PLAN
MAJOR PLANNED ACQUISITIONS/LEASE CONTINUATIONS

SCHEDULE E7

SITE: LAWRENCE BERKELEY LABORATORY **MIE NO.** LBL-85-2 **LAST MIE NO.** None
MIE NAME: Class III Administrative Computer System

PROGRAM B & R CODE: KB **PROGRAM NAME:** Nuclear Physics

MIE DESCRIPTION: A Class III computer system (1 MB) with disk storage system, communications controller, magnetic tape subsystem, printer and other peripherals.

FUNDING PROFILE ($000) (Direct Costs Only)

	PAST	CURRENT	BUDGET	PLAN	OUT-YEARS			
ACQUISITION	FY82	FY83	FY84	FY85	FY86	FY87	FY88	FY89
CAPITAL		--	--	--	--	--	--	--
OPERATING	--	--	--	135	271	271	271	271
CONSTRUCTION		--	--	--	--	--	--	--

NON-ACQUISITION

	FY82	FY83	FY84	FY85	FY86	FY87	FY88	FY89
MAINTENANCE				20	40	40	40	40
OTHER (Specify) *				578	415	462	472	472
TOTAL				733	726	773	783	783
OFFSETS †				(363)	(893)	(1,291)	(1,441)	(1,541)
NET				370	(167)	(518)	(658)	(758)

INSTALLATION DATE (MO/YR) March 1985

MANAGEMENT CLASSIFICATION: X **GENERAL** __ **SPECIAL**

INITIAL PURCHASE EQUIVALENT COST $1,100 **(ALL LEASED ITEMS)**

ACQUISITION STRATEGY:
__ **PURCHASE** __ **LEASE FOR** ____ **YEARS**
__ **LEASE WITH OPTION TO PURCHASE; EXERCISE PURCHASE OPTION (MO/YR)** ____
X **LEASE TO OWNERSHIP; PAYMENTS TO BE COMPLETED BY FY** 1990
__ **OTHER (EXPLAIN):**

PROCUREMENT STRATEGY:
__ **FULLY COMPETITIVE** __ **SOLE SOURCE (Explain)**
X **LIMITED COMPETITION (Explain)**

EXPLANATION: Software compatible with IBM VM and MVS systems and applications software.

MILESTONES: (FOR ITEMS TO BE ACQUIRED IN FY83 THRU FY85)
IMPLEMENTATION PLAN December 1983
SOLICITATION RELEASE May 1984
CONTRACT AWARD October 1984
(JUSTIFICATION MUST BE APPENDED TO THIS SCHEDULE)

* Other includes site preparation and NOMAD license fee (FY 1985 only), software maintenance, operations staff, supplies, and communications (all years). † Offsets come from the gradual elimination of charges for the use of computer services from LLNL, the LBL Central Facility, UCB, and NCSS.

Justification for LBL-85-2

Introduction

The Lawrence Berkeley Laboratory proposes to install a Class III Administrative Computer to support its administrative reporting and management information system needs. These include the financial and business systems which support all of the programmatic work conducted at the Laboratory, including systems for general ledger, payroll, property accounting, personnel, salary administration, effort distribution, budget, accounts payable and all other applications necessary for the conduct of day-to-day-business.

These needs are now met by drawing upon a number of diverse resources including the LLNL Univac 1100/81 computer, the LBL CDC 7600 and 6600 computers, dedicated in-house minicomputers, the purchase of interactive data base services from the University of California, and purchase of commercial timesharing services from National Computer Sharing Systems (NCSS). Such diversity leads to an excessively complex computing environment for administrative data processing, and one that is expensive and extremely difficult to coordinate.

It has also become an extremely uncertain environment as a result of two recent developments:

(1) the establishment of separate DOE contracts for LLNL and LBL where previously there was only one;

(2) the planned release of the CDC 6000 and 7600 computers by October 1, 1984, which means that existing computer applications must be rewritten and transferred elsewhere.

In addition, there is the uncertainty that the University computer center will have the capacity to meet our requirements, or that it will be capable of providing the physical security and privacy of data files on a system that is used for academic instruction and is accessible by students. Many administrative applications are sensitive, or must be processed on a tight schedule, or both. Clearly, neither data protection nor timely output benefit from the present diverse approach. This plan addresses the defects in the present operating style by replacing the many suppliers of computing resources with a single resource to be installed in FY 1985.

ADP Requirements for Administrative Data Processing

The workload requirement for FY 1983 is approximately 1430 NSU's, of which 690 are provided by off-site services and 740 are supplied by the LBL scientific computers and various on-site minicomputers, as shown below:

LBL		740
Scientific Computers	680	
Miscellaneous Minicomputers	60	
Non-LBL		690
LLNL Administrative Systems	390	
University of California	60	
Commercial Services	240	
FY 1983 Total NSU Requirement		1430

A study made of the use of LBL administrative computing services over a six-year period prior to the installation of the LLNL Univac 1100/81 system showed a compound growth rate of approximately 20 percent per year. The rate of growth varied from a low of about 10 percent in a year during which funding cutbacks were experienced, to a high of about 35 percent during a year of modest growth in Laboratory programs. During this period the primary mode of operation was batch processing.

The recent change in the demand pattern towards the use of interactive services indicates that a larger portion of the administrative computing workload will be performed during the normal daytime working hours to support the needs of users while they are at work. The main factor in this shift is the use of data base management systems for the retrieval and manipulation of current data by the users themselves. These new uses of the computer are hardware intensive, and even though they are cost-effective when related to manpower costs, usage of the computer in terms of NSU's is expected to increase faster than was experienced during the period when batch processing was the dominant mode of operation. These considerations, combined with a continuing increase in administrative reporting requirements, produce an estimated compound growth rate of about 30 percent per annum.

A Class II machine could satisfy the current workload, but would be unsuitable for two reasons. First, the projected growth would saturate such a system by the time it is installed in March 1985. Second, the administrative workload is cyclical in nature, rather than of constant level. Scheduled work cannot be performed using average demand requirements, because the need for the computer cannot be spread evenly over a 24-hour day and 7-day week. The main demand comes during normal daytime working hours, at the end of weeks, months, quarters, and fiscal years. To meet these work schedule requirements the computer must be scaled to handle the *peak demand* rather than the average workload. Experience has shown that peak demand, whether measured in terms of computing cycles, jobs submitted, or terminal session hours, is about double the normal workload. A Class III system is therefore the *minimum* that would meet LBL's administrative data processing requirements in FY 1985.

Alternatives Considered

Four other alternatives for the satisfaction of this requirement were considered and rejected:

1. Share time with LLNL on their Univac 1100/81. There are two major disadvantages associated with this alternative. (1) The 1100/81 system does not support NOMAD, the commercially supplied data base management system used by LBL for the generation of personnel reports. (2) LLNL is 50 miles away from LBL, and the computer is located in a limited-access area, entrance to which requires a "Q" clearance.

2. Continue to use the LBL scientific computers. The LBL CDC 6000 and 7600 computers are to be released by the end of FY 1984. It is therefore imperative that the conversion from these systems begin as quickly as possible. However, in order to convert, one must know the target system, and the successor system for the CDC machines has not yet been selected. Furthermore, it is generally undesirable to run both scientific and administrative applications on the same system. The procedures that are necessary to ensure separation of function for sensitive administrative applications interfere with the free access to the full power of the system that is so important to scientific applications.

3. Use commercial services. The cost of commercial services is far too high to be seriously considered. The current use of NOMAD alone, which serves only the Human Resources applications and is less

than 20% of the total workload, is projected to cost $350K in FY 1983. If the use of commercial services is extrapolated to all applications areas, the annual costs would far exceed the operational cost of this acquisition (see Schedule E7 for LBL-85-2).

4. Use the University of California, Berkeley, computer. This has been a useful and welcome supplement to the other sources of administrative data processing, but is not a satisfactory permanent solution for the following reasons:

   - lack of adequate protection from unauthorized access to sensitive data;
   - lack of assurance that adequate capacity could be provided in the future;
   - priority conflicts during times when Laboratory and University workload peaks and deadlines conflict.

Procurement Strategy

The procurement strategy that will be used for this acquisition will be to solicit requests for proposals for an IBM-compatible system.

A substantial amount of processing is performed on the Campus IBM machine using data base operating system files under the SPIRES data base management system. Other work is being done using commercial timesharing services offered by NCSS with the NOMAD relational data base management system. This work involves several essential information systems, including personnel systems for compliance with EEOC regulations, the maintenance of personnel records, and the salary and wage administration for the Lawrence Berkeley Laboratory. Although, in theory, the applications could be converted to run with different hardware and operating systems, the loss of investment in programming and in the cost of retraining the existing data processing staff could not be justified. There are numerous vendors of IBM plug- and software-compatible systems who could easily be responsive to a request for proposal.

Another factor that must be considered in this acquisition is time. One of the principal reasons for the conversion effort that is now under way is the fact that the applications now processed on the Laboratory's CDC computers will not run on *any* replacement. All applications that now run on the CDC 7600 and 6000 computers under the BKY operating system must be converted before the existing equipment is released. Simply stated, there is not time to wait until the administrative computer selection is made in FY 1985 before conversion to the new equipment can commence.

