Coupled-cluster approach to the *ab initio* nuclear quantum many-body problem

9.A. Research Objectives

Our proposed INCITE research has three goals:

- Our main goal is to develop an understanding of the role of three-body nuclear interactions in nuclei into the iron region using nuclear Coupled Cluster algorithms.
- We will also utilize computational resources to understand the deformation and thermal properties of nuclei in the mass 90-120 region using quantum Monte Carlo algorithms.
- We will also develop a microscopic description of bulk properties of nuclei throughout the nuclear chart using a nuclear density functional approach.

In each case, significant computational resources are required to make progress within the next three years, and particularly in FY06. We will describe in the following subsections the scientific objectives of the three research areas.

9.A.1. Nuclear Coupled Cluster Theory (85% of total project)

During the last three years we have developed a set of powerful theoretical tools [1,2,3] for the description of nuclear properties in a many-body framework known as coupled-cluster theory [4,5]. The need for this work is evident from the fact that other ab initio techniques, such as the Green's Function Monte Carlo methods [6] and the no-core shell model techniques [7] have reached or will soon reach their limits of applicability due to the exponential growth in computational need of these techniques when one increases particle number. We are developing new ab initio methods that will overcome this difficulty and allow for a treatment of medium mass nuclei (with up to 100 nucleons).

One of the most promising *ab initio* microscopic theories that can potentially provide a highly accurate description of a variety of many-body physical systems, as small as atomic nuclei and as large as polyatomic molecules, as weakly bound as van der Waals molecules and as strongly bound as atomic nuclei, is coupled-cluster theory. We believe that coupled-cluster theory offers a significant path forward for studying nuclear properties on an ab inito footing far from stability and in mass regions relevant to the RIA experimental programs. While coupled-cluster theory was originally introduced in nuclear physics, it's applications to nuclei have been sporadic [8,9]. We perform this work in collaboration with M. Hjorth-Jensen (Oslo) and P. Piecuch (Michigan State University).

While we have written codes specifically tailored for the nuclear many-body problem, we have utilized the significant developments of coupled-cluster theory that have occurred in quantum chemistry [10, 11, 12, 13, 14,15,16]. With application of these techniques to the nuclear problem, we are now in a position to calculate ground, excited, closed-shell, and open-shell, non-degenerate and quasi-degenerate states of nuclei and certain nuclear properties. We begin in coupled-cluster theory with a reference Slater determinant $|\Phi\rangle$ on which we operate with the exponential of a cluster operator, T which is a hole-particle cluster operator with 1-body, 2-body, and up to A-body components. The similarity-transformed Hamiltonian $\overline{H} = \exp(-T)H\exp(T)$ forms the basic ingredient of the coupled-cluster method. With it, one may calculate the expectation of the energy in the reference state $E = \langle\Phi|\overline{H}|\Phi\rangle$ and the amplitudes of the cluster operators may be found through solving the coupled non-linear algebraic equations $0 = \langle\Phi_{ab\ldots}^{ij\ldots}|\overline{H}|\Phi\rangle$, where $\Phi_{ab\ldots}^{ij\ldots}$ is an n-particle-n-hole Slater determinant built upon the reference state. Here (i,j) are orbital labels below the Fermi surface and (a,b) those above the Fermi surface. If we truncate the T operator at the T_1 and T_2 level (up to two-particle-two-hole correlation amplitudes) then we have coupled-cluster theory in singles and doubles (CCSD), while truncation at the T_3 level yields CCSDT (T=triples), etc. Furthermore, if we diagonalize $\overline{H}$ in the space of 1p-1h and 2p-2h excitations we arrive at equation-of-motion CCSD (EOMCCSD) which enables investigations of excited state information for those states that are principally 1p-1h in character. The CCSD methods scale computationally

as $n_o^2 n_u^4$ where n_0 is the number of single-particle orbitals below the Fermi surface, and n_u is the number of orbitals above the Fermi surface. Thus, both CCSD and EOMCCSD have N^6 scaling with system size.

Full CCSDT calculations [17] are much more expensive methods and scale as N^8 with system size. An accurate method based on moments of the similarity-transformed Hamiltonian has recently been developed. This non-iterative completely renormalized (CR) method allows for corrections to CCSD energies at the triples level and scales as N^7. We have employed these methods, known as CR-CCSD(T) for the ground state and CR-EOMCCSD(T) for excited states [18,19] for both test calculations in ^{4}He and ^{16}O and converged calculations of ^{16}O.

In the ^{4}He test case, we compared to exact Hamiltonian diagonalization calculations in a small space of four oscillator shells. We found that the CR-CCSD(T) and CR-EOMCCSD(T) methods obtain ground- and excited- energies within 0.05 MeV of the exact solution in a small model space. From this study we also saw that, when two-body interactions are employed, triples corrections to the ground-state energy are very small (amounting to less than 1% of the total binding energy in ^{16}O). We also found that nucleon-nucleon interactions alone are unable to obtain either the ground-state binding energy or the excited state structure of the lowest 1p-1h states in ^{16}O. The calculations in [1, 2, 3] pushed technology in an incredible way: we can now perform both ground and excited state coupled-cluster calculations (using CCSD and CR-CCSD(T) methods) in ^{16}O with up to 8 complete oscillator shells. These calculations are converged in model-space and oscillator energy, with a small parameter dependence on the G-matrix starting energy. Our excited state calculations are also converged. We also are able to compute one- and two-body density matrices in order to obtain nuclear properties such as the nuclear charge radius and electron-scattering form factor. Our INCITE computational work will move along the following lines.

Three nucleon forces: The role and importance of the three-nucleon force (TNF) for light nuclei with mass A<=12 is well established by now. We recall that TNFs typically account for additional binding energy (in conjunction with bare two-nucleon potentials), and also change the level ordering. However, the form of the TNFs is less well understood. Current formulations of TNFs are motivated by ideas from effective field theory and from two-pion exchange, and coupling constants are typically determined by fitting spectroscopic data of light nuclei. For a better determination of the TNF it is thus important to test TNFs in heavier systems within ab-initio structure calculations. Coupled cluster theory is a promising method for this endeavour as its computational cost scales much more gently with increasing system size than GFMC or NCSM.

