Report by the Subcommittee on Computational Capabilities for Nuclear Theory

to the

DOE/NSF Nuclear Science Advisory Committee

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I. INTRODUCTION AND OVERVIEW

Concern about the lack of adequate computing capabilities for nuclear theory has been growing since the statement: "Present computer facilities available to the nuclear-science community are not adequate to handle all the required computation for theory", was first voiced in the N.A.S. "Friedlander" Report on "Future of Nuclear Science" (1977). A segment of the nuclear science community initiated workshops in an attempt to understand the computing needs for nuclear theory which led to their consideration of a National Nuclear Computing Center. The Nuclear Science Advisory Committee (NSAC) in developing its Long Range Plan (LRP) in 1979 identified again the continued lack of adequate computing capabilities for nuclear theory. In particular the NSAC Long Range Plan recognized the relatively high priority needs for computing by recommending a construction plan with $12 Million for nuclear theory computing in FY 84 as well as an increase of $3 Million in operating budgets which would be associated with such construction.

In accord with these earlier developments a Subcommittee on Computational Capabilities for Nuclear Theory was appointed in July 1980 with a four point charge:

I. Examine present and future trends for the usage of computers both for nuclear theory calculations and for comparisons of data with theory by nuclear scientists.

II. Evaluate several approaches to computer configurations ranging from a single central facility to many distributed facilities. Combinations of a central facility and

several distributed facilities should be considered.

III. Consider various possible levels of computing capability and recommend the most appropriate configuration and cost for each level of capability considered.

IV. Recommend the optimum choice for the next decade keeping in mind the Long Range Plan for Nuclear Science. This optimum choice should include not only new facilities but also a discussion of the optimum role which could be played by current facilities.

Available to the Subcommittee were previous reports and technical documents which are listed in Appendix A.

The Subcommittee met for the first time on November 5, 1980 and recognized the need for detailed information from the nuclear community. Two surveys were initiated. The first, a telephone survey involving about 100 respondents in various subfields, was carried out by individual committee members and the reports in section III are based to some extent on this telephone survey. The following questions were asked:

1) In the area being surveyed, what are the exciting frontier problems to be tackled?

2) What are the computational capabilities required to properly investigate the above?

3) What fraction of the above exciting problems can be tackled with current computer facilities?

The second survey took the form of a written questionnaire sent to three hundred principal investigators in nuclear theory and experiment. The results of this questionnaire were tabulated by July 15, 1981 at Florida State University and a report on the results is contained in Appendix B of this report. The results of

this questionnaire were helpful in formulating the evaluations obtained in sections IV and V which in turn were discussed at a second meeting of the subcommittee on September 10 and 11, 1981. The major recommendations and conclusions reached by this subcommittee at this second meeting are given in the next section. The detailed nature of computations in nuclear theory are discussed in section III in terms of four subfields which correlate closely with the major subfields of nuclear science considered in the NSAC Long Range Plan. The present and future computational capabilities for nuclear theory are evaluated in section IV according to the six subsections: i) general needs - present and future, ii) educational impact, iii) role of national laboratories, iv) program distribution center, v) new computer languages and vi) new technologies. The costs associated with the various modes of computing are discussed in section V and have been used to provide the estimates of the various funding levels corresponding to each level of computational capability considered in the following section.

This subcommittee is concerned with computational capabilities for calculations by nuclear theorists and theoretical analysis of data with models or reaction codes by nuclear experimentalists. We are not examining the computational needs associated with data collection or the analysis of raw data since the computers used for such purposes are properly considered to be part of the instrumentation of an experimental facility.

II. RECOMMENDATIONS AND CONCLUSIONS

In this section we present first the recommendations appropriate to three distinct levels of computational capability corresponding to: i) a "static" approach, ii) steady increases and iii) a strong initiative. Based upon these three levels of consideration, final recommendations which are in close accord with the Long Range Plan are presented in subsection iv).

i) A STATIC APPROACH TO THE FUNDING OF COMPUTATIONAL NUCLEAR THEORY

As much as any subfield of physics, nuclear theory is and will remain computer-intensive: almost all worthwhile research problems in nuclear theory require substantial amounts of computing. This orientation toward computing has its origin in the basic nature of the intellectual approach to the subject. It has strong implications for the training of graduate students and post-doctoral assistants in nuclear physics.

Computational nuclear theory is strongly coupled to experimental work and is invariably needed to support experimental research in accelerator laboratories. Therefore, the vitality and productivity of most experimental nuclear physics programs depend on the presence of a highly developed computing environment for the associated nuclear theorists. In addition, a vigorous program in computational nuclear theory is needed in order to provide the subject's intellectual underpinnings, without which there would be a drastic decline in general support for nuclear physics as a scientific discipline.

The present level of total support for computing in nuclear theory lies barely above the critical mass. Any scaling down of the totality of existing support for computing in nuclear theory would cause a much larger drop in its ability to contribute to nuclear science. In order to keep activity at its present level, DOE and NSF support for computational nuclear theory must increase, for other current sources of support, such as university subsidies, are rapidly diminishing.

Beyond maintaining the present level of total support through increasing contributions from NSF and DOE, nuclear physics institutions and agencies can achieve some improvements through new flexibility and ingenuity. It takes no massive influx of new funding to:

a) make the computing facilities of the national laboratories more broadly accessible to outside users through the removal of administrative barriers;

b) continue the present modest program of the funding agencies to expand nuclear theorists' access to midi-computers;

c) explore the possibilities of developing common computing facilities with theorists in other areas of physics, as envisioned in the recent Prospectus for Computational Physics;

d) develop a modest dial-in network connecting dispersed nuclear groups with each other and with computers of various capabilities;

e) exploit the educational advantages of such a network by giving students access that will enable them to develop a variety of needed professional skills.

Such a scenario for minimal support cannot be expected to allow computational nuclear theory to make its optimal contribution to nuclear science, but we do think it would allow the nuclear theory community to continue to develop its capabilities, albeit slowly.

ii) STEADY INCREASES IN COMPUTATIONAL CAPABILITY

This level II of computational capability roughly corresponds to a steady improvement which is geared to meet the projected needs as gleaned from the questionnaire, i.e. a factor of two improvement over a five year period. It also is aimed at maintaining maximum flexibility so that several options which may be available in the future remain open as long as possible. The recommendations for such a level of capability are based on the "evolutionary" approach and a two stage procedure is envisaged. In stage one we recommend

a) Funding of midi-computers should be continued at the present rate until up to the order of ten additional facilities are established with provision for connection to existing networks for all such facilities.

b) An interim center should be established as soon as possible with the dual purpose of providing access to a large facility with many of its attendant advantages (e.g., data bases, electronic conferencing, code exchange, etc.) and as a research and development facility which serves as a forerunner for a more powerful centralized facility if this proved to be advantageous. Such an interim center we anticipate would be most economically established at an existing class VI facility.

The costs associated with these two recommendations involve a capitalization of about $3 Million to acquire ten midi-machines and an annual operating budget of up to $2.6 Million. These operating costs are structured as follows:

10 Midi's with network connections	$1.0 Million
A growing level of CPU hrs. (7600 units) on the interim center reaching 5000 by 1984 ($250/hr.)	$1.25 Million (maximum)
Staff: 3 professional + 1 secretary + access to consultants	$0.35 Million

The staff involved in the interim center are needed for repository services, consulting, data bases, etc. The second stage of level II involves a review of the interim center within the first two or three years of its operation. If the nuclear community demonstrates the anticipated benefits of access to a centralized facility then by no later than 1985 we would recommend:

> That the interim center be replaced by more powerful centralized facilities corresponding to about 20,000 CPU hrs. (7600 units). Such facilities could be obtained by sharing a class VI facility with other disciplines.