Funding Considerations

An analysis has been made to determine the best financial basis to use for the acquisition of the equipment. Four methods of acquisition were considered: purchase, straight lease, lease with the option to purchase, and lease-to-ownership.

It can been seen from an examination of Schedule F5 for LBL-85-2 that straight lease and lease with option to purchase are considerably more expensive than outright purchase of the equipment. The fourth alternative, which is a lease-to-ownership arrangement under which payments are made over a five-year period, after which title passes to the government, is more favorable than outright purchase when considering the present value of funds. Since modern equipment will be acquired, the lifetime of the system will extend well beyond the end of the lease period.

Program Conversion

Conversion of the administrative applications programs will entail a major effort. The task is complicated by the multitude of computer systems, the number of languages, and the number of operating systems in current use.

However, the most significant factor in the conversion is that the CDC 7600 and 6000's installed at LBL no longer will be available after FY 1984. Codes for these systems are written in non-standard dialects of FORTRAN and COBOL and run under the unique and highly specialized BKY operating system which was developed in-house and offers only limited compatibility with commercial software.

Conversion has been started by using the University of California, Berkeley's IBM-4341 computer. This computer system was selected because it already is used by LBL for data base management applications using the SPIRES system and because it is connected with the existing Laboratory telecommunications network and can be accessed by the CRT terminals used to access LBL systems.

The software conversion plan will include several efforts. These are:

- Conversion of codes from the LBL CDC systems;
- Conversion of codes from the LLNL Univac 1100/81;
- Implementation of data base management software on the new Class III system (to take the place of commercial services);
- Acquisition of third-party applications software.

The conversion of programs run on the Univac computer is relatively straightforward because these programs have recently been rewritten in the current high level COBOL language and are transportable to IBM-compatible systems through minor coding changes that reflect hardware and job control language differences in the two systems. The use of these existing programs is highly desirable because they are the ones that process our present applications and thus will require no modification to fit the ongoing systems once converted to the new computer. Work is in progress on many of the programs in the general ledger system, and some have already been converted and tested. Other Univac programs also will be modified rather than completely rewritten or purchased from outside sources. A comprehensive list has not been developed, but is expected that well-written applications programs, such as the property management system, that are highly responsive to existing Laboratory administrative needs, will fall into this category.

The purchase of third-party applications software is also being considered. Of particular interest are application packages used in the personnel and payroll areas. Such applications are highly dependent upon outside requirements imposed by legislation and government regulation. These requirements pervade the marketplace so that the changes required to adapt them to the needs of the Laboratory are relatively small. At present, no applications software has been purchased, although payroll and personnel systems are being investigated.

The remainder of the applications software requirements will be met by rewriting existing programs to use more modern techniques, by modifying purchased software, and by completely redesigning and rewriting applications that cannot be converted. Inherent in the process will be the use of modern query language processors, data base management report generators, and other similar general purpose software, the use of which will eliminate the need to convert or rewrite many of the existing administrative data processing applications codes.

Computer Security

Several applications to be processed on the new system will involve data which are sensitive both because the applications involve accounting for and disbursement of funds and because some of the data contain information subject to the Privacy Act. All of these applications exist today, but could be done more safely on in-house equipment. Three examples may clarify the problems:

- Personnel data are processed on computers owned and operated by a commercial organization whose systems are connected to a public communications network;
- Data bases containing financial data are processed on a system which is available to university students for academic work;
- Numerous applications are processed on scientific computers where the separation of functions between programming and operations personnel is not feasible.

The new system will provide the ability to safeguard data through the implementation of physical controls, adequate password protection, the logging of access data, and separation of functions. Compliance with existing computer security regulations will be required in the design of any new software placed on the new Class III Administrative Computer System. Data protection and computer security for this, as for the other systems at LBL, will be under the direction of the Laboratory's Computer Protection Manager.

Other Considerations

This acquisition is not dependent upon any other ADP acquisition or expenditure.

Only about half the administrative data processing is currently accomplished on systems under LBL's operational control. Those systems, the CDC 7600 and 6000's, are currently running at more than 90% of total capacity, averaged over the whole year, and are *always* saturated during the prime shift, when interactive access is attempted.

LBL FY 1985 ADP LONG-RANGE SITE PLAN

SUMMARY OF MAJOR PLANNED ACQUISITIONS/LEASE CONTINUATIONS
(Dollars in Thousands)

SITE Lawrence Berkeley Laboratory - LBL **SCHEDULE E8**

MIE NUMBER	MIE NAME	PAST	CURRENT	BUDGET	PLAN	OUT-YEARS			
		FY 1982	FY 1983	FY 1984	FY 1985	FY 1986	FY 1987	FY 1988	FY 1989
	KB - Nuclear Physics[1]								
LBL-85-3	Class IV Computer System				640 (O)	640 (O)	640 (O)	640 (O)	640 (O)
LBL-85-2	Class III Computer System				135 (O)	271 (O)	271 (O)	271 (O)	271 (O)
	Office of Energy Research								
LBL-85-1	Class VII Computer System				3,300 (O)	3,300 (O)	3,300 (O)	3,300 (O)	3,300 (O)

1 Nuclear Physics is the program with institutional budget responsibility for General Purpose Equipment; however, operating costs will be programmatically shared based on usage.

IDENTIFY THE TYPE OF FUNDS FOR EACH ENTRY: (C) = CAPITAL; (O) = OPERATING; (P) = PLANT (CONSTRUCTION)

LBL FY 1985 ADP LONG-RANGE SITE PLAN

ADPE SYSTEM REUTILIZATION OPPORTUNITIES

SITE Lawrence Berkeley Laboratory - LBL | SCHEDULE E10

UNIT/ SYSTEM NUMBER	ADP SYSTEM/MAJOR SUBSYSTEM	ESTIMATED RELEASE DATE	COMMENTS
1701-04	CDC 6400 (20 PPU)	September, 1983	Owned by Government
1701-04	CDC 7600 (65K + 500K)	October, 1984	Owned by Government
1701-04	CDC 6600 (20 PPU)	October, 1984	Owned by Government
			All opportunities are based on the planned installation of LBL-85-3 in FY 1985.

POINT OF CONTACT: Eric Beals (415) 486-5351
FTS 451-5351

E11. Cost Recovery

The Central Facility recovers all of its operational costs by billing users for the services used. The accounting algorithm for the CDC computers is based upon the Computing Unit, which is a synthesis of CPU and I/O usage, memory occupancy, and, if the job is interactive, connect time. Charge-back for the DEC VAX front-end computers is based upon connect time, CPU and I/O usage, and local storage occupancy. For the text-processing front-end machines, accounting is based on connect time and local storage occupancy. There are additional costs for access, tape and central disk storage, and for output processing handling. Three levels of service priority are available on the CDC machines, with charge-back factors of 2.0, 1.0, and 0.75 times the nominal charge; a reduced rate is applied to weekend and holiday usage. Administrative computing costs are absorbed by Laboratory overhead. The operating costs of all other computers are absorbed by the operating departments or divisions.

E12. Reconciliation

The LBL FY 1984 ADP Long-Range Site Plan was directed towards achieving access to very-large-scale (Class VI or above) computational capability. The access mechanism proposed in that plan was the acquisition of a Class VI computer (LBL-84-1) to become LBL's principal computing resource. During the past year the Office of Energy Research has studied the problem of providing such large-scale resources to all of its contractors. One of the solutions that has been proposed is the establishment of a shared, central facility with access available to all Energy Research contractors. The LBL FY 1985 ADP Long-Range Site Plan is based upon the assumption that such an OER central facility will come into being within the next few years, and that it will satisfy LBL's growing requirement for large-scale computing. As a result, LBL-84-1 has been removed from this year's Plan. In its place a complete proposal for the establishment of a National Center for Energy Research Computing (NCERC) to offer large-scale, very-high-speed computing to all Energy Research contractors is included as LBL-85-1.

LBL-84-1 was also intended to replace the existing CDC 7600, 6600 and 6400 computers, which are the principal LBL general management computers. The LBL FY 1985 ADP Long-Range Site Plan includes provision for replacing these obsolete and operationally expensive systems with a modern, interactive and cost-effective mid-scale Class IV system. This replacement system will satisfy those LBL scientific computing requirements that will not need the unique resources of the NCERC. The replacement system is labeled LBL-85-3.

The implementation strategy associated with LBL-84-1 included an initial system (for service front-end development) that was to be subsequently reutilized for administrative data processing once the total LBL-84-1 system was installed. The present Plan provides for administrative data processing requirements as a separate acquisition which is detailed in the Justification for LBL-85-2.

E13. Examples of Programmatic Uses

Theoretical Predictions of the Properties of Materials

Research and Objectives

It has recently become possible to make *ab initio* predictions of the structural, electrical, magnetic, and mechanical properties of solids using quantum mechanical calculations. This breakthrough was brought about by some major advances in the past few years in the theory of the electronic structure of solids.

The ongoing work at the Lawrence Berkeley Laboratory is motivated by material problems. These calculations involve numerical methods which solve essentially a complex many-body problem. Hence, large-scale computations are required. In these calculations, the structure is determined by minimizing the total energy of the system using a density functional approach. Other properties are then calculated from the electronic energies and wavefunctions.