In a first step, we will treat Hamiltonians with TNFs at the CCSD level, with approximate corrections for three-body clusters. We derived and implemented the coupled cluster equations including a TNF [20]. This is truly new ground, and our results might also prove useful for quantum chemists and condensed matter theorists as effective three-body forces are also generated within molecules and solids when model space truncations are taken into account. For the derivation of the CCSD equations we extended diagram factorization techniques from quantum chemistry. These techniques yield a very compact form of the resulting equations. The second step consists of the efficient numerical implementation of the CCSD equations. This implementation is directly based on the factorized form of the CCSD equations for computations on parallel architectures. In the third step, we will perform structure calculations based on TNFs. Our calculations will be based on different two- and three-nucleon forces and target different nuclei. As examples we mention V_{lowk} with its TNF obtained from fit to triton and the alpha particle, G-matrix based two-body forces from bare potentials augmented by the Urbana and/or Tucson-Melbourne TNFs, and effective Hamiltonians that originate from similarity transformed bare interactions. Nuclei of interest will be Oxygen-16, mid-shell nuclei like Silicon-28, and possibly heavier nuclei like Calcium-40. We will also study the corresponding neighbor nuclei which differ by one in their mass.

The results will indicate (i) what part of the structure in heavier systems is affected by the TNF, and (ii) enable a better determinion of the TNF itself through possible deviations between theory and experiment. Another important question concerns computational reductions of the TNF. Studies within the

NCSM show that those three-body matrix elements which can be written as density dependent two-body matrix elements are the most important ones. Insight in this matter will enable us to extend calculations with TNF to larger model spaces, and might also help us to understand effective two-body interactions in traditional shell-model problems with a core.

9.A.2. Auxiliary Field Monte Carlo (10% of total project)

Calculations of the structure and excitation spectra of nuclei have also been carried out using Hamiltonian diagonalization techniques (also configuration-interaction calculations in chemistry). The diagonalization occurs in a model space spanned by many-body basis states. These states are usually constructed near the Fermi surface of a given nucleus. For example, for ^{54}Fe, one assumes a frozen core of ^{40}Ca and works in the basis states of the 'fp' shell, which consists of the 20 single-particle neutron and proton orbitals above ^{40}Ca. Application of this approximation has been extremely successful for understanding properties in medium-mass nuclei. As with any Hamiltonian diagonalization problem, it suffers from applicability when the model-space becomes too large. Present limitations are of the order of 2 billion basis states. For a review, see [21].

Medium-mass nuclei in the A=80-120 region are beginning to be explored using realistic shell-model interactions projected into a given set of single-particle basis states that lie near the fermi surface. We turn to the very successful Shell Model Monte Carlo (SMMC) method [22] which recasts the interacting shell model problem into a multi-dimensional integration problem. Importantly, the SMMC method also enables studies of thermal nuclear properties important in various contexts. These methods are based on a Monte Carlo evaluation of the path integral obtained by a Hubbard-Stratonovich transformation of the imaginary-time evolution operator. The many-body problem is thus reduced to a set of one-body problems in fluctuating auxiliary fields [23]. The SMMC method has recently been used in conjunction with electron-capture calculations during core collapse [24]. We are also investigating the ground-state structural properties of nuclei in the mass 80 region within the fp-gds model space [25], and their thermal properties [26]. By FY06 we will have completed a study of the rotational properties of N=40 nuclei as well.

With the exception of rare earth studies (see, e.g., [27]), SMMC calculations were traditionally performed in shell model spaces for which the neutrons and protons occupied the same single-particle orbitals and for which the interaction maintained good isospin. We have relaxed these restrictions in the recent thesis work of Cem Ozen. Dr. Ozen has developed a working pn-SMMC code and is now calculating nuclear properties in the Zr and Mo isotopes above the ^{88}Sr core. We are using realistic interactions [28] developed for this model space. The pn-SMMC results agree with standard diagonalization results the region [29] for nuclei that have only a few valence nucleons.

By performing this effort, we will be able to investigate nuclear structure using the SMMC technique for a wider class of problems than we have studied before. Specifically, we will be able to study neutron rich nuclei more efficiently by restricting the proton space appropriately. We shall be able to use realistic interactions generated in the proton-neutron formalism rather than in the isospin formalism, and we will be able to investigate for the first time thermal properties of nuclei far from stability. Since nuclei that electron capture during the later stages of supernova collapse are quite neutron rich, we should for the first time be able to study weak processes in these nuclei using the SMMC methods.

Another avenue of our ongoing research efforts involves circumvention of the quantum Monte Carlo sign problem. All realistic shell-model two-body interactions have an associated Monte Carlo sign problem in the SMMC method. This problem was initially overcome by extrapolation techniques [30]. We are investigating other ways of overcoming or at least delaying to low temperatures the sign problem. One promising method involves shifting the contour of integration [31] to pass through the (imaginary) stationary point. This stationary point is taken to be the Hartree-Fock minimum for the given nucleus. Our preliminary results indicate that we can reach meaningful results to about T=0.5 MeV in fp-shell nuclei without extrapolation. In contrast, the standard SMMC approach breaks down completely at a very high

temperature of T=3.0 MeV in fp-shell calculations. Once we fully test the SC-SMMC method we will apply it to iron group and gds nuclei. This enabling technology will allow us to calculate, for the first time, various nuclear properties without resorting to extrapolation techniques.

9.A.3 Nuclear HFB Calculations (5% of total project)

The study of nuclei far from stability is an increasingly important part of nuclear physics. The new experimental developments inevitably require safe reliable theoretical prediction of nuclear properties throughout the whole nuclear chart - from the proton drip-line through the beta stability line and the r-processes path, to the neutron drip line and to the uncharted territory of super-heavy elements.

One solution of the problem is a no-core shell-model mass table fit based on a G-matrix or some finite-range effective interaction. This could incorporate all required symmetries to the problem and will generate information for ground and excited states, electromagnetic transitions, level densities - all being physical quantities of crucial importance for understanding the nature of produced experimental data. Our coupled-cluster approach described above follows this approach and aims to extend the ab-initio description of nuclei from light toward medium mass and heavier nuclei. In order to gain a global picture of the nuclear landscape we use modern nuclear density functional theory (DFT) which is based on an Skyrme-type functionals and solved via self-consistent Hartree-Fock-Bogoliubov (HFB) calculations. These methods are mainly restricted toward ground-state properties, and have already achieved a level of sophistication and precision which allows analysis of experimental data for a wide range of properties and for arbitrarily heavy nuclei. For instance, self-consistent models are now able to reproduce measured nuclear binding energies with an impressive rms error of roughly 700 keV [32]. However, much work remains to be done.