Additional capitalization costs are estimated at $5 Million and a suitable staff (35 FTE) would involve an increase in operating costs of about $2 Million. If both stages occurred then the total operating budget during stage two would be between $3 - $4 Million per year. Capitalization costs to establish both stages would be about $8 Million. These estimated costs are significantly below the Long Range Plan

recommendations particularly when it is remembered that the latter are phrased in FY 79 dollars whereas our estimates are in current dollars.

iii) STRONG INITIATIVE

The recommended level III capability is designed around a very general computational system where a number of computer facilities are linked together by means of an information network. The heart of this system - the principal node - consists of a large CLASS VI central computer with large capacity and capability. Regional nodes may contain cost effective midi-computers for additional computing capacity or intelligent I/O stations with advanced graphics and printing capabilities. A large number of simple/inexpensive dial-up connections are also provided.

Some of the long recognized advantages of a large central computer facility which can serve the needs of a large body of users with common goals and interests include:

-increased cooperation and enhanced sharing of data, codes and information. Reduces duplication of effort.

-provides underprivileged (university?) users with access to the same powerful computing capability as some of the large national labs.

-allows for movement of people from universities to labs or from one lab to another with no loss of productivity.

-increases both scientific and administrative flexibility - i.e., one can quickly and easily respond to changes, new priorities or other important programmatic needs.

-can provide capabilities which might not be justifiable on an individual basis otherwise:

i) large capacity

ii) good software systems

iii) good documentation

iv) good consulting

v) special purpose hardware and software for file storage, graphics, etc.

vi) support for special applications

-a coherent cost-effective approach for most if not all computations in nuclear theory.

There is currently a large body of experimental nuclear physics data which theory is unable to properly address in part due to unavailability of adequate computing capability. New accelerators and experimental facilities are under construction and being designed. If nuclear theory is to keep pace and possibly lead research in some of these new areas of physics, it must plan for and support funding of the most up-to-date tools for attacking these problems. An aggressive and prompt establishment of a Level III capability would provide both a national visibility for the funding agencies and serve as a unifying influence in the nuclear community. Level III cost estimates are as follows:

	Capital Costs $K	Yearly Operating Costs $K
I. LOCAL ENVIRONMENT		
i. Network Node. Small local computers such as VAX, IBM, SEL, etc. Tie in existing facilities and fund additional 10^+ units over a period of time.	3,000	1,000

		Capital Costs $K	Yearly Operating Costs $K
ii.	Network I/O stations including e.g. DEC 11/44 with a printer, disk, 30-40 terminal ports. 10 units.	1,500	100
iii.	Dial-up terminals to individual users, including a mix of Video/Graphics capabilities up to 1200 baud. 100 units.	300	50
II.	CENTRAL FACILITY		
i.	Class VI central computer e.g. CRAY including 1.0 million word memory, 9600 mbyte disks.	9,000	350
ii.	Central Mass Storage	1,000	100
iii.	Local Network for Central Facility. Including in addition a local I/O station and copy of a typical node computer such as a VAX.	1,000	50
iv.	Network Hardware and Communications Network Lease.	500	240
v.	Manpower Cost (50 FTE)		3,000
vi.	Supplies and Services		450
vii.	Building Lease		150
	TOTALS	16,300 K$	5,490 K$

iv) OPTIMUM CHOICE

The computational level consistent with the Long Range Plan lies between levels II and III considered above. In view of the nuclear community indicating many diverse opinions and because changes in computer technology are occurring rapidly we recommend:

a) That stage one of level II be adopted for the short term period ending in about 1984/1985.

b) That an evolutionary approach towards level III be adopted for the rest of the decade keeping in mind that the actual level reached would depend upon the experience gained from the interim center.

The above recommendation is aimed at meeting projected needs with a realistic budget outlay. It has the advantage of maintaining maximum flexibility at each stage. In particular the approach to level III can involve an appropriate fraction of a central facility which is shared with other disciplines. Clearly the improvements in computer technology in 1985 and beyond will alter many of our thoughts and it would be inappropriate for this committee to make too detailed a recommendation for this part of the decade.

Current facilities could be optimally integrated into the overall approach according to the ideas a) - e) discussed in level I above. In particular it is desirable to:

- Make the computing facilities of the national laboratories more broadly accessible to outside users through the removal of administrative barriers.
- Allow currently existing midi-computers to be connected to existing networks.

We believe the above recommendations are in accord with the computing

needs of the nuclear community and are cost effective within the guidelines of the Long Range Plan.

III. NATURE OF COMPUTATIONS IN NUCLEAR THEORY

As the fields of physics advance, theoretical investigations naturally evolve from a stage of analytical solutions to where numerical solutions become essential. At any one time, different subfields are in different stages of this process. However, in general, large scale computation becomes necessary as the systems of interest become more complex. For example, complexity increases as one moves from a few degrees of freedom to many degrees of freedom; or from low order expansions to high order expansions. It is important to note that complexity arises not from "a poor choice of problems" but inevitably as theory advances. This increasing complexity is well evidenced in the various subfields discussed in the following subsections:

i) LIGHT IONS AND INTERMEDIATE ENERGY

A good deal of this area is devoted to the classical study of nuclear structure using various probes. For these investigations computation tools are absolutely essential. Types of codes in use for calculating cross sections now range from ordinary DWBA calculations to sophisticated many-coupled-channel approaches. For the analysis of neutron radii the multiple scattering approaches to proton and pion elastic scattering are being pushed very hard. The inclusion of many effects is leading to

understanding of the data and, it would appear, the extraction of neutron radii, but some phenomenology, and a good deal of computer time will be required. Kaon scattering will have its own advantages and a similar program will be needed for this new probe. For all of the reaction studies, shell model calcula- must be done, a process inherently requiring the use of a computer. A large program of coherent ("sub-threshold") pion production to specific nuclear states is underway at IUCF, TRIUMF and LAMPF and the interpretation of this data will require computers for both the reaction mechanism and the shell model calculations (apparently) required. The observation of a correlated nucleon pair following pion absorption in flight (a possible probe of nucleon-nucleon correlations in nuclei) has not been pursued to its fullest due, at least partly, to the lack of adequate codes. This last is, in turn, due partly to lack of computing facilities.

Leaving the realm of (almost) purely nucleonic description, many workers in this field are including mesonic and/or N^* degrees of freedom into their calculations. This last is one way of including modifications of the nucleon-nucleon interaction due to the presence of the nuclear medium. These effects are of moderate size in several cases and more careful investigation will require the continuing development of scattering and reaction theories including these additional degrees of freedom.

Other investigators in the area are turning to the problem of how to include quark degrees of freedom into these calculations as well, but this work is only beginning. Some workers are focusing on

specialized areas such as parity violations. The amount of computing to be done to solve the models which will eventually evolve in this area is difficult to estimate.

A better developed area of the physics of quarks in nuclei is the field of hypernuclei. To investigate the effect of replacing one light quark with a strange quark, nuclear structure physics must be redone. The payoff from these studies is very high, apparently allowing us to measure the interaction of a quark directly. To make these studies, reactions involving strangeness change must be calculated [(π,K), (K,π), (γ,K), (p,K) etc]. Many of the techniques for calculating these cross sections may be carried over but new ideas will be needed as well and both the reaction codes and hyper-nucleus shell model codes will require considerable amounts of computing time.

Anti-protonic induced nuclear reactions may well provide a new method for introducing a large amount of energy (~2 GeV) with almost zero momentum. The analysis of these multi-pionic final states may provide a method for "x-raying" the nucleus. While this idea is still embryonic, it is difficult to imagine this data being interpreted without the use of considerable amounts of computer time.

In the nucleon-nucleon interaction many investigators are attracted by the question of the possible existence of di-baryons. This potentially exciting subject requires three-body calculations for its interpretation since the features observed occur near the threshold for Δ production and could conceivably be explained by this mechanism alone. The known resonance

in the π-nucleon channel and the supposed resonance in the nucleon-nucleon channel require the strict application of 3-body unitarity, hence the need for 3-body calculations. In addition, the solution to the di-baryon problem will require the use of all possible experimental data bearing on it. In order to correlate these thousands of data a computer must be used to reduce the number to a suitable usable form (e.g. phase shifts).