One of the major difficulties involved in the determination of properties of condensed matter systems starting from the constituent atoms is that very high precision is required. For example, to obtain the vibrational properties (e.g., phonon frequencies) of a crystal, a precision of one part in ten million is needed for the energy of each atom in systems which typically contain 10^{23} strongly interacting atoms. A major development which was made here at LBL and which makes these major calculations possible is the pseudopotential formulation of the problem. In this approach, the core electrons which do not influence the properties of the solid phase are removed from the problem. Focusing only on the valence electrons, the calculations become tractable, and it is no more difficult to treat the very heavy elements than the light ones.

With only the atomic number and atomic mass as input, we can now calculate with high accuracy the structural properties such as the lattice constants, bulk moduli, phonon frequencies, the Gruneisen parameters, electron-phonon interactions, etc., and, in some cases, predict solid-solid structural phase transformations for systems with not too many atoms in the unit cell of the crystal. From the calculations, we can also obtain the electronic structure, the magnetic structure, and the optical and transport properties of the system. Thus far, we have performed calculations on semiconductors, metals, insulators, semi-metals, and some selected surfaces. Agreement betweeen theory and experiment is typically at a few percent level.

The success of this approach, therefore, has been extremely encouraging. With the proper computing facilities, many objectives and possibilities appear to be within reach. One could predict structures. One could "fabricate" materials theoretically and search for those with desirable special properties. Many materials have desirable properties only at high pressures. Theory could help in understanding the high pressure phase and in finding ways to bring back the materials to zero pressure while retaining the desirable properties. One could search for high transition temperature superconductors. Theoretical calculations provide information on the electron-phonon interactions. The object is then to find materials with strong electron-phonon interactions which would give a high transition temperature.

The method also can be applied to study the structural and electrical properties of surfaces and interfaces which are systems of great importance in the areas of device applications and catalysis. The most basic (and unsolved) problem in surface physics is the determination of the atomic structure. Almost all other properties depend critically on determining the atomic arrangement. Systems of particular interest in the semiconductor area are: reconstruction of the clean surfaces, interfaces between semiconductors (heterojunctions), and interfaces between semiconductors and metals

(Schottky barriers). Another area of vital interest in surface science and catalysis is the properties of clean and adsorbate-covered transition metal surfaces.

The advantage of the theoretical calculations (as opposed to experimental measurements) is that it is possible to scan many systems which is impractical to do experimentally. This is especially true for high pressure or surface experiments where the characterization of the sample is generally difficult.

Figures LBL-E7 and LBL-E8 and Table LBL-E4 depict some results for the covalent semiconductors. As seen in Figure LBL-E7, the *ab initio* calculated structure (i.e., the lowest energy structure) for Si is the measured diamond crystal structure with both the lattice constant and the bulk modulus in excellent agreement with experiment. Figure LBL-E8 illustrates that the type of structural transformation and the pressure and volume at which Si transforms from the semiconducting diamond phase to the metallic β-tin phase are correctly predicted. In addition to the static structural quantities, excellent charge density for the electrons is obtained. This is illustrated for graphite in Figure LBL-E9. A list of materials and systems which have been examined using the pseudopotential approach is presented in Table LBL-E5.

Computing Requirements

The major limitations of the CDC 7600 computer for problems of the type we do is space and speed. The calculations involve repeated diagonalization of large matrices and the Fourier transform of large arrays. Hence, although the theoretical methods that we develop are applicable to any system, we have been limited to systems with few atoms per unit cell. The reason is that the computer memory required in a calculation is generally proportional to N^2 and the time required to N^3 where N is the number of atoms in the cell of a periodic system. Many important problems of interest (such as those related to surfaces discussed above) simply cannot be attacked with the present facilities. A Class VI or larger machine at LBL would open up many new avenues of research in this area.

Scientific Personnel

Professors Marvin L. Cohen, Leo M. Falicov, and Steven G. Louie; approximately 20 postdoctoral fellows and graduate student research assistants.

Table LBL-E4

Static Structural Properties.

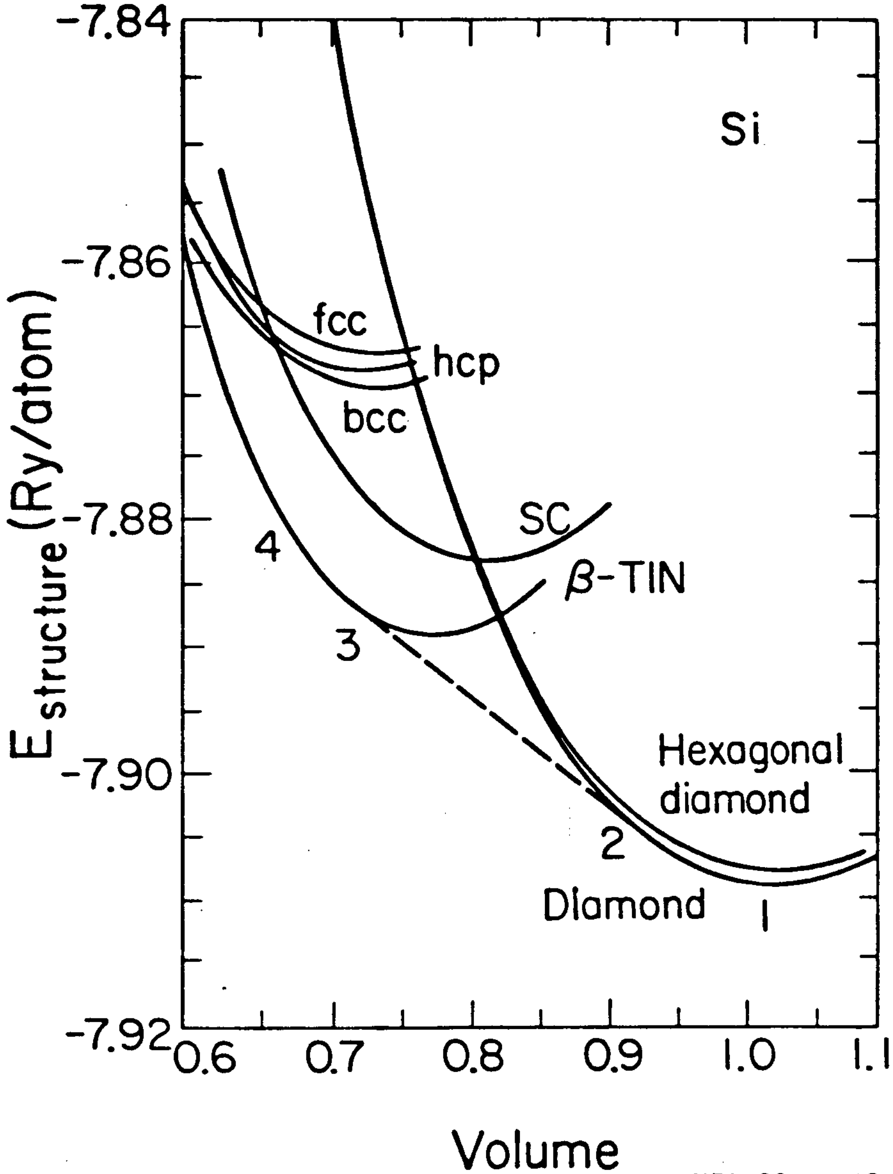
	Lattice Constant (Å)	Cohesive Energy (ev)	Bulk Modulus (Mbar)
Si			
calc.	5.45	4.67	0.98
expt.	5.43	4.63	0.99
% diff.	0.4%	1.0%	-1.0%
Ge			
calc.	5.66	4.02	0.73
expt.	5.65	3.85	0.77
% diff.	0.1%	4.0%	-5.0%
C			
calc.	3.60	7.57	4.41
expt.	3.57	7.37	4.43
% diff.	0.8%	3.0%	-1.0%

Table LBL-E5

List of Systems for which Theoretical Calculations Have Been Performed on their Structural Properties using *ab initio* Pseudopotentials.