The quest for the nuclear energy density functional, including dynamical effects and symmetry restoration, is one of the main themes and goals of the proposed project. . Developing a universal nuclear density functional will require a better understanding of the density dependence, isospin effects, and pairing, as well as an improved treatment of symmetry breaking effects and many-body correlations.

By employing various criteria (agreement with measured masses, radii, low-lying excited states, giant vibrations, rotational properties, and other global nuclear characteristics) our goal is to find an optimal parametrization of the functional. During last years, our group was laying out theoretical foundations and constructing computational tools to tackle this ambitious task. Our load-balancing routine allows us to calculate the entire deformed even-even mass table in a single 24 wall-clock hour run (or approximately 4,800 processor hours on an old SP-3 at ORNL called Eagle) [33].

Most of the currently used Skyrme forces correctly reproduce generic trends in nuclear masses, but they may differ in their descriptions of other quantities. Moreover, they often significantly differ in parameters or coupling constants. This suggests that yet-unresolved correlations may exist between these parameters, and only certain combinations thereof (probably a small number of them) are important. Such correlations would explain the fact that widely different parametrizations lead to fairly similar results. The most often used families of Skyrme or Gogny interactions are nowadays considered as two particular realizations of an effective interaction. The modern approach uses a formulation based on the energy density functional theory [34]. Here, one of the still unsolved questions is an appropriate selection of experimental data that would allow for more-or-less unique determination of the coupling constants defining the energy functional. To this end, one usually uses certain constraints obtained by extrapolating nuclear data to an infinite system and selected data for finite nuclei. Such a strategy does not seem to converge to a unique solution, and leads to a plethora of parametrizations currently available in the literature.

Recently, important indications on how to construct the nuclear energy functional have been obtained within the chiral perturbation theory based on the QCD Lagrangian treated within the effective field theory (see, e.g., [35]). It seems that main physical features of the functional can indeed be obtained from such a fundamental approach. Even if one still has to readjust and fine-tune the parameters for a precise description of nuclear data, one can gain an important insights into the structure of the functional, especially the dependence of the coupling constants on nuclear densities.

We are convinced that the present stage of theory requires constructing new energy density functionals supplemented by a complete error and covariance analysis. We believe that it is not sufficient to ``predict'' properties of exotic nuclei by extrapolating properties of those measured in experiment. We must also quantitatively determine errors related to such an extrapolation. Moreover, for an experimental work it is essential that an improvement gained by measuring one or two more isotopes be quantitatively known. From theoretical perspective, we must also know the confidence level with which the parameters of the functional are determined. Analysis of this type constitutes a standard approach in other domains of physics, but they are seldom performed in theoretical nuclear structure research.

Up to now massive HFB calculations are mainly based on zero-range Skyrme forces. An open question is whether going away from the stability line one should use the same force parameters or even the same effective forces. Obviously new fitting calculations are required and most probably one should include new terms. Present Skyrme density functionals include about 14 unknown parameters. One can fix about 5 of them using infinite nuclear matter properties and the rest should be fitted to known nuclear masses, radii and other ground state data. So, one has to fit about 10 parameters to produce the known 2135 measured masses with the best possible accuracy. Then, one can calculate all 9200 nuclei within the whole mass table.

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9.B. Significance of Research

The U.S. nuclear physics community continues to pursue the development of technologies and facilities that will explore unstable nuclei. The principal experimental focus of present and proposed low-energy nuclear research facilities is on understanding nuclear properties far from stability. Information gleaned from experiment will complement ongoing nuclear theory efforts to understand the nuclear force, the mechanism of nuclear binding, and implications of nuclear theory and measurements on astrophysical processes. The science to be addressed by this INCITE proposal will enable us to pursue research to help answer several long-standing questions in nuclear theory research. Three of these questions are: *How are nuclei assembled from their fundamental building blocks and interactions? How do complex systems exhibit such astonishing simplicities and regularities? How many elements and nuclei are yet to be discovered?* These three questions for the field focus on the microscopic theory of nuclei. Nuclear scientists strive to derive the properties of atomic nuclei from the interactions of protons and neutrons, or ultimately, from quarks and gluons [1]. Indeed, nuclei are *the only link* between QCD and the atomic and macroscopic world. This approach — starting from basic components to create a complex system — is a common one in science and is shared by chemists and materials scientists, whose building blocks are atoms and molecules, and biologists and biophysicists, who work with large macromolecules like proteins that make up cells and complex organisms built on their constituent cells and molecules.

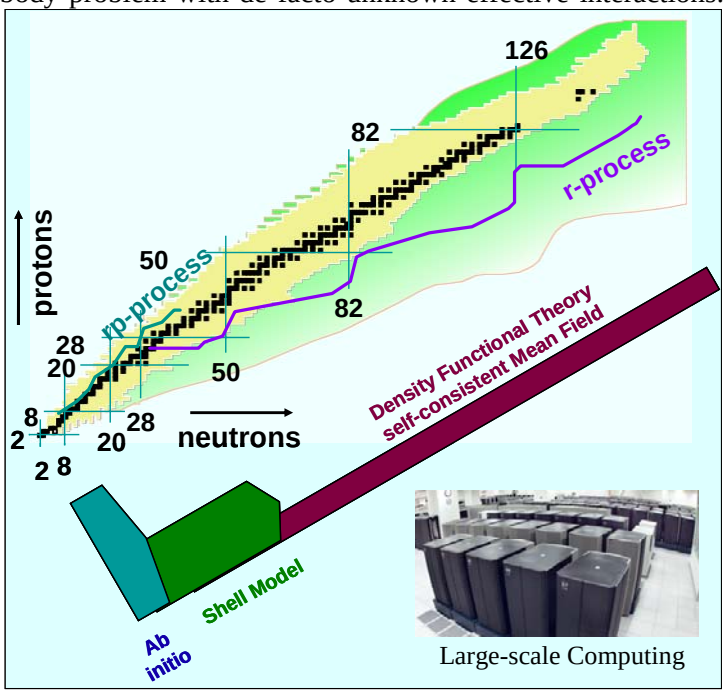
Nuclear properties often display striking regularities—such as energy levels that mirror nearly perfect rotational motion—which point to the purity of particular quantum states. Likewise, nuclei display structural changes with neutron and proton number; sometimes these changes are abrupt, sometimes gradual. Understanding these regularities in terms of symmetries of the many-body system, and their breaking, as well as in a microscopic framework, is a truly challenging problem. Deficiencies in our present understanding have surfaced as we study nuclei that have vastly different ratios of protons to neutrons compared with stable nuclei. Today, we have limited knowledge of just how many neutrons can be added to a stable nucleus before it becomes unable to hold more. We need new theoretical and experimental tools to make progress in the future.