On an even more fundamental (but related) level, one of the most important problems facing the nucleon-nucleon area is the derivation of the nucleon-nucleon interaction from the basic quark constituents. Those calculations will involve (at least) six bodies and the possibility of using modern computer techniques to solve the confinement problem is a very exciting (and speculative) one.

The computing time needed to carry out these programs is expected to be in excess of 3,000 hrs./yr. of 7600 time. The "excess" is because none of the speculated extensions have been included. Only programs with concrete time estimates have been counted.

While the existence of good graphics capability and large core were common requests, the single largest need for special requirements was an algebraic manipulator such as MACSYMA or diagram calculation programs such as SCHOONSCHIP.

ii) COMPUTING NEEDS FOR HEAVY-ION THEORY

Collisions between complex nuclei confront the theorist with the problem of understanding nuclei under the unusual conditions of high excitation energy, angular momentum, deformation, isospin asymmetry, and density. In such complex situations, even the

"normal" pattern of behavior expected on the basis of known nuclear properties is difficult to define, so that detailed realistic simulations are an indispensable tool, even if only to establish the background against which exotica may be identified. The breadth of phenomena to be described, from low-energy fission to interactions at relativistic energies, implies that a variety of models, studied with both analytical and numerical methods, are necessary for a complete understanding.

For systems formed at low bombarding energies (E/A less than about 20 MeV), static simulations play an important role. The potential energy and inertia of a nucleus as functions of its shape, temperature, and angular momentum are amenable to calculation using macroscopic (liquid drop), microscopic (constrained Hartree-Fock), and macroscopic-microscopic (Strutinsky method) models. To date, computational limits have allowed exploration of only a small portion of the full parameter space involved. Thorough studies would entail some 300-400 hours of CDC 7600 time.

Dynamical simulations of low-energy heavy-ion collisions involve a variety of computationally intensive models. For peripheral collisions, DWBA and coupled channels calculations treating many partial waves and intrinsic states of the nuclei are necessary to understand experimental cross sections and to extract useful structure information from them. A vigorous program, even just exploiting existing codes, might entail some 150-200 hours of CDC 7600 time per year.

For central collisions at low energies, the Time-Dependent Hartree-Fock (TDHF) method is the principal microscopic formulation. Calculations of this type involve the evolution of single-particle wavefunctions for each nucleon of the colliding system and hence

require both a large memory (about 2 million words) and high speed; they are, however, naturally suited to vector computation. A typical calculation for an intermediate mass system such as Kr+La requires about 90 minutes of CRAY-1 time per impact parameter. An extensive investigation of larger systems, including studies of prompt particle emission from the early stages of the collision and variation of the effective inter-nucleon interaction, could easily consume 5 hours of CRAY-1 time per week; extension of these methods to spontaneous fission might require a similar amount of time. Formalisms for extending and correcting the TDHF picture (functional integral methods, two-body collision terms) are available, although their realistic application is impossible with the present computer capabilities. Similarly, the reduction of the TDHF picture to a macroscopic nuclear fluid dynamics can only be achieved by a detailed comparison of microscopic quantum calculations with classical Liouville and fluid dynamical results in realistic situations.

High-energy heavy-ion collisions (E/A greater than about 100 MeV), present an entirely different set of problems to be treated with a correspondingly different set of methods. Intranuclear cascade calculations, classical equations-of-motion methods, and nuclear hydrodynamics are the primary tools here for investigating the extent of equilibration, the influence of the nuclear equation-of-state, and the possible existence of exotic phenomena such as pion condensation. Since these models involve tracing the evolution of each nucleon or bit of nuclear matter in the system, their realistic implementation, including three spatial dimensions and mesonic degrees of freedom, requires large amounts of computer time; some 400-500 hours of CDC 7600 time might be required for a

thorough exploitation of existing codes. Moreover, as more exclusive characterizations of collision products become possible experimentally, more detailed simulations and high statistical accuracy in these stochastic calculations are required.

In the intermediate energy regime (E/A between 20 and 200 MeV), there is as yet no adequate computatonal method, or even formalism, suited to describe heavy-ion collisions. However, it will most likely involve an interpolation between the mean-field dominant at low energies and the nucleon-nucleon collisions important at high energies. If past experience is any guide, model calculations in restricted geometries and with schematic interactions will be possible with the facilities currently available to workers in the field, but realistic calculations directly comparable to experimental data will require access to state-of-the-art computers.

iii) ELECTROMAGNETIC PHYSICS

Electromagnetic probes - photons and electrons - play an important role in exploring our understanding of nuclear structure in both few-body and complex nuclei. Their interaction with matter is weak and the best understood of the elementary probes. The scattering processes are directly related to the local charge and current densities and information on nuclear structure follows from measurement in a direct and unambiguous fashion. In the case of electron scattering, momentum transfer is varied for fixed energy transfer, thus mapping out in precise microscopic detail the spatial distribution of nuclear charge and magnetism; limited only by the wavelength corresponding to the momentum transfer.

Fundamental objectives of nuclear structure physics include

the development of a fundamental theory of the nucleon-nucleon (NN) force and the application of this force in predicting the observed properties of nuclei. The spectrum of activity in electromagnetic physics is aimed at these broad objectives. In the few-body systems, detailed models based more or less on first principles have been constructed and tested. In complex nuclei such a direct approach is not possible and one often uses a mean-field theory with a density-dependent interaction, such as the density-dependent Hartree-Fock approximation. At a more fundamental level, simple model relativistic quantum field theories have been constructed which attempt to deal with the nucleus directly as a relativistic many-body system.

Large basis shell model calculations continue to be very important for confronting our current understanding of nuclear structure with some of the very precise electron scattering data now available. The interpretation of form factor data is in many cases severely limited by the detailed theoretical calculations which are often required. The predictions of the interacting boson approximation (IBA) model which has had a great success in explaining level systematics and transition rates in rotational and transitional nuclei is now being critically tested in several experiments. An experiment such as (e,e') can in fact probe detailed microscopic predictions of this model. Such specific predictions are not in fact available to date, partly due to the lack of sufficient computing capability. These types of frontier large scale calculations require large computer memories, massive off-line storage and 100's of hours of 7600 CPU time.

Precise electron scattering results have clearly indicated

the short-comings of current density-dependent Hartree-Fock calculations for rotationally deformed nuclei as well. Theoretical possibilities for improving this and other similar difficulties in other nuclei include the use of unrestricted Hartree-Fock calculations for nuclear ground states; unfrozen core for rotational nuclei; Hartree-Fock with variation after projection applied to rotational states; and generator coordinate calculations applied to open-shell nuclei. All of these forefront calculations will depend heavily on the availability of computers with large virtual memories, large mass storage and in most cases require some ten's of hours of equivalent 7600 time for typical problems.

The few body problem, stimulated by precise measurements of charge and magnetic form factors to regions of high momentum transfer, is again of forefront theoretical interest. Included here are the Faddeev calculations for two-body low energy photodisintegration of $^3He(^3H)$ using NN interactions with tensor forces and including both E1 and E2 transition operators. Calculations would be done with both separable and state-of-the-art local interactions. Of similar interest are Faddeev calculations for complete (2- and 3-body breakup) low energy electrodisintegration of ^3He and ^3H. A more difficult problem is the two-body photodisintegration of ^4He in a complete 4-body calculation with separable interactions.

Mesonic exchange and relativistic effects are of course necessary ingredients in a complete understanding of the structure of both light and complex nuclei. The relativistic wave function calculations involve large integral-differential equations whose solutions are most naturally done on a "vector machine". As such, advances in this area will be limited and severely restricted

to those researchers at national laboratories, for the most part, where such facilities are normally available for other purposes.