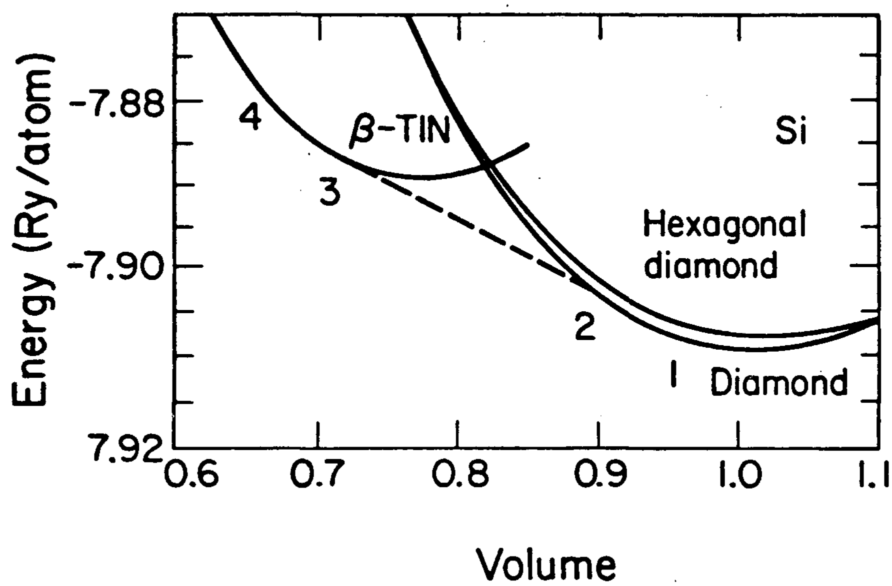
Covalent Semiconductors	Si, Ge, Sn
Compound Semiconductors	AlAs, AlP, GaAs, GaP
Metals	Al, Be, Mo, Nb, Zr
Insulators	C
Semi-Metals	Graphite
Surfaces	Si, Ge, C

Figure LBL-E7



XBL 831-1113

Figure LBL-E8

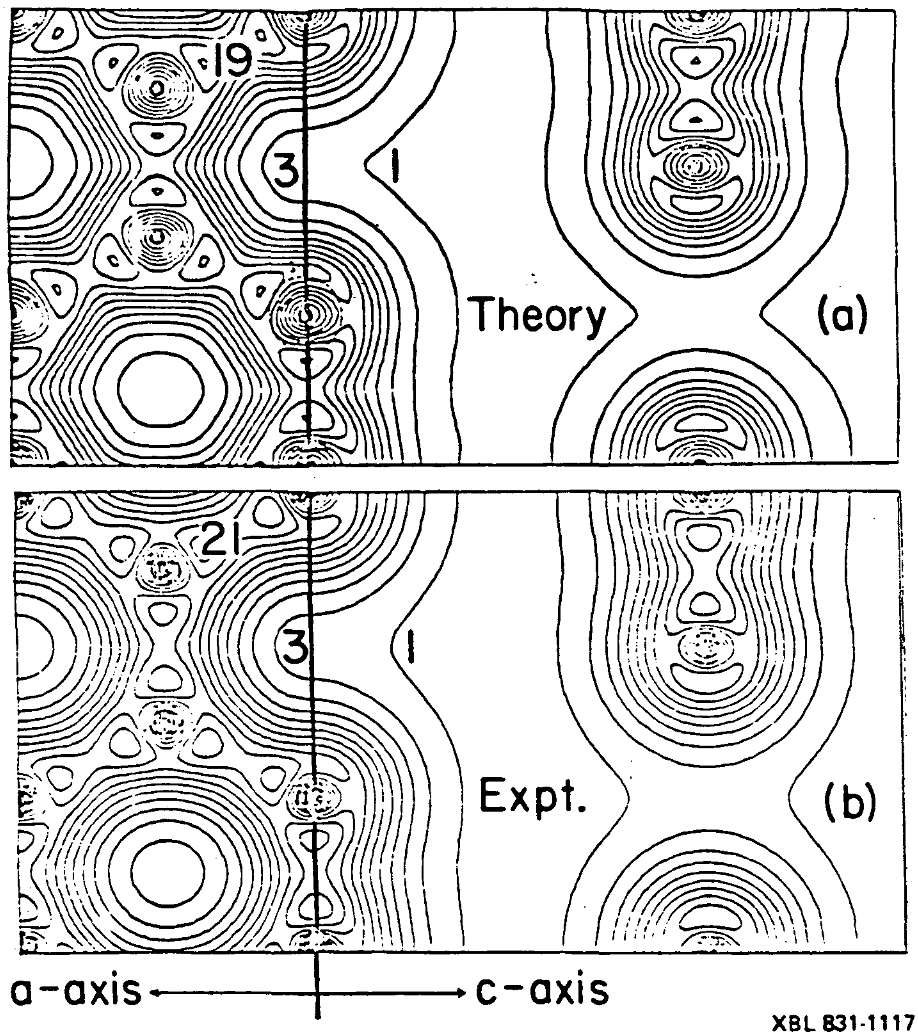


Transition volumes and pressure for Si

	Volumes diamond	Volumes β-tin	Pressure (Kbar)
calc.	0.928	0.718	99 ± 10 %
expt.	0.918	0.710	125
% diff.	1.1%	-1.1%	-20%

XBL 831-1115

Figure LBL-E9



Nuclear Deformation Energies

The binding energy (or mass) of an atomic nucleus may be considered as made up of a "local" part, akin to the energy of a drop endowed with a surface tension, and a "nonlocal" part (Coulomb energy, proximity energy and shell effects[1]). The two leading terms in the local (liquid-drop) part are a shape-independent volume energy and a surface energy proportional to the surface area of the shape in question. Together with the electrostatic energy of a uniform distribution of electric charge, these contributions represent the major part of the potential energy of a nuclear system.

Even though some of the most important features of the deformation energy of a charged drop have been adequately studied and tabulated, there are others that are still not well understood -- more than forty years after the introduction of the deformable liquid-drop model in connection with nuclear fission. The need for a better understanding and a quantitative tabulation of nuclear deformation energies becomes more acute with the increased interest in the physics of nucleus-nucleus collisions, in which a variety of configurations, not enountered in fission, make their appearance. The present work aims at alleviating this need by presenting what amounts to three-dimensional tabulations (deformation-energy maps) based on a careful choice of three deformation degrees of freedom (corresponding to a mass asymmetry variable, an elongation or fragment-distance variable, and a necking or fragment-deformation variable).

The production of 665 computer-drawn potential-energy maps together with 150 maps of other nuclear properties of interest has been finished. (The

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[1]W. J. Swiatecki, Prog. Particle and Nucl. Phys. 4, 383 (1980); Lawrence Berkeley Laboratory preprint, LBL 8950, (March 1979).

atlas of maps has been printed as a Lawrence Berkeley Laboratory document, LBL-12811, May 1982.) Each map refers to a fixed mass asymmetry and displays the property of interest as a function of the elongation/distance and the neck/fragment-deformation variables. The maps span the range of virtually all possible systems accessible though the collision of any two nuclei in the periodic table.

Figure LBL-E10 is one of these maps. Contours of equal deformation energy are plotted against the distance or separation variable "RHO" and the fragment-deformation or neck variable "DECK". The contours are spaced at 0.002 of the surface energy of the sphere (665.09 MeV in this case). The map refers to a mass asymmetry corresponding to the heavier fragment having a fraction 0.7714 of the total mass. The total system has a fissility parameter $x = 0.825$, corresponding to a nucleus close to ^{252}Cf. Configurations of approaching spheres are along the abscissa. The spheres touch at RHO = 1. Shapes formed by portions of intersecting spheres are along the edge sloping up at 45° and end up as a single sphere at the left-hand tip of the map, where the larger sphere has swallowed up the smaller one. The upper curved boundary of the map corresponds to an elongating spheroid with one tip blunted by a portion of a sphere. Scission configurations (in the form of two tear-drop fragments with tips in contact) are just below the ridge running from the configuration of tangent spheres at RHO = 1 to the right-hand edge at DECK $\simeq$ 0.7.

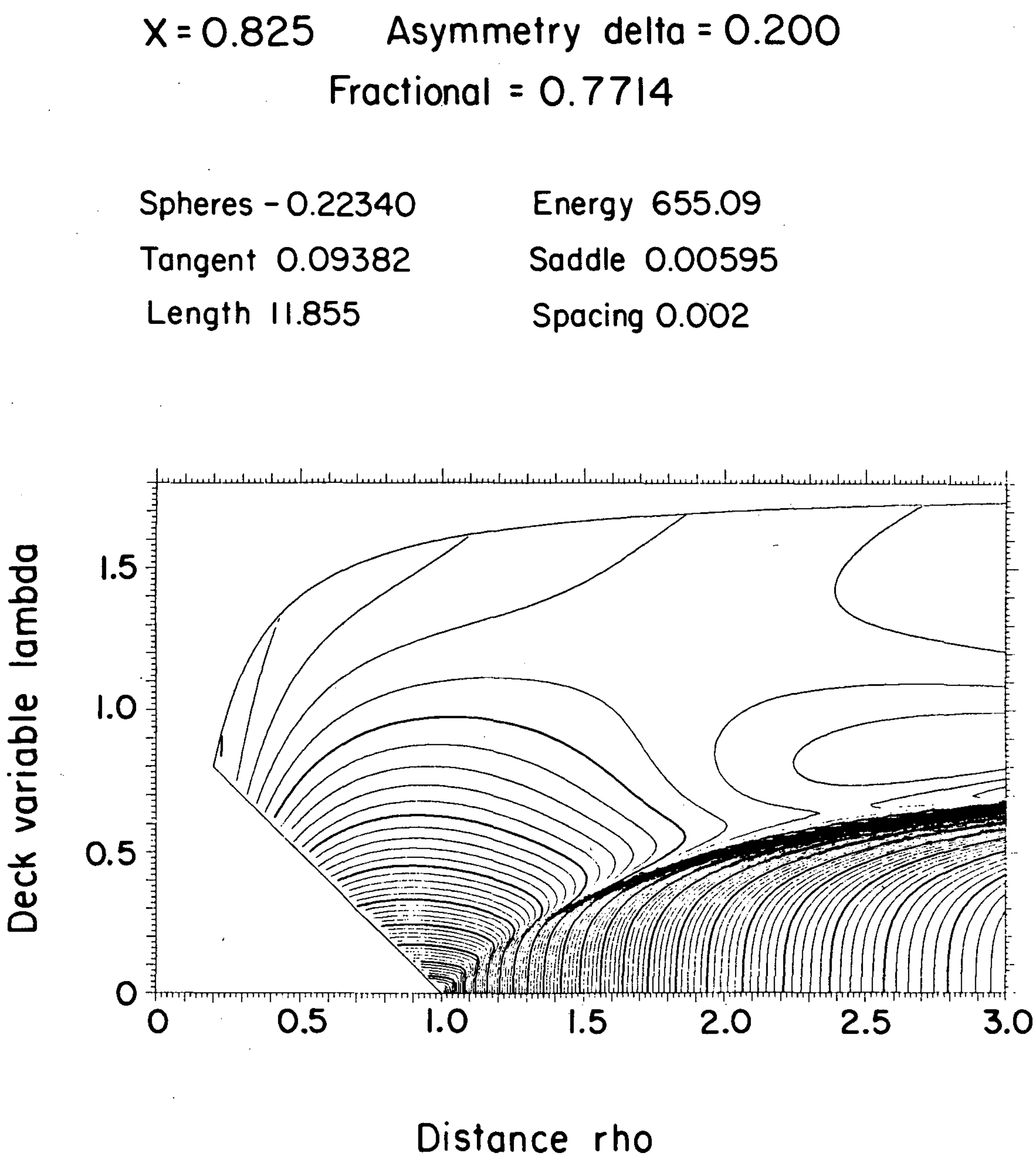
The availability of such maps enables one, for the first time, to assess at a glance the main features of the driving forces involved in nuclear fission or in the fusion or reseparation of any two nuclei in the periodic table. The accuracy of the computer-generated maps is such that, provided the locations of the contours are read off with sufficient precision, the maps represent, in effect, a tabulation of the relevant quantitites to several significant figures.