Nuclear structure theory strives to build a unified and comprehensive microscopic framework in which bulk nuclear properties, nuclear excitations, and nuclear reactions can all be described. A new and exciting focus in this endeavor lies in the description of exotic and short-lived nuclei. The extreme isospin of these nuclei and their weak binding bring new phenomena to the fore which isolates and amplifies important features of the nuclear many-body problem. The new arena of nuclei with large neutron excess is therefore key to building a unified theoretical foundation for understanding the nucleus in all its manifestations—from the stable nuclei that exist around us to the most exotic nuclei, and even to exotic forms of nucleonic matter which exist, e.g., in neutron stars.

Currently, a variety of nuclear structure research facilities within the United States, in Europe, and in Japan provide experimental data concerning the properties of both exotic and stable nuclei. In order to address astrophysical questions related to nuclear physics, the National Science Foundation (NSF) recently created the Joint Institute for Nuclear Astrophysics. In addition to the current U.S. facilities, efforts are ongoing to build the Rare Isotope Accelerator (RIA), the next-generation low-energy nuclear facility in the U.S. RIA is a near-term number-three priority of the U.S. Department of Energy, Office of Science (and the top priority within the Division of Nuclear Physics).

RIA and other exotic beam facilities allow unique insights into the quantum many-body nature of nuclei by providing access to their most extreme manifestations and by providing precise control of the number of neutrons in these systems. Recent theoretical and experimental achievements, coupled with the experimental discoveries that RIA will provide, are focusing new attention on a number of unsolved issues in nuclear structure and offer excellent scientific opportunities for the next decade and beyond. Given the advent of research on radioactive nuclei, particularly with the coming of the RIA, it is extremely important to prepare nuclear theory for its realization.

Understanding nuclei and predicting nuclear behavior requires one to solve the complicated many-body problem with de facto unknown effective interactions. While this statement is obvious, its implementation has been quite difficult due to the computational challenges involved. Various methods have been employed; these are broadly classified, along with the nuclear landscape in Fig. 1. The research that will be conducted in this INCITE proposal maps well onto this figure and will range in scope from theoretical work on effective interactions for nuclear structure, to the application of techniques for solving the nuclear many-body problem, to the relation between microscopic theory and macroscopic symmetries. The specific methods that will be pursued include nuclear coupled-cluster methods, shell-model techniques (quantum Monte Carlo based algorithms), and self-consistent mean-field theories based on density-functional theory (inducing superconducting correlations). These are invaluable tools for furthering our understanding of nuclear properties and will enable exciting research at the frontier of nuclear theory. The practical implementation of these methods requires excellent computational capabilities and parallel computing resources. By utilizing and developing new theory and computational tools, this INCITE award will provide the community with reliable, quantitative predictions for nuclear structure and guide future experimental efforts.



Large-scale Computing

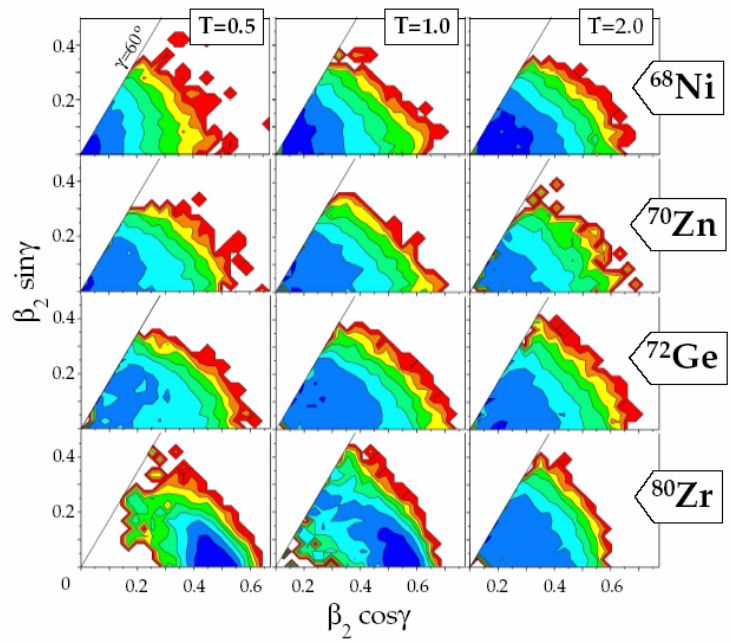
9.B.1. Significance of Nuclear Coupled-Cluster work in this proposal

What is the role of the three-body nuclear force on medium-mass nuclei ranging from ^{16}O to ^{60}Ca?
Recent indications from GFMC and NCSM calculations indicate that three-body forces are necessary to obtain an understanding of light nuclear systems (through mass 12) [2,3]. Probing the effects that the three body forces will have on medium mass nuclei has not yet occurred, although some conjectures have been put forward [4]. We know from few-nucleon experimental data [5] that three-nucleon forces should exist and from Effective Field Theory that they are systematically derivable [6]. In fact, since the nucleon is a composite particle, three-body forces must exist. Our current understanding of their effect on the nuclear many-body problem is that they account for some fraction of the nuclear binding (not accounted for using bare two-body forces alone), and that they may affect spin-orbit splitting [7] in nuclei. It has recently been conjectured that three-body forces will also impact orbital momentum properties of nuclei [8]. These properties affect sub-shell closures in systems like ^{22}O and ^{48}Ca. For example, ^{16}O is a closed shell nuclei (the closure is N=Z=8, 0s-0p orbitals). The N=Z=20 nucleus ^{40}Ca is also closed shell (0s-0p-1s0d orbitals). The sub-shell closure above ^{16}O is at ^{22}O (closed $0d_{5/2}$ orbital). All two-body interactions fail to produce the spectrum of ^{22}O (and ^{48}Ca which has a closed N=28 sub shell). This physics is highly relevant to rare-isotope nuclear properties as in the very recently measured ^{42}Si [9].