In summary one should also note that in addition to the mostly theoretical problems indicated above, the analysis of experimental electromagnetic physics data is itself very computation intensive. Of particular importance is the necessary unfolding of experimental spectra for radiative, bremsstrahlung and dispersive effects. Dispersion (coupled-channel) type calculations have so far been done on only a few nuclei. This is due mostly to the limited availability of computing capability. The detailed interpretation of some of our form factor data is already hampering our ability to extract purely nuclear structure information. Such dispersion calculations can take upwards of 100 hours of 7600 time for a typical nucleus.

iv) GENERAL THEORY

A) Nuclear Structure Calculations

Many-body wave functions of discrete nuclear states are the basic ingredient for understanding and correlating nuclear reactions through these states. The measurement program of spectroscopy constitutes the largest fraction of research effort at most accelerator laboratories. The theoretical program based on mean field potentials and effective residual two-nucleon interactions is largely a computational effort. This effort is clearly limited in the U.S. by computer resources. Most large basis shell model computer programs have been developed and used in Europe.

A relatively new and productive area of experimental investigation is the intercomparison of inelastic scattering cross

section of different probes at intermediate momentum transfer. The angular distributions of (e,e'), (p,p'), and (π,π') for the same discrete states are being analyzed to extract information on the small components of wave functions and on the effective NN interaction that generates them. The challenge to theory to explain the many systematic trends observed in the data is not being met at a rate to promote synergism.

New theoretical approximations such as the Interacting Boson Model have helped to clarify the important symmetries of low lying vibrational and rotational states, but the computationally intensive Hartree-Fock and Random Phase Approximation remain the main tools of analysis for most structure studies.

A new and exciting development in nuclear structure calculations is the application of Monte-Carlo methods for the variational or exact treatment of many-body problems. These calculations employ a biased random sampling of many-body configurations to produce such results as the binding energy and charge density of the nuclear ground state. To date, there have been computationally intensive variational calculations of ^{4}He with a realistic v_{14} potential and exact calculations of ^{4}He using only a central inter-nucleon potential. These results have been important in establishing the need for three-body forces and in setting bench-marks against which approximation schemes can be tested. Attempts to extend these methods to larger systems must deal with the difficult constraint of the Pauli principle and are likely to be even more prodigious consumers of computer time.

B. Few Nucleon Interactions

The nuclear force problem is confronted most forcefully when

proposed NN potentials are used to predict structure and response functions of the A = 2, 3, and 4 nuclei. The past decade has seen critical tests of the independent nucleon pair assumption. The new insights, especially from charge and magnetic form factors, have broadened our view about the nature of nuclear constituents.

Calculations of few nucleon interactions involve a great deal of numerical work. Global phase shift analysis of nucleon and meson scattering data, Faddeev solutions for three-body bound and continuum states, and meson exchange currents with isobar components in the wave function are all areas of investigation that require large amounts of numerical work. Future efforts with relativistic formulations and four body systems will require even more computer power.

The related area of nuclear matter calculations with new NN potentials has been stimulated by comparing the results of quite different computational approaches: hypernetted chain, Brueckner-Bethe-Goldstone perturbation series, and variational calculations. An effective three-body force in the nuclear Hamiltonian seems to be required to reproduce the average nucleon binding energy and normal nuclear density.

C. Quarks and Gluons in Nuclei

A main new area of research in the next several years will be the search for the influence of subnucleon constituents on nuclear structure and dynamics. It is not immediately clear to what extent this research will require extensive numerical calculations. One guesses however that since the total number of particles and fields in a given nucleus increases over the nucleon-meson description the number and complexity of the equations to be solved

on a computer will increase, possibly dramatically. In addition relativistic formulations will exclude many simplifying approximations used in the solution of the Schroedinger equation of motion.

Bag models of the nucleon have been successful in explaining its excited states using analytic methods. But interacting bags do not have spherical symmetry and thus extensive numerical boundary condition calculations will be required (a la TDHF).

IV. PRESENT AND FUTURE COMPUTING NEEDS FOR NUCLEAR THEORY

i) PRESENT COMPUTING MODES, FUNDING, AND NEEDS

The increasing sophistication and complexity of nuclear models and the experiments which they purport to describe implies that computation plays a major (and growing) role in modern nuclear theory and data analysis. Indeed, the importance of computing is evident in the results of our survey questionnaire, which showed a total nuclear science usage of 3824 CPU hours (7600 units) last year. This time was used by some 400 theorists and some 200 experimentalists, splitting the time between them very nearly in proportion to their numbers. Thus, one nuclear scientist currently uses some 6 hours of CPU time annually, although the variation in individual use is most likely large.

Present nuclear-science computer usage involves a number of different types of calculations, spanning all sub-fields. However most (about 85%) experimental users are engaged in the interpretation of reaction data using coupled-channels, DWBA or nuclear structure codes. Theoretical users concentrate in the same areas (about 70%), although there is also substantial activity in few-body and many-body calculations and in reaction models specific to heavy-ions (TDHF and nuclear hydrodynamics).

Our survey showed that the environments in which nuclear scientists compute vary considerably. About 2/3 of the theorists and 4/5 of the experimentalists are at universities, the balance being at national laboratories. Approximately 50% of our respondents compute on a main-frame machine (> 0.5 NSU). The remainder use a diversity of smaller machines, with a significant fraction of these (~40%) computing on VAX-size facilities. Anecdotal evidence sug-

gests that this latter fraction is growing rapidly. About 40% of our users compute on campus-wide facilities, 40% use laboratory or departmental machines, and the remaining 20% compute at remote locations (about 1/3 of these involve distances greater than 500 miles). Theorists seem to be more heavily dependent on campus or remote facilities (2/3) than are experimentalists (1/2). Almost all scientists responding indicated that they had access to some kind of interactive system, although usage for both theorists and experimentalists seems to be a mix of about 60% in a batch mode and 40% in an interactive mode. Greater than half of our respondents have access to more than one machine.

No single item emerges as a major source of frustration for those scientists responding to our questionnaire. Particularly high on the list were insufficient storage capacity, graphics, and throughput. Lack of documentation seemed to be a problem for only a small number of users.

To some extent, the funding agencies have recognized the importance of computation in nuclear science. The NSF annual computing budget is $145K ($57K for theory, $88K for experiment), while the DOE funding is $669K ($480K for theory, $209K for experiment). Nuclear scientists were able to obtain an additional $915K from other sources last year ($645K theory, $216K experiment), predominantly "invisible money" in the case of universities. These additional sources are clearly very important, as they amount to more than the total agency contribution. In all, there was a total annual expenditure of $1749K for 3824 CPU hours, which amounts to some $450 per CPU hour.

Within the next five years, the present situation is likely to change in several respects. First, the demand for computer time

will undoubtedly grow; our respondents indicated that they would need approximately twice as much CPU time annually within five years. Second, the technological trend is toward smaller, more cost-efficient machines, meaning that a fair fraction of the present usage is likely to move to more personal environments (e.g., laboratory or department machines). Finally, anecdotal evidence suggests that the "invisible money" which is so important to university scientists is disappearing, due in part to the general shift away from large machines.

ii) THE EDUCATIONAL IMPACT OF COMPUTERS IN NUCLEAR THEORY

Although the subcommittee has dealt primarily with computers as research tools in nuclear theory, it is well to mention also the big role which computers and computing play in the education of new generations of nuclear theorists. Ready access to modern computing facilities is essential if the U.S. is to train competitive research physicists in nuclear theory. Our students must learn to write sophisticated programs, modify and test codes obtained from elsewhere, and use computers in somewhat the same manner in which experimental nuclear physicists use accelerators. As aids to instruction, computers also have a significant place in nuclear theory. It appears to this subcommittee that if it were intended to stifle nuclear theory, nothing would be more quickly effective than the isolation of our students from up-to-date computing facilities.

iii) THE ROLE OF NATIONAL LABORATORIES IN FILLING NUCLEAR THEORY COMPUTING NEEDS

While many national laboratories have very substantial

computing facilities, these are often not available for non-weapons related work. Two examples are Oak Ridge (there people doing basic research must go outside the lab for additonal computing) and Livermore (basic researchers are buying time from Los Alamos).

An exception to this rule is the Los Alamos National Laboratory. This situation has developed over the last two years because an open partition exists for unclassified computing. It is expected that LLNL will be in a similar position in about 2 years.

Thus two types of help are possibly available from national laboratories.