This is an example where, without the use of computers and the associated plotting techniques, an essential aid to our understanding of nuclear processes could not have been provided.

Scientific Personnel

W. J. Swiatecki, Lawrence Berkeley Laboratory and J. Blocki, Institute of Nuclear Research, Swierk, Poland.

Figure LBL-E10



XBL 831-1116

LBL FY 1985 ADP LONG-RANGE SITE PLAN

FINANCIAL ALTERNATIVE ANALYSES

(Dollars in Thousands)

SITE: Lawrence Berkeley Laboratory - LBL
ITEM: Class IV Computer System
MIE NUMBER: LBL-85-3

PURCHASE OPTION
FISCAL YEAR

SCHEDULE F1

	TOTALS	1985		1986	1987	1988	1989	1990	1991	1992	1993
•PURCHASE COST	2600	2600									
•MAINTENANCE COST	752		94	94	94	94	94	94	94	94	
•RESIDUAL VALUE	(151)									(151)	
CONSTANT COSTS	3201	2600	94	94	94	94	94	94	94	(57)	
DISCOUNT FACTORS		1.000	[.953]*	0.867	0.788	0.716	0.651	0.592	0.538	0.489	0.445
PRESENT VALUE COSTS											
•ANNUAL		2600	90	81	74	67	61	56	51	(28)	
•CUMULATIVE		2600	2690	2771	2845	2912	2973	3029	3080	3052	

LEASE OPTION
FISCAL YEAR

SCHEDULE F2

	TOTALS	1985	1986	1987	1988	1989	1990	1991	1992	1993
•LEASE COST	6992	874	874	874	874	874	874	874	874	
•MAINTENANCE COST	. . . . *included in lease cost* . . .									
CONSTANT COSTS	6992	874	874	874	874	874	874	874	874	
DISCOUNT FACTORS		[.953]*	0.867	0.788	0.716	0.651	0.592	0.538	0.489	0.445
PRESENT VALUE COSTS										
•ANNUAL		833	758	689	626	567	517	470	427	
•CUMULATIVE		833	1591	2220	2846	3413	3930	4400	4827	

*SEE TABLE 2 FOR MONTHLY DISCOUNT FACTORS

LBL FY 1985 ADP LONG-RANGE SITE PLAN

FINANCIAL ALTERNATIVE ANALYSES

(Dollars in Thousands)

SITE: Lawrence Berkeley Laboratory - LBL
ITEM: Class IV Computer System
MIE NUMBER: LBL-85-3
EXERCISED AFTER 36 **MONTHS**

LEASE WITH OPTION TO PURCHASE
FISCAL YEAR

SCHEDULE F3

	TOTALS	1985	1986	1987	1988	1989	1990	1991	1992	1993
• LEASE	2535	780	780	780	195					
• MAINTENANCE	752	94	94	94	94	94	94	94	94	
• PURCHASE COST	2600				2600					
• LEASE CREDITS	(1300)				(1300)					
• RESIDUAL VALUE	(151)								(151)	
CONSTANT COSTS	4436	874	874	874	1589	94	94	94	(57)	
DISCOUNT FACTORS		[.953]*	0.867	0.788	0.716	0.651	0.592	0.538	0.489	0.445
PRESENT VALUE COSTS										
•ANNUAL		833	758	689	1138	61	56	51	(28)	
•CUMULATIVE		833	1591	2280	3418	3479	3535	3586	3558	

LEASE-TO-OWNERSHIP OPTION
FISCAL YEAR

NUMBER OF MONTHS 60

SCHEDULE F4

	TOTALS	1985	1986	1987	1988	1989	1990	1991	1992	1993
• LEASE	3200	640	640	640	640	640				
• MAINTENANCE	752	94	94	94	94	94	94	94	94	
• RESIDUAL VALUE	(151)								(151)	
CONSTANT COSTS	3801	734	734	734	734	734	94	94	(57)	
DISCOUNT FACTORS		[.953]*	0.867	0.788	0.716	0.651	0.592	0.538	0.489	0.445
PRESENT VALUE COSTS										
•ANNUAL		700	636	578	526	478	56	51	(28)	
•CUMULATIVE		700	1336	1914	2440	2918	2974	3025	2997	

*SEE TABLE 2 FOR MONTHLY DISCOUNT FACTORS

SCHEDULE F5

SITE: LAWRENCE BERKELEY LABORATORY
Item. Class IV Computer System
MIE NUMBER LBL-85-3

SUMMARY OF FINANCIAL ALTERNATIVE ANALYSES

ANALYSIS PARAMETERS:

Estimated Installation Date	Oct 1, 1984
Estimated Removal Date	Oct 1, 1992
Analysis Period	8 years
Lease Credit Schedule	50% for 3 year lease

SUMMARY OF COMPARATIVE COSTS
(Dollars in thousands)

OPTION	Constant Dollar Costs	Present Value Costs	Cost Ratio	Break-even Point
A. Purchase	3201	3052	1.00	--
B. Lease	6992	4827	1.58	Nov. 20, 1988
C. Lease with option to purchase	4436	3558	1.17	Jan. 1, 1988
D. Lease to ownership	3801	2997	.98	--

Assumptions:

1. Purchase price is $2,600,000.
2. Maintenance equals 3.6% of purchase price per year.
3. Lease cost equals 30.0% of purchase price per year.
4. Lease to ownership can be financed under University of California full payout lease over a period of 60 months at an interest rate of 8.5% per annum.

LBL FY 1985 ADP LONG-RANGE SITE PLAN

FINANCIAL ALTERNATIVE ANALYSES

(Dollars in Thousands)

SITE: Lawrence Berkeley Laboratory - LBL
ITEM: Energy Research Computing Facility
MIE NUMBER: LBL-85-1

PURCHASE OPTION
FISCAL YEAR

SCHEDULE F1

	TOTALS	1985		1986	1987	1988	1989	1990	1991	1992	1993
•PURCHASE COST	13,400	13,400									
•MAINTENANCE COST	6,400		800	800	800	800	800	800	800	800	
•RESIDUAL VALUE	(777)									(777)	
CONSTANT COSTS	19,203		800	800	800	800	800	800	800	23	
DISCOUNT FACTORS		1.000	[.953]*	0.867	0.788	0.716	0.651	0.592	0.538	0.489	0.445
PRESENT VALUE COSTS											
•ANNUAL		13,400	762	694	630	573	521	474	430	11	
•CUMULATIVE		13,400	14,162	14,856	15,486	16,059	16,580	17,054	17,484	17,495	

LEASE OPTION
FISCAL YEAR

SCHEDULE F2

	TOTALS	1985	1986	1987	1988	1989	1990	1991	1992	1993
•LEASE COST	38,560	4,820	4,820	4,820	4,820	4,820	4,820	4,820	4,820	
•MAINTENANCE COST	. . . .	*included in lease cost* . . .								
CONSTANT COSTS	38,560	4,820	4,820	4,820	4,820	4,820	4,820	4,820	4,820	
DISCOUNT FACTORS		[.953]*	0.867	0.788	0.716	0.651	0.592	0.538	0.489	0.445
PRESENT VALUE COSTS										
•ANNUAL		4,593	4,179	3,798	3,451	3,138	2,853	2,593	2,357	
•CUMULATIVE		4,593	8,772	12,570	16,021	19,159	22,012	24,605	26,962	

*SEE TABLE 2 FOR MONTHLY DISCOUNT FACTORS

FINANCIAL ALTERNATIVE ANALYSES

(Dollars in Thousands)