The basic scientific question then is how does a realistic three-body force affect this problem? This is an extremely important question in nuclear structure today and can be addressed microscopically presently only through coupled-cluster techniques. Hence, the bulk of our proposed effort focuses on the issue of the role of the three-body force in medium mass nuclei.

9.B.2. Significance of Nuclear Auxiliary Field Monte Carlo calculations

What are the thermal, rotational, and pairing properties of mass 80-120 neutron rich nuclei?
The only viable method that includes all many-body correlations for a given nuclear system in this mass region and is able to probe the thermal properties of nuclear systems is the nuclear version of the Auxiliary Field Monte Carlo method (known as Shell Model Monte Carlo, SMMC) [10]. One particularly interesting region of the nuclear chart is in the mass 80-120 (from zirconium to tin). The region is famous for shape-coexistence phenomena and the onset of highly deformed intrinsic ground-states [11]. An understanding of neutron capture probabilities on nuclei in this region is also important for the Science Based Stockpile Stewardship Program [12]. Very neutron rich nuclei in this region (for example ^{110}Zr) lie on the neutron-rich r-process nucleosynthesis path (a stellar process that produces about ½ of the elements heavier than iron in the universe) where neutron capture also plays an important role. Since many of these capture rates cannot be directly measured, theory actually plays a key role in determining them.



The SMMC technique will be used to probe the thermal properties of these nuclei. As an example, we mention the deformation changes that occur when one heats nuclei in this region [13]. We show in the figure deformation plots for several nuclei in the mass 70-80 region with 40 neutrons. In the figure, β describes how deformed the nucleus is while γ indicates whether the nucleus is oblate (γ=0) oblate (γ=60) or soft (uniform filling in γ). ^{68}Ni and ^{70}Zn are fairly spherical nuclei while ^{72}Ge exhibits shape-coexistence. ^{80}Zr is very well deformed (and prolate) as is seen in the figure. At intermediate temperatures (middle column) all nuclei retain some of their ground-state character, but the shape distributions become softer in the γ-direction. At the higher temperature of T=2.0 MeV the four N=40 systems considered become soft in both β and γ, filling uniformly the phase space in the β–γ plot.

Of particular importance to neutron capture is the level density information, which can be directly probed by the SMMC method [14]. The SMMC technique is the only method that uses realistic nuclear interactions to probe nuclear properties as a function of temperature.

9.B.3. Significance of Nuclear HFB mass-table calculations

What is the nuclear energy density functional that will enable predictive mass-table calculations?

Density functional theory (DFT) is built on theorems showing the existence of universal energy functionals for many-body systems, which include, in principle, all ground-state many-body correlations. Condensed matter physicists and computational chemists have developed such functionals for the Coulomb interaction that describe properties of a wide range of systems with chemical accuracy.

In nuclear physics, self-consistent methods based on the DFT, e.g., the Hartree-Fock-Bogoliubov theory with Skyrme parameterizations, have achieved a level of sophistication that allows analyses of experimental data for a wide range of properties and for arbitrarily heavy nuclei. For example, HFB calculations were recently used to explore the rich physics exhibited by super-heavy nuclei [15].

The achieved accuracy and predictive power of mean-field calculations, however, still leaves much to be desired. For example, two-neutron separation energies for Sn isotopes resulting from Hartee-Fock-Bogoliubov calculations utilizing a wide range of Skyrme potentials match experimental data where it exists. However, each of the various Skyrme potentials extrapolates to different results as one advances to the neutron drip line where data do not exist to constrain theory. The quest for a truly universal DFT of nuclei, including dynamical effects and symmetry restoration, is one of the main themes of theoretical nuclear structure worldwide.

To make progress, a concerted effort will be required to study new functionals when applied to finite nuclei and infinite or semi-infinite nuclear matter. For instance, in the particle-hole channel, one would like to enrich the density dependence of the effective mass in order to differentiate between its value in the bulk and at the Fermi surface. Another goal is to understand connections between the symmetry energy and isoscalar and isovector mean fields, and in particular the influence of effective mass and pair correlations on symmetry energy versus isospin. Such an understanding will allow us to better determine isospin corrections to nuclear mean fields and energy density functionals. In the self-consistent method, the average nucleonic field is obtained from the nucleonic density. Consequently, in the nuclear state with nonzero angular momentum, the self-consistent potential acquires time-odd components. These terms are expected to play a significant role at very high angular momentum when the nucleus is strongly polarized, but they should also influence properties of beta decay and the ground states of odd-mass and odd-odd nuclei. Addressing these challenges will require us to exploit advances in the study of microscopic inter-nucleon interactions, in the development of many-body computational techniques, and in raw computer power, as well as to further develop DFT itself as applied to finite, self-bound systems.

We outline in 9.C our proposed calculations and computational readiness.

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9.C. Computational Approach

9.C.1. Nuclear Coupled Cluster Theory (85% of total project)

Our computational methodology was briefly described. During the last three years we have developed a set of powerful theoretical tools [1,2,3] for the description of nuclear properties in a many-body framework known as coupled-cluster theory [4,5].

The nuclear coupled-cluster CCSD code was written over the course of the last 3 years and was specifically targeted for a distributed memory environment. We could not use quantum-chemistry implementations of CC theory for a variety of reasons, including the differing types of symmetries involved in the calculations. We therefore wrote our own CCSD (and excited state, and triples corrections) codes. Our workhorse is the CCSD algorithm. We describe below its various features and the techniques used to solve the CCSD problem.

- *Programming languages, libraries, and other software used:*

The Nuclear CCSD code was written in Fortran90 with MPI. It contains BLAS and LAPACK routine calls. The code also uses parallel I/O (via MPI-IO calls). The nuclear CCSD code was built from scratch. Chemistry codes cannot be adapted to the nuclear problem since the nuclear forces are spin and isospin dependent. Thus, standard algorithmic savings in chemistry brought about by the symmetries of the Hamiltonian (e.g., use of a spin-orbital basis) cannot be employed for nuclei.