The first is of a short term nature. Individual contractors with DOE (possibly NSF) support may submit a proposal to buy time on computers at Los Alamos National Laboratory. These proposals will be considered on an indivudual basis and time would be sold with a non-interference understanding (permission to use the time could be withdrawn at any time, presumably because it was needed for national defense). The rates charged for time would, hopefully, be the internal ones, although this is not completely clear. This option exists at the present time.

The second possibility is for some laboratory to conclude an agreement with DOE and/or NSF to supply time. This would allow the establishment of an interim computing center with the advantages of central program libraries, code transportability and universal availability. If later it were decided to create our own computing center or join with another group such a change need not be noticed by the user.

The selection of a site for such an interim center should

consider such features as: availability of a class VI computer, existence of an interactive system, ability to supply graphics capability, connection to one or more nets (ARPANET, TYMNET, TELENET, etc.) and a central mass storage facility. These qualities are essential for a useful center for remote use. (One might be able to bypass the graphics but it was noted as very desirable by many respondents.)

No single laboratory could supply all of these features today but, taking into account planned development, all of the requirements will be available in late 1982 or 1983 when such an interim center might reasonably be started. Below are listed some possibilities with the present limitations.

Los Alamos - Has only 7600's in the open partition at the present. Will have 4-5 Crays in 1982. One of them may go in the open partition. Network connections in 1982.

Livermore - Has no open partition (1983?)

Sandia at Livermore - Has no mass storage system. Runs from tapes only.

National Center for Atmospheric Research (Boulder) - Batch oriented system. Tends to run long monolithic jobs.

This list is by no means exhaustive but represents the major national class VI facilities which may be interested in such a possibility. (Los Alamos has already expressed interest in such discussions).

It should be mentioned that certain state facilities may be candidates for both the interim center and a nuclear theory computing center. Two such possibilities (somewhat future) are at Colorado State University in Ft. Collins, Colorado and at University of Massachusetts in Amherst, Massachusetts. Both have plans for

a CDC cyber 205.

iv) PROGRAM DISTRIBUTION CENTER

Since the community of nuclear theorists is comparatively small, informal direct trading of computer programs is an effective mode of sharing the work of different groups. Nevertheless, it is surely true, as the 1979 report on Computer Needs for Nuclear Theory (chaired by W. MacDonald) observed, that "access by all nuclear physicists to a computer system with libraries of subroutines for the standard calculations of nuclear physics can reduce considerably the wasteful duplication of effort and the drudgery of this programming..." At present, no such generally accessible system exists in the U.S.

There are, however, some computer program libraries available to nuclear theorists, and it may be useful to give a brief description. Most prominent is the COMPUTER PHYSICS COMMUNICATIONS PROGRAM LIBRARY in the Queen's University of Belfast, Northern Ireland. This service has existed since 1969, is associated with the European physics Journal COMPUTER PHYSICS COMMUNICATIONS, and, as of a year ago, contained 510 programs in its file. Although it is generally believed that this library contains mostly programs in atomic and molecular physics, nuclear physics, with 157 programs, is the largest single subfield represented in the collection. Atomic physics, with about 140 programs, is second. Upon request and payment, the programs are sent to the customers as card images on magnetic tape. Most programs are in Fortran, but Algol, Basic, and PL/1 are also used. The demand from individuals ordering nuclear physics programs from the Belfast library can be gauged from the information that 938 requests for nuclear physics programs have been received;

200 of these came from the U.S.

Besides serving individual customers who order specific programs when they need them, the library has twenty-four subscribers, who regularly receive copies of all programs. Five of these subscribers are in the U.S.: ANL, Georgia Institute of Technology, Georgia State University, LASL, and the National Magnetic Fusion Energy Computer Center at Livermore. The current cost is approximately $300 per volume (two volumes per year). The programs are fully described in COMPUTER PHYSICS COMMUNICATIONS.

Users of the CPC Program Library appear to be well satisfied by the efficiency and reliability of this service. Orders are promptly executed, and the programs are generally in good condition and can be used with few difficulties. It is acknowledged that high editorial standards are rigorously maintained, and this accounts for the consumer satisfaction. At the same time, these conditions also explain some of the drawbacks associated with this library. The editorial process is so exacting, and the demand for full documentation of programs so strict, that a nonnegligible fraction of potential contributors appears to be deterred from submitting good programs.

Anyone designing a new central program library systems must be mindful of these experiences: The conflicting demands of thorough documentation, to render the product widely and readily usable and capable of modification, against the need to keep the effort of preparing the programs within acceptable bounds. This problem is not a chimera, for it is well known that carefully devised user programs, such as nuclear data compilations, can founder when they do not manage a proper balance between dependability and completeness on one hand and timeliness and rapid availability on the other.

Since the CPC Computer Program Library is a well established and generally successful venture, which performs a valuable service, it is surprising that the number of subscribing institutions is so small.

A second service of a similar nature is the National Energy Software Center at Argonne National Laboratory. This center, which is the successor of the Argonne Code Center established in 1960, principally serves the DOE, the NRC, and its contractors, but is open to other subscribing organizations as well. The bulk of the approximately 800 programs, which are maintained in this library, is in the area of nuclear technology. Some thirty programs can be classified as pertaining to nuclear theory. The Center at ANL communicates with other data banks and software centers, both in the U.S. and abroad, but in most of these interactions the emphasis is on the energy mission of the sponsoring agencies.

Given this background of existing library services, and in view of the experience nuclear physicists have had with them, what unmet needs are there that a new program distribution center (or an old, reorganized one) should address? The answer to this question depends strongly on the value which the community of nuclear theorists places on the kind of service which such a library would be able to provide. Several different scenarios can be imagined.

At one extreme, a central national computer facility could be primarily a repository of programs directly accessible to the users, who are connected with the center by a network. The center would function much as a library of books, although to be useful it would have to be vigilant in providing critical control of the "accessions" to the library. While the library would maintain the software, the physics initiative and the construction of

programs would be entirely the responsibility of the users.

In other models, the center would accept increasing responsibility for the computational aspects of the programs, for the numerical analysis, and perhaps even for the physics of the problems under study. An example is the Computational Science Division of the Daresbury Laboratory, in which a staff of scientists provides support to a number of collaborative university projects. This example also illustrates the importance of authoritative scientific leadership of such a center, it it is to be effective as other than a passive depository of externally generated programs.

Past experience and future projections suggest that it would be sensible to develop the library function of any new center in gradual stages. Instead of designing a system that might on paper seem ideal for the nuclear theory community, it would be better to make a modest and modular start, letting the demand determine the eventual direction and magnitude of growth of this enterprise.

v) NEW COMPUTER LANGUAGES IN NUCLEAR THEORY

A. For Numerical Computation

At present, most numerical calculations in nuclear theory are programmed in UNSTRUCTURED FORTRAN. It is likely that the next five years will see such calculations move first to STRUCTURED FORTRAN and then to NATURAL SCIENTIFIC FORTRAN. The move to Structured Fortran will be hard on veteran programmers but will produce shorter development time and greater reliability, portability, and modifyability. Structured Fortran is a first modest step toward the structure of Scientific English, and will likely pave the way for the next, larger, step to Natural Scientific Fortran. That language will accept commands that look exactly

like the instructions one would write on a scratch pad for a graduate student to do the calculation. This capability will greatly improve ease of entry and debugging, not to mention portability, etc. In addition, the "program" will often be incorporated into the text of the subsequent paper submitted for publication, since it will already look just like the formal section of the paper.

As pocket computers replace programmable calculators in the next few years, those physicists who use them will switch to BASIC. As this happens, BASIC will likely evolve into a structured language more appropriate to scientific calculations. The current hybrid language BASCAL is a first step in the direction.

Other recently developed languages such as PASCAL, ADA, C, and FORTH, will likely have little impact on nuclear physics calculations during the next five years.

B. For Formal Manipulations

Nuclear theorists will start making greatly increased use of programs that will aid them in making formal mathematical manipulations. The first major use will be in evaluating Feynman Diagrams, both formally and numerically. Currently, this means learning the command language of SCHOONSCHIP, ASHMEDAI, REDUCE, SMP, or MACSYMA. Such programs will become widely available and will be used as theorists learn the "language". In addition, there is some evidence that the type of program represented by Reduce, Macsyma, and MuMath will begin to replace the present human manipulations involved in complex formal integrations and differentiations. It is quite likely that something like MuMath may be incorporated into pocket calculators.