SITE: Lawrence Berkeley Laboratory - LBL
ITEM: Energy Research Computing Facility
MIE NUMBER: LBL-85-1
EXERCISED AFTER 36 **MONTHS**

LEASE WITH OPTION TO PURCHASE
FISCAL YEAR

SCHEDULE F3

	TOTALS	1985	1986	1987	1988	1989	1990	1991	1992	1993
• LEASE	12,060	4,020	4,020	4,020						
• MAINTENANCE	6,400	800	800	800	800	800	800	800	800	
• PURCHASE COST	13,400			13,400						
• LEASE CREDITS	(6700)			(6700)						
• RESIDUAL VALUE	(777)								(777)	
CONSTANT COSTS	24,383	4,820	4,820	11,520	800	800	800	800	23	
DISCOUNT FACTORS		[.953]*	0.867	0.788	0.716	0.651	0.592	0.538	0.489	0.445
PRESENT VALUE COSTS										
•ANNUAL		4,593	4,178	9,078	573	521	474	430	19	
•CUMULATIVE		4,593	8,772	17,850	18,423	18,944	19,418	19,848	19,859	

NUMBER OF MONTHS 60

LEASE-TO-OWNERSHIP OPTION
FISCAL YEAR

SCHEDULE F4

	TOTALS	1985	1986	1987	1988	1989	1990	1991	1992	1993
• LEASE	16,495	3,299	3,299	3,299	3,299	3,299				
• MAINTENANCE	6,400	800	800	800	800	800	800	800	800	
• RESIDUAL VALUE	(777)								(777)	
CONSTANT COSTS	22,118	4,099	4,099	4,099	4,099	4,099	800	800	23	
DISCOUNT FACTORS		[.953]*	0.867	0.788	0.716	0.651	0.592	0.538	0.489	0.445
PRESENT VALUE COSTS										
•ANNUAL		3,906	3,554	3,230	2,935	2,668	474	430	11	
•CUMULATIVE		3,906	7,460	10,690	13,625	16,293	16,767	17,197	17,209	

*SEE TABLE 2 FOR MONTHLY DISCOUNT FACTORS

SCHEDULE F5

SITE: LAWRENCE BERKELEY LABORATORY
Item. Energy Research Computing Facility
MIE NUMBER LBL-85-1

SUMMARY OF FINANCIAL ALTERNATIVE ANALYSES

ANALYSIS PARAMETERS:

Estimated Installation Date	Oct. 1, 1984
Estimated Removal Date	Oct. 1, 1992
Analysis Period	8 years
Lease Credit Schedule	50% for 3 year lease

SUMMARY OF COMPARATIVE COSTS
(Dollars in thousands)

OPTION	Constant Dollar Costs	Present Value Costs	Cost Ratio	Break-even Point
A. Purchase	19,023	17,495	1.00	--
B. Lease	38,560	26,962	1.54	Sept.1988
C. Lease with option to purchase	24,383	19,859	1.14	Sept., 1987
D. Lease to ownership	22,118	17,209	.98	Nov., 1992

Assumptions:

1. Purchase price is $13,400,000.
2. Lease to ownership can be financed under University of California full payout lease over a period of 60 months at an interest rate of 8.5% per annum.

LBL FY 1985 ADP LONG-RANGE SITE PLAN

FINANCIAL ALTERNATIVE ANALYSES

(Dollars in Thousands)

SITE: Lawrence Berkeley Laboratory - LBL
ITEM: Class III Administrative Computer System
MIE NUMBER: LBL-85-2

PURCHASE OPTION
FISCAL YEAR

SCHEDULE F1

	TOTALS	1985		1986	1987	1988	1989	1990	1991	1992	1993
•PURCHASE COST	1100	1100									
•MAINTENANCE COST	317		19	40	40	40	40	40	40	40	18
•RESIDUAL VALUE	(64)										(64)
CONSTANT COSTS	1353	1100	19	40	40	40	40	40	40	40	(46)
DISCOUNT FACTORS		1.000	[.935]*	0.867	0.788	0.716	0.651	0.592	0.538	0.489	0.445
PRESENT VALUE COSTS											
•ANNUAL		1100	18	35	32	29	26	24	22	20	(20)
•CUMULATIVE		1100	1118	1153	1185	1214	1240	1264	1286	1306	1286

LEASE OPTION
FISCAL YEAR

SCHEDULE F2

	TOTALS	1985	1986	1987	1988	1989	1990	1991	1992	1993
•LEASE COST	2957	183	370	370	370	370	370	370	370	184
•MAINTENANCE COST	. . . .	*included in lease cost* . . .								
CONSTANT COSTS	2957	183	370	370	370	370	370	370	370	184
DISCOUNT FACTORS		[.935]*	0.867	0.788	0.716	0.651	0.592	0.538	0.489	0.445
PRESENT VALUE COSTS										
•ANNUAL		171	321	292	265	241	219	199	181	82
•CUMULATIVE		171	492	784	1049	1290	1509	1708	1889	1971

*SEE TABLE 2 FOR MONTHLY DISCOUNT FACTORS

LBL FY 1985 ADP LONG-RANGE SITE PLAN

FINANCIAL ALTERNATIVE ANALYSES

(Dollars in Thousands)

SITE: Lawrence Berkeley Laboratory - LBL
ITEM: Class III Administrative Computer System
MIE NUMBER: LBL-85-2
EXERCISED AFTER 36 **MONTHS**

LEASE WITH OPTION TO PURCHASE
FISCAL YEAR

SCHEDULE F3

	TOTALS	1985	1986	1987	1988	1989	1990	1991	1992	1993
• LEASE	990	165	330	330	165					
• MAINTENANCE	320	20	40	40	40	40	40	40	40	20
• PURCHASE COST	1100				1100					
• LEASE CREDITS	(445)				(445)					
• RESIDUAL VALUE	(64)									(64)
CONSTANT COSTS	1901	185	370	370	860	40	40	40	40	(44)
DISCOUNT FACTORS		[.935]*	0.867	0.788	0.716	0.651	0.592	0.538	0.489	0.445
PRESENT VALUE COSTS										
•ANNUAL		173	321	292	616	26	24	22	20	(20)
•CUMULATIVE		173	494	786	1402	1428	1452	1474	1494	1474

NUMBER OF MONTHS 60

LEASE-TO-OWNERSHIP OPTION
FISCAL YEAR

SCHEDULE F4

	TOTALS	1985	1986	1987	1988	1989	1990	1991	1992	1993
• LEASE	1354	135	271	271	271	271	135			
• MAINTENANCE	320	20	40	40	40	40	40	40	40	20
• RESIDUAL VALUE	(64)									(64)
CONSTANT COSTS	1610	155	311	311	311	311	175	40	40	(44)
DISCOUNT FACTORS		[.935]*	0.867	0.788	0.716	0.651	0.592	0.538	0.489	0.445
PRESENT VALUE COSTS										
•ANNUAL		145	270	245	223	202	104	22	20	(20)
•CUMULATIVE		145	415	660	883	1085	1189	1211	1231	1211

*SEE TABLE 2 FOR MONTHLY DISCOUNT FACTORS

SCHEDULE F5

SITE: LAWRENCE BERKELEY LABORATORY
Item. Class III Administrative Computer
MIE NUMBER LBL-85-2

SUMMARY OF FINANCIAL ALTERNATIVE ANALYSES

ANALYSIS PARAMETERS:

Estimated Installation Date	Mar 1985
Estimated Removal Date	Feb 1993
Analysis Period	8 years
Lease Credit Schedule	50% for 3 year lease

SUMMARY OF COMPARATIVE COSTS
(Dollars in thousands)

OPTION	Constant Dollar Costs	Present Value Costs	Cost Ratio	Break-even Point
A. Purchase	1353	1286	1.00	--
B. Lease	2957	1971	1.53	52 mo.
C. Lease with option to purchase	1901	1474	1.15	35 mo.
D. Lease to ownership	1610	1211	0.94	N.A.

Assumptions:

1. Purchase price is $1,100,000.
2. Maintenance equals 3.6% of purchase price per year.
3. Lease cost equals 30.0% of purchase price per year.
4. Lease to ownership can be financed under University of California full payout lease over a period of 60 months at an interest rate of 8.5% per annum.

SECTION G. SITE STRATEGY, COMMENTS AND POINTS OF CONTACT

G1. Site Strategy

The principal goal of this Plan is to provide the computing resources required to serve the scientific research programs of the Laboratory in the most cost-effective manner. The Plan is based on the concept of a distributed computing network consisting of access to a large-scale, high-speed computing resource, modern interactive computing resources, satellite computers, and workstations.

The specific components of the network are:

1. A flexible and efficient communications network interconnecting the various components of the distributed system. This network will incorporate many of the presently used communications facilities.

2. Access to a large-scale, high-speed computing resource for those research programs which require Class VI or above services. The proposal for the National Center for Energy Research Computing in this Plan is an example of such a resource.

3. A modern mid-scale interactive computer system in the Central Facility satisfying those computing requirements that fall between the capabilities of the large-scale resource and the satellite computers. This system will also provide the focus for other laboratory-wide services such as graphics, COM, and mass-storage.

4. Distributed satellite computers available for the specialized needs of individual Divisions or research groups. Satellite systems will utilize a standard network protocol for communications with the laboratory-wide distributed system.