- *Description of the underlying mathematical formulation:*

Coupled-cluster techniques solve for ground- and excited-states of a quantum many-body system at a given level of many-body sophistication. Modern formulations of coupled-cluster techniques rely on a basis expansion as described in Section 9A.1. One solves for the excitation amplitudes within the basis. The equations, as described in [1] are coupled, non-linear, algebraic equations for the excitation aplitudes that must be solved iteratively. A compact mathematical statement of the problem is given by the expression $f_i(t_1, t_2) = 0$, where the set of unknown amplitudes (one-particle-one-hole and two-particle-two hole excitation amplitudes t_1 and t_2) must be found. The equations are closed if one assumes that any higher order amplitudes (three-particle-three-hole amplitudes in this case) are zero.

- *Algorithms and numerical techniques employed*

The number of unknowns in these equations for ^{16}O in 8 oscillator shells is 603,720; this number grows substantially for ^{40}Ca; in 7 shells the comparable numbers are: for ^{16}O, 345,160 unknowns, and for ^{40}Ca, there are 2,072,608 unknowns (the largest problem we have attempted to tackle to date). Regardless of the number of unknowns the number of iterations needed to obtain converged results (to six digits) apparently remains fairly stable regardless of the nucleus involved. We use Moller-Plesset perturbation theory [6] to obtain an initial guess for the amplitudes. We have also implemented an iterative acceleration technique known as direct inversion in the iterative subspace (DIIS) [7] to speed convergence. Normally 20 or less iterations are needed to solve the equations to 10^{-6} accuracy.

A complete calculation for a give nucleus proceeds in the following manner. First, one must generate the effective two-body interaction for the problem. The nuclear interactions typically have very repulsive (in some cases hard) core potentials. Bare NN potentials (which describe the two-body interactions among protons and neutrons) cannot be directly used in the CC approaches. One must first renormalize these interactions to the model-space in which one is working. This can be done in several ways including a standard infinite sum of ladder diagrams (the G-matrix approach [8]) a Hamiltonian similarity transformation and projection to the model-space [9], and a renormalization group (RG) method that obtains only the low-momentum part of the interaction [10]. This step is not numerically intensive and can be performed on a small cluster or workstation. The output from this step, the effective-two body interaction, is then used in the CCSD approach. The RG approach, also known as V_{lowk}, will be utilized to investigate three-body effects. This particular renormalization contains a momentum cutoff parameter, and one must check that results are independent of this parameter when three-body forces are included.

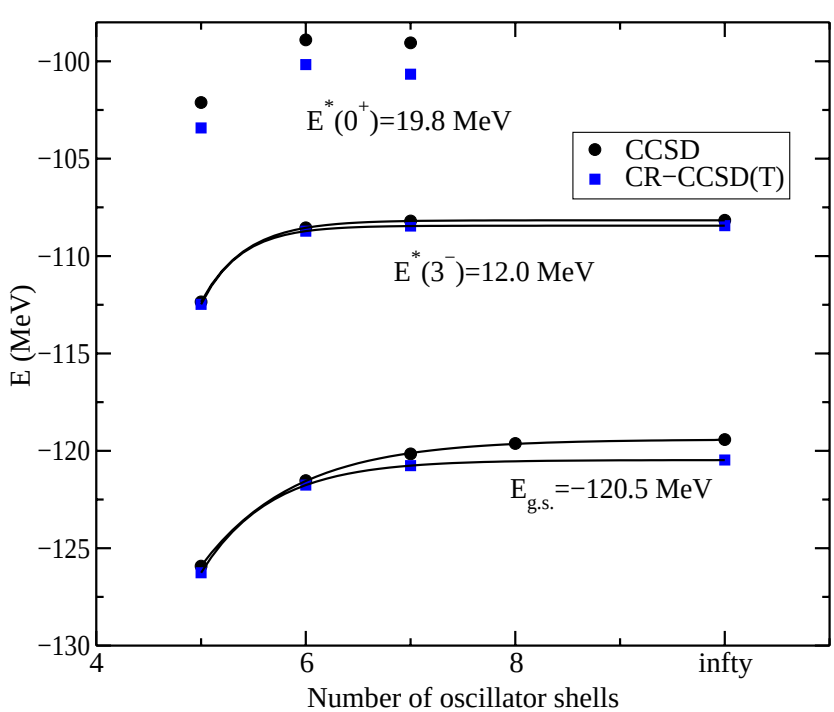
Second, the two-body interactions obtained from the first step are calculated in a 'coupled' representation and must be decoupled. This step is performed within the parallel CCSD code. The scattering of two quantum-mechanical particles must conserve certain symmetries, one of which is, for example, the total two-particle angular momentum of incoming particles before they interact must be the same as the outgoing angular momentum after they interaction. In order to be used in the CCSD approach, the matrix elements must first be uncoupled. This procedure is performed by first reading in the coupled matrix, and using a master-worker algorithm to spread the work of decoupling. Once matrix elements have been decoupled and MPI-I/O written to a file, the resulting 4-index array of matrix elements is block-distributed among the processors with a MPI-I/O read. This turns out to be an extremely efficient (and crucial) part of the overall algorithm.

The final step involves calculation of the CCSD amplitudes. The present code uniformly distributes the interaction matrix elements across processors on two of the four indices. Each processor maintains a complete copy of the amplitudes. Thus each processor performs a partial sum of the equations to obtain new amplitudes. An all-reduce (addition) is used to obtain the new copies of the amplitudes for the next iteration step. While the keeping one copy of the amplitudes for each processor means that as we go to larger model spaces, memory use becomes an issue, the overall Flops performance of the code has benefited from this strategy. For non-iterative triples corrections we transport the resulting CCSD amplitudes and decoupled Hamiltonian to collaborators at Michigan State for analysis.

- *Parallel implementation and readiness*

The workhorse of this project is our nuclear CCSD code. It was developed on the SP-3 platform at NERSC (Seaborg). It has also been run on the 256 processor shared memory SGI Altix machine (RAM, Itanium2 processors running at 1.5 GHz) at ORNL. The computational requirements strictly scale as as $n_o^2 n_u^4$ where n_0 is the number of single-particle orbitals below the Fermi surface, and n_u is the number of orbitals above the Fermi surface. We have checked that this scaling holds as one performs calculations in larger nuclei or as one increases the model space. The EOMCCSD method also obtains this scaling.