C. Scientific Text Processing

It is likely that nuclear theorists will gradually move toward the use of scientific text processors during the next five years, in some cases typing entire manuscripts themselves, in other cases just doing the editing after initial entry by a typist. This will save money, time, and personnel problems for those physicists who wish to use editing to improve their papers' powers of communication. For this they will use a formatting language, one that has evolved from the present TROFF, TEK, etc. Already, papers formatted with TROFF commands can be transmitted to the AIP for direct entry into their electronic typesetter.

D. Electronic Conferencing, Messaging, and Information Retrieval

As travel becomes more expensive and research budgets come under further strain, it is likely that electronic conferencing and information retrieval will take over some of the functions of present conferences. For this, physicists will have to learn the command languages of those electronic systems. Such systems will be lineal descendents of CONFER, EIES, RIM, DIALOG, SPIRES, etc.

vi) NEW TECHNOLOGIES

The continued rapid development of computer power through the end of this century seems assured. Much of this power is achieved by the ever increasing size of chips ranging from LSI to VSI to ULSI (ultra-large scale integration) arising from the associated technologies in silicon, GaAs and cryogenic Josephson junctions. At the other end of the scale "personal" computers are rapidly becoming pocket size computers with considerable power. Due to the general interest of the public at large in

personal computers the much needed software to use them will be developed rapidly.

New architectures may play an important role in computers to be developed over the next decade. Such new architectures are aimed at improving raw speed either by developing a high degree of parallel processing or by designing a specialized architecture which embodies some features of the "physics of the problem". Coupled microprocessors are envisaged as a possible scheme for several physics problems (e.g. Hydrodynamics) but such a technology will not be easily used in the next decade except by the hard bitten computer experts.

In the near future (1982-83), video disks are expected to become available and promise to revolutionize mass storage systems. Estimates are that initially, a read-write unit will cost ~$150K, a read unit, ~$50K; and the disk itself ~$1K. A few years after their introduction, the costs are expected to drop to ~$50K, $6K, and $100, respectively. Video disks are about the size of an ordinary phonograph album and will initially have capacities of 10^{11} bits per disk increasing to 10^{12} bits per disk after they have been on the market for a few years. Video disks will also facilitate wide distribution of selected data bases, since multiple copies can be made in much the same way as phonograph records are reproduced.

V. COST CONSIDERATIONS

There are over 600 Nuclear Theory Computers Users. Each costs the U.S. about $75,000/year, totalling about $45 million/year and increasing every year. The cost of a good computing environment for these users is roughly equal to a 10% increase in their productivity. Increasing productivity means:

1) Eliminating the frustrations listed in question 7 of the questionnaire (Appendix B).
2) Eliminating unnecessary duplication of effort.
3) Avoiding software conversion.
4) Increasing throughput.
5) Providing bigger/faster computers to the "underprivileged" as well as the privileged.

In considering the various options for nuclear theory computations it became clear that a pluralistic approach is needed to meet the manifold modes of computing required by various members of the community.

Cost estimates of midi-computers turns out to be very sensitive to the environment in which they might be placed. University groups, particularly those with underutilized permanent staff members for hardware and/or software support. believe that a typical midi-computer complex can be satisfactorily maintained for an annual cost as low as 10% of the purchase price.

Such a cost effective environment is not always available and annual operating budgets as high as 40% of the purchase price have been estimated. In most University environments midi-computers require no operators, floor space and power may be available at no extra cost, University discounts and matching funds can reduce capitalization costs and collaboration with other campus machine

groups may produce sizable additional discounts.

Cost estimates of larger machines are also somewhat uncertain, e.g., a CDC 7600 has an estimated capitalization cost of $3-4 Million and a stand alone operating cost/year of about $1.5 Million; a CRAY (~4 X 7600) has an estimated capitalization cost of $6-11 Million and a stand alone operating cost/year of about $2.0 Million. Detailed estimates of various costs associated with setting up a network involving a principal node, and/or regional computers with network nodes are given in Tables A and B below. The manpower typically associated with a central facility and a regional facility are listed in Table C. As noted above the costs of the smaller components such as a network node are very variable - the values given in Tables A and B are regarded as maximum values. It should also be emphasized that large central computers such as CRAY and CYBER-200's come in various "sizes". Two such sizes are listed in item 5 of Table A.

It is difficult and often misleading to compare the "performance ratio" of small machines to the large vector machines. Such a ratio is very job dependent and if scaled relative to cost becomes very environment dependent. In general one can find extremes wherein a small computer will be highly advantageous and opposite extremes wherein a large computer is absolutely required to complete the computations in a reasonable time. Between the two extremes the performance ratio relative to cost ratio appears to be similar for the small and large machines.

The addition of array processors to midi-computers can be important in improving the overall performance of the smaller machines. Array processors cost from $50K - 250K and while they are highly "specific", there are applications in which such an addition

will provide a tenfold increase in power at no more than double the cost. It should be emphasized that at present array processors are not trivial to use productively. This software barrier is being lowered and no doubt such array processors will, in the next few years, become equally easy to use as their host facilities are today.

Table A

Capital Costs or Lease

1. Terminal concentrator for dial-up	$40 K
2. Network I/O stations	
DEC 11/44 with printer, disk, 30-40 terminal ports	$150 K
3. Network Node	
VAX, 1.5 mbyte memory, RP06, printer, 8 ports	$300 K
4. Regional Computer,	
0.5 million word mem, 2400 mbyte disks	$3-4 million
5. Cnetral Computer (CRAY)	
0.5 million word mem, 3600 mbyte disks	$6 million
2.0 million word mem, 9600 mbyte disks	$10.5 million
6. Lease 16 TYMNET ports	
$450/port + $2300 for TYMCOM	$10 K/month
7. Lease 4800 baud telephone line + modems	
short (20 - 50 miles)	$300/month
long (500 + miles)	$1000/month
8. Lease 50 kbit/sec DDS for 1000 miles	$8000/month
9. Central Mass Store	$1 million
10. Local Network for Central Facility	$500 K

Table B

Operating Expenses

	$ K/year
1. A VAX Network Node	
Part-time staff, Maint., Supplies	$125
Network connection	25
	$150
2. A Regional Computer Facility	
Maint. of Computer	$350
Network connection to other facilities	200
Supplies and Services	400
Manpower (25 FTE)	1500
Building Lease	100
	$2550
3. A Central Computer Facility	
Maint. of Computer	$350
Maint. of File Storage System	200
Maint. of Local Network	50
Total Network Lease costs	600
Supplies and Services	600
Manpower (50 + FTE)	3000
Building Lease	100
	$4900

Table C

Manpower

Regional Facility

Director

Software Supervisor

Hardware Supervisor

Operations Supervisor

Program Manager

2 Secretaries

10 Operators (2 per shift, 24 hrs/day, 365 days/year)
(accounting, output mailing, billing, etc.)

4 Engineers or engineering techs.

4 Systems Analysts

25

Central Facility

Same as above plus

6 Consultants (1 for every 100 users)

3 Network software programmers

3 File Storage software programmers

3 Utility software programmers (debuggers, compilers, etc.)

5 Documentation Editors

5 Special Applications (Graphics, DBMS, CAD/CAM, etc.)

50

Appendix A

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Appendix B

Report on the Results of a Questionnaire on Nuclear Theory Computing

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July 15, 1981

Introduction

This report presents the results obtained from a questionnaire (Appendix C) mailed to three hundred principal investigators in nuclear science. The names of these investigators were provided and categorized as theory and experiment by the program officers of the National Science Foundation and the Department of Energy. One hundred and twenty responses were obtained with three of these containing unanswered forms as the respondents felt their participation was unappropriate. Most of the questionnaires returned represented the answers or feelings of a group. The response at about the 40% level is perhaps misleading because at several institutions one of the investigators answered for all the principal investigators at their institution.