5. Work stations ranging from simple terminals to sophisticated microprocessor based systems and having the capability for program development, debugging and execution, interactive graphics, word processing, and electronic mail.

This distributed network system is an extremely flexible and versatile structure which permits a variety of diverse computational needs to be satisfied. The multiple levels of computation are intended to complement and enhance each other, and to promote more efficient utilization of overall computational resources. Although individual computing needs change frequently, the network system permits users to dynamically utilize the computational resources most suitable to their current problems.

This Plan represents an evolution from last year's Plan caused by the following considerations:

> The LBL FY 1984 ADP Long-Range Site Plan was directed towards achieving access to very-large-scale (Class VI or above) computational capability. The access mechanism proposed in that plan was the acquisition of a Class VI computer (LBL-84-1) to become LBL's principal computing resource. During the past year the Office of Energy Research has studied the problem of providing such large-scale resources to all of its contractors. One of the solutions that has been proposed is the establishment of a shared, central facility with access available to all Energy Research contractors. The LBL FY 1985 ADP Long-Range Site Plan is based upon the assumption that such an OER central facility will come into being within the next few years, and that it

will satisfy LBL's growing requirement for large-scale computing. As a result, LBL-84-1 has been removed from this year's Plan. In its place a complete proposal for the establishment of a National Center for Energy Research Computing (NCERC) to offer large-scale, very-high-speed computing to all Energy Research contractors is included as LBL-85-1.

LBL-84-1 was also intended to replace the existing CDC 7600, 6600 and 6400 computers, which are the principal LBL general management computers. The LBL FY 1985 ADP Long-Range Site Plan includes provision for replacing these obsolete and operationally expensive systems with a modern, interactive and cost-effective mid-scale Class IV system. This replacement system will satisfy those LBL scientific computing requirements that will not need the unique resources of the NCERC. The replacement system is labeled LBL-84-2.

The implementation strategy associated with LBL-84-1 included an initial system (for service front-end development) that was to be subsequently reutilized for administrative data processing once the total LBL-84-1 system was installed. The present Plan provides for administrative data processing requirements as a separate acquisition labeled LBL-85-2.

Detailed discussions of the implementation strategies for LBL-84-2, LBL-85-1, and LBL-85-2 are contained in Section E 7.

G2. General Comments/Critical Issues

None

G3. Points of Contact

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Appendix A.

Performance of the MIDAS Prototype

The goal of the MIDAS project is the development of a computer system specifically aimed at dealing with the problems associated with the reduction and analysis of scientific data. The system is designed to provide a highly interactive, graphics-oriented, multi-user environment capable of handling relatively large data bases for each user. The architecture is organized in such a fashion that multiple users can operate independently and simultaneously, without any significant effect on the speed of individual data processing.

For problems involving sequential data analysis the proposed parallel processor approach should provide each real-time user with a processing power at least an order of magnitude greater than is currently available on LBL's best upper mid-range computers (DEC VAX or ModComp Classic) or roughly equivalent to one CDC 7600. The design organizes CPU's into subsystems consisting of ten processors and is capable of supporting at least five subsystems, if required. The total processing power of a full system should therefore be equivalent to approximately 50 of the best of our current mid-range computers. This processing power may be dynamically distributed among many users or allocated to fewer users with more demanding problems. The total resources of the facility could, if desired, be focused on a single problem.

An important design goal of this facility is the creation of a highly modular hardware and software environment. In this environment the high technology devices can be isolated in such a manner as to facilitate their relatively low cost replacement as need and future technological advances dictate. The system is, therefore, capable of planned growth, both in terms of rapidly changing technology and with the needs of the user community.

Architecture

As described previously,[1,2,3,4] the MIDAS design is based on a hierarchy of multiple, high-level processors which permits the high-speed parallel analysis of experimental data. The basic structure of data, discrete event packets, makes its analysis ideally suited to parallel processing. In this parallel framework events are analyzed simultaneously and asynchronously by multiple CPU's, as opposed to the serial, one-event-at-a-time, approach of conventional computers. Such a design is now practical due to the commercial availability of high-level CPU's at relatively modest cost. The system combines interactive graphics capability, high-speed computation, and large mass storage capacity to guarantee a rapid response time to each user. For a currently typical data analysis problem, a turnaround time of under 1 minute for every magnetic tape equivalent of data processed is considered a desirable goal to reach. This requires that each user have available, on demand, a processing power approaching that of the CDC 7600. The system design is intended to provide a highly effective interface between the computer and the scientist, thereby minimizing the real time necessary to complete a given analysis problem. The key features this data analysis facility is designed to provide are as follows: 1) highly interactive performance; 2) high-speed processing; 3) optimized I/O operations; 4) modular construction; and 5) ease of usage.

The basic philosophy of the architecture involves three independent levels of computer processing in a general tree structure, integrated with an independent intelligent mass storage system. The first processing level has a single multi-tasking computer referred to as the "primary computer". The main function of this level is to handle all user interaction and to manage all resources of the system. The problem of interactive analysis is conceptually divided at this level into interactive requirements, handled by the primary computer, and a batch analysis phase handled by level two, the "secondary computer" system.

This secondary system may consist of up to five computers, which, although dynamically allocable, are independently devoted to the solution of only a single analysis problem at a time. The function of the secondary computer is to receive a specific batch analysis problem from the primary, to break the problem into components (e.g., input, output, arithmetic transformation, spectrum generation, etc.) and to load the problem into the elements of a third processing level, known as the "multiprocessor array". Having set up the problem and started the processing, the secondary computer will constantly monitor and, if necessary, control, the operation of the multiprocessor array as well as maintain contact with the primary computer.

A multiprocessor array (which exists for each secondary computer) consists of at least eleven somewhat specialized, high-speed processors, a multi-bussed memory area for data, and a local storage area for results. The assumption is that once an analysis problem is specified, data-events are all analyzed in a parallel fashion, rather than serially as would be done in a conventional computer. At least eight of the eleven processors would be powerful, pipelined CPU's whose function is to perform mathematical transformations of the data base. Each of these CPU's would have a processing capability equivalent to the most powerful computers currently used by the LBL Nuclear Science Division. Thus, a general system containing 5 distributed or secondary systems, would have at least 40 processors of this type in multiprocessor arrays.

Separate from these three processing levels, the design also incorporates an intelligent, multi-bussed, parallel processing storage environment. At least 5 intelligent controllers would oversee the storage and retrieval of user data and results from various mass storage devices. Initially these devices would consist of magnetic tapes, large discs, and bulk histogramming memory.

Development

The development of the **MIDAS Project** was planned in three stages: Phase 1, the development of a working prototype; Phase 2, the creation of a fully operational model; and Phase 3, an expansion of the architecture into a complete multi-user system. Construction of the Phase 1 MIDAS prototype was begun in May 1980 and, after passing all tests, became operational in January 1982. The hardware cost of this initial system was approximately $110K. This prototype utilized three commercial mid-range CPU's to demonstrate the feasibility of the basic parallel-processor approach. The central processing units of commercial mid-range computers, which include floating-point and pipeline hardware, can be obtained at about one-tenth the cost of a complete computer system utilizing the same CPU. A major advantage of utilizing powerful commercial CPU's is the availability of software support, particularly in the form of support for high-level languages such as FORTRAN.

In the prototype system user programs are compiled and assembled in a standard manner by the Secondary CPU. Complete binary copies of this program are then downloaded by the Secondary into each parallel CPU (Programmable Arithmetic Processor) for execution. During execution, a special processor, the Input Formatter, independently directs the incoming information into separate blocks of external memory (the data area). A hardware switching unit, the Conductor, supplies new information to each CPU, on demand, by switching a new block into its memory map. Calculational results are collected from the 'completed' memory blocks by the Output Formatter and stored in a common bulk memory unit, the Storage Memory. All of these processors operate simultaneously and asynchronously. Results of the analysis are available to the user from the Secondary computer by means of a second access port on the Storage Memory.

In January 1982 benchmark tests were conducted on the Prototype System to compare its performance both with our current computers (Mod Comp IV/25) and with performance predicted by our software models. Based on results of software simulations, the performance of the system was expected to be dependent on the relative amounts of I/O versus CPU utilization of each problem. For this reason, testing was conducted utilizing several (very different) existing codes under different calculational conditions. This involved converting several existing large-scale programs to run in a MIDAS environment. These included EVA (an Event Analysis language originally developed in Copenhagen); ORDER, the analysis portion of the MINUS3 system running at the SuperHILAC and 88-inch Cyclotron; SATURN, a Monte Carlo fission simulation code; and an analysis program used to reduce data taken by the Bevatron's Plastic Ball apparatus. In order to assist in utilizing MIDAS, sophisticated program translation and debugging tools have been created to facilitate program conversion and development. These include a generalized translater program which converts higher-level, free-form FORTRAN or RATFOR-type codes into ModComp-standard FORTRAN which can then be compiled and run on MIDAS. Substantial program simplification occurred in the course of converting these programs due to the architecture of MIDAS, which permits some operations (particularly those involving I/O, such as event unpacking) to be performed by specialized hardware devices rather than by software.