The code performance can be summarized by quoting a relevant number: on 100 processors of the SGI Altix, 0.2 Tflops of performance was obtained in N=8 shells (480 single-particle orbitals) in ^{16}O, and converged calculations were obtained within 10 wall-clock hours. The per-processor performance of this run was 2 Gflops (34% of theoreti- ak). Thus, for ^{16}O and 480 particle states, 2 Tflop-hours eded to obtain a converged l-state result. The conver- with oscillator shells is shown) in the Figure to the left for round and excited state calcu- [3]. We note that the first l lies at about twice its ex- ntal value. The inclusion of a ody interaction should sig- tly improve this description. f the INCITE time will be perform additional calcula- n the following nuclei: ^{22}O, Ca, ^{48}Ca, ^{60}Ca, ^{56}Ni, ^{42}Si. As entioned in 9b, this choice of is motivated by the need to tand how three-body forces both masses, spin-orbit split- nd the intruder-extruder prob-



lem encountered when one only uses two-body NN interactions. The total computational time required for these calculations will be approximately 400,000 MPP[1] equivalent processor hours to complete this part of the project. The CCSD code has been run at NERSC on up to N=7 (336 single particle orbitals) for ^{40}Ca. One caveat on Seaborg is that memory becomes an issue for ^{40}Ca and above nuclei. For these nuclei, optimally 8 Gbytes/processor is necessary. This will require us to make extensive use of the large memory nodes on Seaborg, or to utilize fewer processors per node on the standard nodes. (We will likely find memory savings opportunities in the code before we compute the larger nuclear systems proposed – ^{60}Ca and ^{56}Ni.) A recent test calculation on Seaborg indicated a 379 Mflop/processor rating utilizing 4 processors per node (1024 processors total, 256 used in computing) for ^{40}Ca. Memory requirements for lighter nuclei may make the XT3 at ORNL a good candidate for running some of this effort.

In order to assess the influence of the three-body interactions on the above list of nuclei, we will first perform CCSD calculations with an approximate two-body equivalent of the three-body interaction. We will perform these calculations at two cut-off parameters. This equivalent form of the three-body interaction should amount to an effort that is equivalent to the standard CCSD runs. We will require 3.2 million MPP equivalent processor hours to make this assessment (for both ground- and excited-state information) for all nuclei in our list at N=7 and for ^{40}Ca and ^{42}S at N=8.

The full inclusion of the three-body interaction at the CCSD level (V3CCSD) will require significantly more computing resources. We will first tackle this problem for the N=6 basis (224 single-particle states). We know that the scaling of the most expensive V3CCSD terms in the amplitude equations are of order $n_o^2 n_u^5$ and $n_o^4 n_u^4$ (there are likely ways to decrease these rather large factors). This scaling means that to investigate the effect of the three-body interaction on ^{16}O and ^{22}O will require approximately 1,200,000 MPP equivalent hours.

For this part of the project, we therefore propose the following three-year computational strategy. Our request is for 2.25 million MPP equivalent hours per year in FY06, FY07, and FY08. During the first year we will compute all nuclei in our list for the N=7 basis set (smaller basis set sizes will account for about 20% of our request) using the approximate 3-body inclusion and test the cut-off parameter dependence in ^{16}O. We will also begin calculations of the V3CCSD (full inclusion of V3 at the CCSD level) equations for ^{16}O. During FY07 we will complete the N=8 basis state runs, finish the V3CCSD runs for ^{16}O and start the ^{22}O V3CCSD runs. During FY08 we will complete the V3CCSD runs for oxygen and also calculate, for the first time in an ab initio framework ^{28}Si at the V3CCSD level.

The theoretical development and implementation of the nuclear CCSD effort was originally begun under ORNL LDRD funds (FY02/03). ORNL SEED money funds (FY05/06) partially support our V3CCSD efforts. Through the LDRD and SEED funds, we have developed useful connections with David Bernholdt and Robert Harrison from ORNL concerning certain aspects of the numerical implementations.

9.C.2. Auxiliary Field Monte Carlo (10% of total project)

- *Programming languages, libraries, and other software used:*

The nuclear Shell Model Monte Carlo code was written in Fortran90/95 with MPI. It contains BLAS and LAPACK routine calls.

- *Description of the underlying mathematical formulation:*

Monte Carlo evaluation of the path-integral requires several steps. The evolution operator is an exponent of a matrix representation of the one-body Hamiltonian which describes how particles behave in the fluctuating fields. There are two one-body Hamiltonian matrices (one for protons and one for neutrons) for each time-slice of the path integral. If the imaginary time, which is measured in units of inverse en-

[1] [1] An MPP hour at NERSC is equivalent to one wall clock hour, while the CCS/ORNL (the IBM Cheetah (3.5 times the NERSC IBM-SP) and the SGI-Altex (4 times the NERSC IBM-SP) computers are a factor of 3.5-4 faster than Seaborg at NERSC.

ergy, is taken to infinity, then we recover ground state information on the system; otherwise, we obtain information on the thermal average of the system. Because of the natural gap between ground- and excited-states in nuclear systems (particularly in those with an even number of particles), an imaginary time of 2 MeV^{-1} (in nuclear units) allows for ground-state calculations. The imaginary time is discretized, typically in steps of 1/32 which obtains reasonable convergence.

- *Algorithms and numerical techniques employed:*

We thus perform the following operational steps for each Monte Carlo sample. First, we generate the one-body Hamiltonian matrix (which depends on the fluctuating auxiliary fields), then we exponentiate it to obtain the matrix representation of the evolution operator for a given imaginary time step. We must then multiply all such time-slices together to produce the imaginary-time evolution matrix, U. We must take the determinant of (1+U) in order to formulate the probability that is used to determine whether to accept or reject the Metropolis random walk for a given auxiliary field. These steps are performed several times per recorded sample to obtain statistically independent samples.

- *Parallel implementation and readiness:*

The SMMC code performs separate Metropolis random walks on each processor, making the code rather efficient in communications overhead. For each sample, the code performs a global reduce operation (this has the effect of synchronizing the code when each sample is taken). The global reduce is over only about 50 variables (observables such as energy, level-occupation numbers, and various transition operators).

The SMMC code has matured significantly in the last 10 years. Published benchmarks from 1997 indicate the average MF rating (per processor) was 36 Mflops on the IBM-SP2 Thin66. Today, the code (with continuing software and hardware performance enhancements) performs at roughly 300 Mflops/processor (and up to 350 depending on the application) on Seaborg. Further enhancements beyond raw speed have given the code another factor of 10 in overall efficiency. Code memory requirements are roughly 200Mbytes/processor.