We feel the present study reached and was responded to by a major fraction of nuclear theorists and experimentalists with a significant interest in nuclear theory computing (defined here as computational calculations by nuclear theorists and theoretical analysis of data with models or reaction codes by nuclear experimentalists). The total number represented by the survey response amounts to over six hundred computer users. Nuclear theorists from thirty-five universities and eight national laboratories responded. Nuclear experimentalists from thirty-two universities and six national laboratories responded. Overall this study reached over three times as many respondents as the 1979 survey in this area by Koshel and MacDonald.

The results are presented here in the order as they appeared in the questionnaire. The results in question 2 were obtained by using

a simple conversion procedure based on the table of computer equivalents to a CDC 7600 given in Appendix D. While such a conversion is probably not very reliable for a given individual case the average error is presumably much less. Since only totals are used here we feel the procedure used is adequate.

The present report is to be used as a source of information for the NSAC subcommittee on Computing Capabilities for Nuclear Theory. This report presents the tabulated results and does not attempt to interpret them since the full subcommittee will be involved in the interpretation of such data.

Results

1] Give estimates of the following:

i) Annual budget for computing operations

$ NSF, $ DOE, $ Other (specify)

ii) Annual usage (in hours): CPU time , Elapsed time (if available)

iii) Projected annual usage five years hence (in hours): CPU time

The results for each section of this question are presented in Tables 2 and 3. The only unusual response occurred for section iii) under experiment where a large projection of 2000 hrs was listed by a single respondent. Elapsed times were not given by enough respondents to make a useful statement.

Table 2

Annual Budget in Thousands of $

	NSF	DOE	OTHER*	TOTAL
Theory	57K $	480K $	654K $	1191K $
Expt	88K $	209K $	261K $	558K $
Total	145K $	689K $	915K $	1749K $

*other sources were primarily "invisible" money in the case of universities.

Table 3

Current and Projected Usage (CPU hrs.)*

	Current usage	Projected usage
Theory	2449	4857
Expt	1375	3814
Total	3824	8671

*units of CDC 7600.

2] What kind of computer (e.g. CYBER 74) are your estimates based on?

This information was useful not only to provide the list of computers given below in Table 4 but also to convert CPU hours to CDC 7600 CPU hrs. to obtain the results given above in Table 3. Except for the Vax usage most usage is on main frame computers.

Table 4

Machine	No. of respondents with access (3 only)
CDC 7600	20
VAX 11/780	18
IBM 370/158 or 165	18
IBM 3033	7
CRAY 1	5
IBM 370/168	5
IBM 360/65	5
AMDAHL 470	4
CYBER	4
IBM 3032	3
CYBER 170/750	3
DEC 1041	3
IBM 360/44	3
PDP 11/34	3
CYBER 71	3

3] Where is your computer located? Give multiple answers if more than one.

Laboratory☐ , Department☐ , Campus ☐ , Remote☐ ,

specify place_____ miles distant_____

The results for the locations in terms of number of responses are given in Table 5 below. The distance away for remote locations covered the range $^{1}/_{4}$ → 4,000 miles with 9 respondents being over 500 miles.

Table 5

Computer Location

	Theory	Expt	Total
Laboratory	23	25	48
Department	4	6	10
Campus	44	22	66
Remote	20	8	28

4] How many computer theory users are in your group?

This question caused some confusion for experimentalists answering the questionnaire - possibly some did not carefully note the definition of nuclear theory computing at the beginning of the questionnaire. However, enough experimental respondents did appear to understand the question so that the numbers have some validity. The number of users is broken down into theory and experiment at Universities and National Laboratories in Table 6.

Table 6

Computer Theory Users*

	Universities	National Laboratories	Total
Estimates from Theory respondents	260	130	390
Estimates from Expt respondents	181	46	227
TOTALS	441	176	617

*includes experimentalists involved in analysis of data using nuclear models or reaction codes

5] (a) What is your ratio of usage for batch versus interactive?

(b) Describe briefly your computing environment.

The answers to part a) are essentially identical for theoretical and experimental respondents namely 60% batch and 40% interactive. Almost all respondents had some interactive capability and more than a half of them had access to more than one machine.

6] What kinds of calculations do you perform? (e.g. TDHF, nuclear structure, coupled channels, few body problems, nuclear matter, nuclear astrophysics, nuclear reactions - data interpretations, etc.)

Since some respondents are doing several kinds of calculations the tabulation given below in Table 7 simply is in terms of the number of people listing a given subfield. Subfields not given in Table 7 (e.g. fission) had responses of $\lesssim 3$. The computer usage associated with each area could not be reliably extracted in this questionnaire.

Table 7

Number of responses by subfield

Subfield	Theory	Expt	Total
Nuclear Reactions-data interpretation	11	30	41
Coupled channels	23	16	39
Nuclear reactions-mechanisms	24	13	37
Nuclear Structure	25	11	36
Few-Body	17	4	21
Nuclear Matter	11	1	12
Nuclear Astrophysics	5	3	8
TDHF (Time dependent Hartree Fock)	6	1	7
Nuclear Hydrodynamics	6	1	7

7] What are your group's major frustrations arising from current facilities? Check one or more.

i) Lack of Compatibility with other systems

ii) Lack of throughput

iii) Lack of documentation

iv) Too many system changes

v) Inadequate accessibility

vi) Insufficient graphics

vii) Insufficient storage capacity: high speed core ☐, disc on line ☐ , disc off line ☐ .

viii) Other (specify)

Table 8 shows the number of responses to each of the above items. On the average each respondent checked two frustrations. Clearly the various frustrations occur with about equal weight so that no particular problem stands out as special.

Table 8

Responses to itemized list of major frustrations

i)	Lack of compatibility	21
ii)	Lack of throughput	27
iii)	Lack of documentation	16
iv)	Too many system changes	24
v)	Inadequate accessibility	23
vi)	Insufficient graphics	27
vii)	Insufficient storage capacity	30
viii)	Other	29

8] What new types of nuclear theory computing facilities would be most beneficial to you? Give brief reason(s) for choice.

i) A single large class 6 central facility (e.g. CRAY I) with remote access from anywhere in the U. S.

ii) A few midi-computers (e.g. Vax 11/780, SEL 32/77) with remote access capabilities located at sites with large groups and an appropriately reduced version of (i).

iii) Many midi- and mini-sized computers distributed amongst many groups but with remote access capabilities at appropriate places.

iv) Other (specify)

There was no overwhelming desire for any of the options listed as i), ii) and iii). The comments of respondents who chose iv) were also very divisive. Many of the respondents choosing option (i) are from small institutions and based their choice on their belief that they would not have a big enough group to have their own

machine. Some of the respondents indicated under question 11 (additional information and comments) that access to a large class 6 machine was occasionally necessary. The numbers of respondents checking the various options are tabulated in Table 9. A few respondents to the questionnaire did not answer this question.

Table 9

Preference for new facility options

Option	#
(i)	36
(ii)	22
(iii)	27
(iv)	19

9] How important is the documentation and availability of other group's programs to your work?

Very important ☐ Often important ☐ Occasionally important ☐

The number of responses by category are given by Table 10.

Table 10

Documentation and Availability of Programs

Category	number checked
Very important	20
Often important	30
Occasionally important	53

10] Should a "translation" center and network connections for distribution of programs be set up?

Yes No Other (specify)

Here the response shows a significant yes vote of 67 compared to a 24 no vote and 7 other. It is hard however to reconcile the responses to questions 9 and 10.

11] Additional information and comments.