Performance was, therefore, tested under three classes of conditions. The first class of problems involved programs with heavy I/O demands; the second set of problems included calculations with relatively balanced I/O and CPU requirements; the third class of problems involved completely CPU-bound calculations, with minimal I/O operations. Table 1 summarizes the results of the benchmark tests. These tests were first run on the prototype consisting of three parallel CPU's (Programmable Arithmetic Modules). A fourth CPU, incorporating new memory which enables this CPU to perform fetches from local memory 20% faster than the three original CPU's, was later added and the benchmark tests were repeated. The EVA program was used as representative of I/O-intensive operations; the ORDER program was run with two different analysis conditions - one case incorporating basic histogram building (moderately I/O-intensive) and another case including extensive gated-spectra and pseudo-parameter creation (mostly CPU-intensive). The SATURN code was included as a completely CPU-limited program. Table 1 indicates that in a CPU-limited environment MIDAS performance shows approximately linear increase in speed with number of CPU's, as would be expected. In I/O intensive problems, however, the increase is far more dramatic, showing a processing throughput more than 50% greater than would be predicted by a strictly linear increase with the number of CPU's. The comparison tests were performed by analyzing real experimental data on both the prototype facility and existing computers.

Work on the Phase 2 model, shown in Figure 1, began in February 1982 and is currently in the final stages of testing. To develop the Phase 2 model, the original prototype was expanded to incorporate ten active processors. A fourth CPU was added to the prototype in March, 1982, and a fifth in May. Projections of the performance of a Phase 2 System running an 'average,' or class 2, program are shown in Table 2. These projections are based on an emulation of the system utilizing the measured benchmark performances. A projection based on a CPU bound problem run on both the CDC 7600 and the MIDAS prototype indicates that the processing power of a single Phase 2 subsystem should be the equivalent of about 85% of a 7600. Total estimated capital equipment cost for the completion of Phase 2 is $390K (inclusive of Phase 1). This working system will support one or two interactive users performing CPU-intensive operations. The Phase 2 model will ultimately constitute a single Distributed Subsystem within the Phase 3 facility. By utilizing additional Distributed Subsystems, the Phase 3 system is capable of considerable expansion, both in terms of processing power and the number of simultaneous users supported.

Summary

The utilization of multiple processors operating in parallel, such as employed in the MIDAS architecture, provides an alternative to achieve necessary high-speed computation in the future. Multiprocessor systems will, by definition, always have the potential of greater computational power than any traditional serial architecture. Focusing this power, however, and applying it to single problems or applications is not simple and is the subject of a great deal of current research. **MIDAS** is based on the concurrent operation of multiple asynchronous processors. This specialized computer facility is intended to provide a highly-interactive environment which will permit problems to dynamically utilize multiple processors in the manner appropriate for the calculation.

Conceptually, a multi-processor architecture can operate in either a parallel or a pipeline mode. In parallel operation all processors execute the same program concurrently, but asynchronously, with each processor accessing separate data packets. In pipeline operation different phases of the calculation execute in each CPU. In this latter mode all processors operate in parallel, with results being passed between processing stages. These modes of operation contrast with an 'array processor' architecture in which instructions are executed synchronously and in parallel. The MIDAS architecture permits parallel, pipeline, or array processing to be configured and intermixed in a dynamic and extremely flexible fashion. The architecture is also able to easily accommodate specialized hardware processors (e.g., custom VLSI processors), as required.

The MIDAS Project is designed to fill a specific need within the nuclear science community. Experience at other research institutions and examination of current computer performance suggest that this need cannot reasonably be filled by currently available computers in any cost-effective manner. Effort at both SLAC and CERN is being devoted to the parallel operation of several, specially-designed, CPU's (emulating an IBM 370/168) to analyze experimental data. Given current computing trends, research and development into the application of parallel processing will certainly have broad applications in other areas besides nuclear science.

References

1. A Specialized, Multi-User Computer Facility for the High-Speed, Interactive Processing of Experimental Data, Creve C. Maples, IEEE Transactions on Nuclear Science, NS-26, 4580 (1979).
2. The Design of MIDAS - A Modular Interactive Data Analysis System, Creve Maples, William Rathbun, Daniel Weaver, and John Meng, IEEE Transactions on Nuclear Science, NS-28, 3746 (1981).
3. The Utilization of Parallel Processors in a Data Analysis Environment, Creve Maples, Daniel Weaver, William Rathbun, and John Meng, IEEE Transactions on Nuclear Science, NS-28, 3880 (1981).
4. A Fast Time-Sliced Multiple Data Bus Structure For Overlapping I/O and CPU Operations, W. Rathbun, C. Maples, J. Meng, and D. Weaver, IEEE Transactions on Nuclear Science, NS-28, 3875 (1981).

Table 1

Results of Benchmark Tests on MIDAS Prototype System

	Running Time in Seconds (Ratio)			
	I/O Limited	Average Mix		CPU Limited
Single Computer	272 (6.3)	612 (5.5)	2314 (4.9)	(~4)
MIDAS (3)*	49 (1.1)	159 (1.4)	673 (1.4)	(1.4)
MIDAS (4)*	<43> (1)	112 (1)	472 (1)	(1)

*Indicates number of parallel CPU's

Table 2

MIDAS - Relative Performance

	Problem: Average CPU and I/O Mix		
	Time (sec.)	Relative Speed	I/O Rate (KB/sec)
1 PAM	480	(1)	26
2 PAMs	241	2.0	52
3 PAMs	159	3.0	83
4 PAMs	112	4.3	115
•			
•			
(8 PAMs)	(53)	(9.0)	(243)

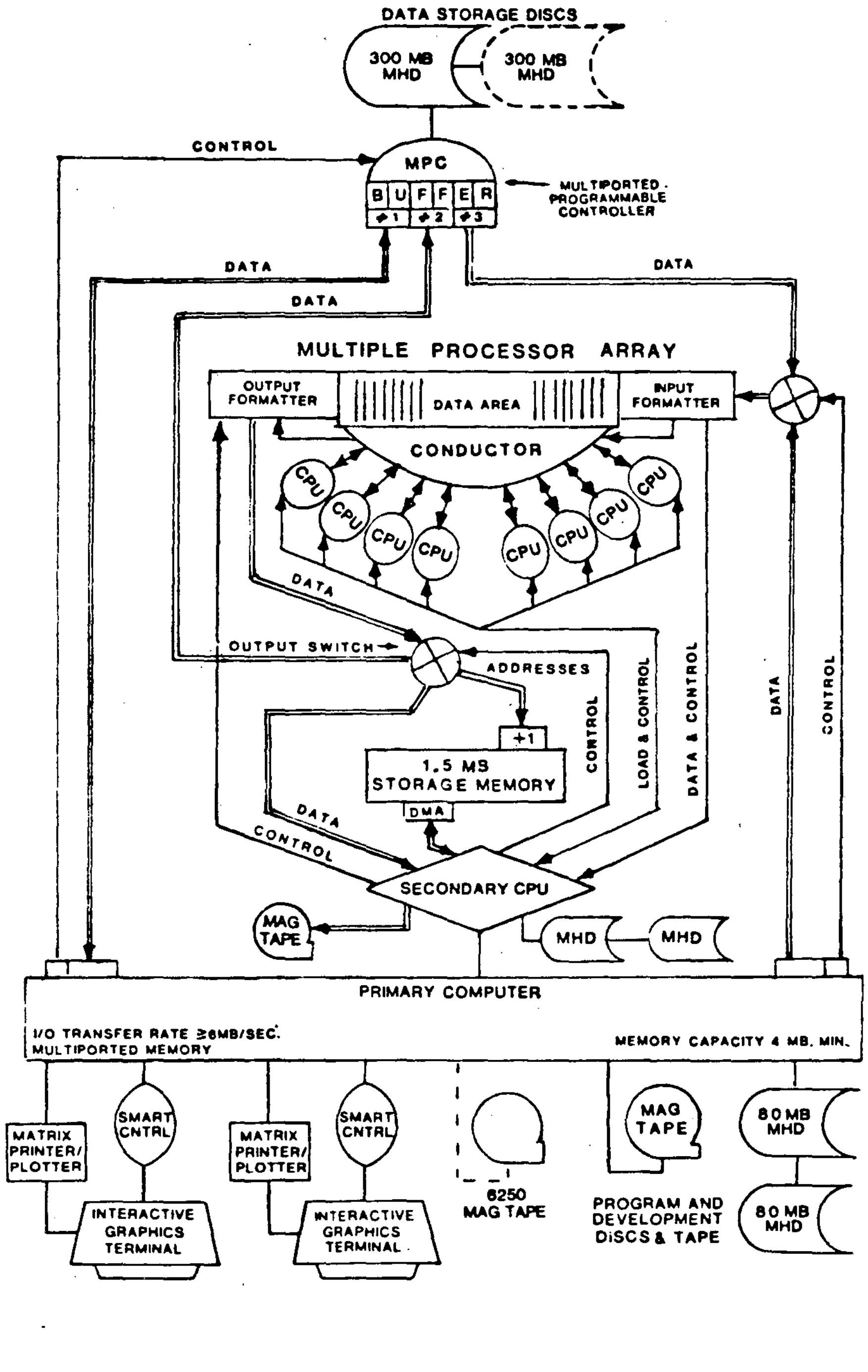

Figure 1. The layout of the MIDAS phase 2 system, currently in final testing.

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