We list twenty of the comments which appeared to be of most interest.

a) "A single central facility is best for us because we have little chance of supporting a mini or midi with technical help."

b) "Remote access for options ii) and iii) might be rather low priority."

c) "Option (i) would allow us to benefit from specialized and sophisticated languages such as MACSYMA."

d) "The rapid advance of computing capabilities at low facility investment make option (iii) an attractive alternative."

e) "I think the bureaucracy of such a monstrosity (option i) would render it little accessible except to a small subset of the theorists who would need access. A user needs to go to the facility occasionally."

f) "I do not have major problems with computing at present. However it would be useful for me occasionally to have access to a very large machine."

g) "The Vax is so powerful that even really big jobs can be run (overnight or in stages) if (as rarely happens) it becomes necessary for a particular problem."

h) "My situation is adequate but it would be useful to be tied in to computers at other laboratories.

i) "Option (i) appears to be the best compromise for nuclear theorists (like myself) isolated in smaller universities."

j) "At least for the moment we are fairly satisfied with the computer available in the campus."

k) "Option (ii) serving large groups (or regional groups) will cut down on network costs and connecting problems. Large capacity jobs will still need access to a large class 6 facility."

l) "I prefer to use midi-computers that I have direct access to; but it is useful to have a powerful machine available for occasional use."

m) "The VAX or SEL is totally uninteresting, however, sharing a 205 with others is interesting."

n) "We have been able to perform useful calculations locally only by virtue of having "unlimited" computing time on the campus computer. However, our system is overcommitted to administrative and teaching functions compared to research; it is effectively too slow to allow for the most sophisticated and massive (e.g. Monte Carlo) calculations."

o) "Option (ii) - ease of access + the big number crunching abilities as necessary. You can do an awful lot of cost effective computing on a 780, particularly with an array processor."

p) "Option (i) - need large computations with collaborators in different cities."

q) "The major problem for nuclear theory is the trend of university computing centers toward zero batch, which = zero production of nuclear theory #'s."

r) "A good software library similar to that offered by Computer Physics Communications and a mini-computer system with remote access to the documentation and source programs is more important than a giant number cruncher."

s) "Option (iii) - I think this will be the best choice for the long term future, because of the advent of high density chips. There will, however, still be a need for a few supercomputers available to all users."

t) "Option (i) - better maintenance of documentation".

The above comments offer a range of views which is consistent with the answers to question 8.

Appendix C

Questionnaire and information mailed to Principal Investigators in nuclear science.

Department of Physics
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May 4, 1981

Dear Dr.

Please find enclosed a short list of questions concerning nuclear theory computing (defined here as computational calculations by nuclear theorists and theoretical analysis of data with models or reaction codes by nuclear experimentalists). The information obtained from your answers will be very useful to the NSAC subcommittee on Computing Capabilities for Nuclear Theory.

For your information the charge to this subcommittee is also enclosed. It is vital to this subcommittee to have direct input from the community, otherwise our final recommendations (which we are asked to provide to NSAC by September 1981) will not be properly representative. I know questionnaires represent a short term nuisance, but we believe this one is sufficiently important to the community that it is worth answering.

Sincerely,

D Robson

D. Robson

DR:lc

Charge to the DOE/NSF Nuclear Science Advisory Committee Subcommittee on Computational Capabilities for Nuclear Theory

Forefront theoretical nuclear research requires the existence and efficient operation of advanced computational facilities. In the Nuclear Science Advisory Committee Long Range Plan, the nuclear theory working group pointed out "nuclear theory in the U.S. is hampered considerably by the lack of good computing capability required by modern theory" and recommended "funding to provide computing capability which would remedy this situation."

The Subcommittee will determine the computational needs of forefront theoretical nuclear research in the United States and examine the ability of existing facilities to meet those needs. If deficiencies are found, then the Subcommittee will identify and evaluate options to remedy the deficiencies. The options considered shall include upgrade and/or modification of existing computational facilities. In the course of its work, the Subcommittee will specifically:

I. Examine present and future trends for the usage of computers both for nuclear theory calculations and for comparisions of data with theory by nuclear scientists.

II. Evaluate several approaches to computer configurations ranging from a single central facility to many distributed facilities. Combinations of a central facility and several distributed facilities should be considered.

III. Consider various possible levels of computing capability and recommend the most appropriate configuration and cost for each level of capability considered.

IV. Recommend the optimum choice for the next decade keeping in mind the Long Range Plan for Nuclear Science. This optimum choice should include not only new facilities but also a discussion of the optimum role which could be played by current facilities.

Questionnaire for Nuclear Theory Computing

If you use more than one computer, please indicate relative usage under question 2. Use section 11 for clarification purposes. Please return by May 15, 1981 in the enclosed envelope.

1. Give estimates of the following:

   i) Annual budget for computing operations

   $ NSF, $ DOE, $ Other (specify)

   ii) Annual usage (in hours): CPU time __ __ __ , Elapsed time __ __ __

   (if available)

   iii) Projected annual usage five years hence (in hours): CPU time __ __ __

2. What kind of computer (e.g. CYBER 74) are your estimates based on?

3. Where is your computer located? Give multiple answers if more than one.

   Laboratory ☐ , Department ☐ , Campus ☐ ,

   Remote ☐ : specify place _____ miles distant _____

4. How many computer theory users are in your group?

5. (a) What is your ratio of usage for batch versus interactive?

   (b) Describe briefly your available computing environment.

6. What kinds of calculations do you perform? (e.g. TDHF, nuclear structure, coupled channels, few body problems, nuclear matter, nuclear astrophysics, nuclear reactions-data interpretation, etc.)

7. What are your group's major frustrations arising from your current facilities?

   Check one or more:

   i) Lack of compatibility with other systems

   ii) Lack of throughput

   iii) Lack of documentation

iv) Too many system changes

v) Inadequate accessibility

vi) Insufficient graphics

vii) Insufficient storage capacity: high speed core ☐ , disc on line ☐ , disc off line ☐

viii) Other (specify)

8. What new types of nuclear theory computing facilities would be most beneficial to you? Give brief reason(s) for choice.

i) A single large class 6 central facility (e.g. CRAY I) with remote access from anywhere in the U.S.

ii) A few midi-computers (e.g. VAX 11/780, SEL 32/77) with remote access capabilities located at sites with large groups and an appropriately reduced version* of (i).

iii) Many midi- and mini-sized computers distributed amongst many groups, but with remote access capabilities at appropriate places.

iv) Other (specify)

9. How important is the documentation and availability of other group's programs to your work?

Very important ☐ Often important ☐ Occasionally important ☐

10. Should a "translation" center and network connections for distribution of programs be set up?

Yes ☐ No ☐ Other (specify)

11. Additional information and comments:

*A possible opportunity will occur at Colorado State University in December 1981. They have less than 1/3 of a CYBER 205 subscribed at the present time so some fraction of such a facility with a central software repository could by considered.

APPENDIX D

COMPUTER EQUIVALENCE TABLE *

Manufacturer	Model	Relative Capacity	Nominal Capacity (NSU's)
CRI	CRAY-1	4.0	40,000
CDC	STAR-100	1.8	18,000
CDC	7600	1.0	10,000
IBM	3033	.95	9,500
IBM	360/370/195	.95	9,500
UNI	1100/82	.88	8,800
UNI	1100/44	.88	8,800
CDC	CYBER 175	.70	7,000
IBM	360/168-3	.58	5,800
IBM	370/168-1	.53	5,300
IBM	360/91	.51	5,100
IBM	370/165-II	.50	5,000
UNI	1108	.29 1/	2,900
IBM	3031	.24	2,400
CDC	6600	.22	2,200
CDC	CYBER 174	.22	2,200
IBM	370/158	.20	2,000
IBM	360/75	.20	2,000
CDC	CYBER 74	.18	1,800
IBM	IBM 360/65	.16	1,600
DEC	PDP KL10	.14	1,400
CDC	CYBER 73	.12	1,200
DEC	VAX 11/780	.12	1,200
CDC	6400	.11	1,100
HIS	66/40	.11	1,100

Manufacturer	Model	Relative Capacity	Nominal Capacity (NSU's)
IBM	360/44	.07	700
DEC	PDP KI10	.06	600
DEC	PDP KA10	.04	400
IBM	360/50	.036	360
DEC	11/70	.036	360
DEC	11/45	.033	330

1/ Specifically UNI 1108 complex at SLA.

*SOURCE: Department of Energy FY1981-1985 ADP Long Range Plan