We performed several benchmark calculations over the course of the last year using the SMMC code. These calculations were performed on very large systems consisting of either 30 (gds) or 50 (fp-gds) single-particle states for both neutrons and protons. All calculations were performed on Seaborg at NERSC. For comparison, the corresponding matrix diagonalization that would be required in standard shell-model diagonalization procedures would be of rank 1.3E10 for gds or 2E16 for fp-gds. Depending on the type of measurements taken, the performance of the code is given in the following table (data taken with poe on Seaborg). I had to change from MP_PIPE_SIZE=64 to MP_PIPE_SIZE=32 to make the final 2048 processor run.

Processors	Job size / MC samples	Time to complete	Speed/processor	Aggregate speed
256	Ni56, fp-gds / 5120	3.3 hours (wall)	285 Mflops	72.9 GFlops
256	Ni68, fp-gds / 5120	3.3 hours (wall)	284 Mflops	72.7 GFlops
256	Ni78, fp-gds / 5120	3.3 hours (wall)	283 Mflops	72.4 Gflops
128	Ni68, fp-gds / 4096	5.8 hours (wall)	271 Mflops	34.7 Gflops
16	Ni68, fp-gds / 32	0.5 hours (wall)	315 Mflops	5 Gflops
512	Mo92, gds / 16384	0.7 hours (wall)	311 Mflops	159 Gflops
1024	Mo92, gds / 32768	0.7 hours (wall)	317 Mflops	325 Gflops
2048 (MP=16)	Mo92, gds / 65536	0.9 hours (wall)	241 Mflops	493 Gflops
2048 (MP=32)	Mo92, gds / 65536	0.74 hours (wall)	298 Mflops	610 Gflops

As mentioned in 9.A.2, SMMC calculations will be used to explore the properties of nuclei in the mass 80-120 region. To perform one calculation for one nucleus in this region using the newly developed pn-SMMC technology requires 7,000 MPP equivalent processor hours. 200,000 MPP equivalent processor hours per year would then allow us to perform a fairly comprehensive study of thermal, rotational, pairing, and deformation properties of about 30 nuclei in this mass region. We expect significant insight into the nature of medium-mass neutron rich nuclei to be gained from such calculations.

9.C.3. Nuclear HFB Calculations (5% of total project)

- *Programming languages, libraries, and other software used:*

The Nuclear HFB code was written in Fortran90 with MPI. It contains BLAS and LAPACK routine calls.

- *Description of the underlying mathematical formulation:*

The solution of self-consistent mean-field equations for weakly bound paired nuclei requires a correct description of the asymptotic properties of nuclear quasiparticle wave functions. In the present implementation, this is achieved by using the single-particle wave functions of the Transformed Harmonic Oscillator, which allows for an accurate description of deformation effects and pairing correlations in nuclei arbitrarily close to the particle drip lines. The program uses the axially Transformed Harmonic Oscillator single-particle basis to expand quasiparticle wave functions. It iteratively diagonalizes the Hartree-Fock-Bogolyubov Hamiltonian based on the Skyrme-forces and zero-range pairing interaction until a self-consistent solution is found.

- *Parallel implementation and readiness:*

Presently we have a fast code for spherical HFB calculations [11] which takes almost 10 CPU minutes per nucleus as well as a code for axially deformed HFB calculations [12] with acceptable processor speed - about 1 CPU hour per nucleus. All CPU predictions are based on an Intel Xeon 2.8 GHz processor. On the Power-4 IBM processor (e.g. the processors in Cheetah), this code obtains 1.2 GFlops/processor. Memory needs for these codes is small: less than 100 Mbytes. These codes are compute intensive and have very little need for communications.

Our strategy for numerical treatment of the problem is the following:

- First step: One performs more expensive axially deformed HFB calculations for all 1754 nuclei with available experimental data - the resulting total energy for a nucleus can be denoted as $E(\beta_0)$. One also calculates the same nuclei but constrained to a spherical symmetry - the resulting total energy for a nucleus can be denoted as $E(0)$ - in order to define the deformation energy $E_{def} = E(0) - E(\beta_0)$. This generates a quasi-experimental set of data $E_{\exp}^{sph} = E_{\exp} - E_{def}$ which can be used on the second step. (MPP equivalent time: 14,000 hours)
- In the next step, one performs the fit of the energy density functional to the quasi-experimental set of data $E_{\exp}^{sph}$ for the same 1754 nuclei but using spherical HFB calculations which are relatively fast. If necessary, one could repeat these steps several times. (MPP equivalent time: 6,000 hours if one performs 10 iterations)
- Final Step: At the end one would perform complete proton drip-line to neutron drip-line axially deformed mass table calculations. In order to have information for the ground state of e.g. 9200 nuclei lying between the drip lines over the range $Z, N \geq 8$ and $Z \leq 120$, one should calculate each nucleus 3 times (starting with oblate, prolate and spherical initial conditions, the ground state is the one with the lowest total energy) which make about 27600 calculations. (MPP equivalent time: 55,200 hours).

For this part of the project, the total project time is then 75,200 MPP equivalent hours (during year 1). We will also investigate the feasibility of performing exact particle-number projection within the HFB scheme, which will begin in year 1. The total time requested to perform the mass-table analysis and to perform initial exact particle-number calculations is then 100,000 MPP equivalent hours per year.

Suggested Implementation of this project on several platforms

The three codes described above have different computational requirements and therefore it would be best to run them on different machines. We believe the following breakdown would be in order.

The major effort in this project will be the CCSD portion with the three-body interaction study. This part of the project will have a major impact in the low-energy nuclear physics field and will help us understand the role of the three-nucleon interactions in medium-mass nuclei. The project requires machines with significant available memory per processor. We believe two machines will be in order for this project: a) Seaborg and its follow-on machines at NERSC, and the Cray XT3 at ORNL. While we have not performed tests on the XT3 at this time (the machine is not yet completely built) we believe our Seaborg experience should make the transition to the XT3 fairly straightforward.

The SMMC codes require several hundred Mbytes per processor. We believe that we can optimize memory for the ANL BGL machine. The code should run on that platform as fast as it runs on Seaborg. We have discussed with colleagues who perform Green's Function Monte Carlo calculations on that machine, and they have seen performances similar to Seaborg performance. We therefore request 200,000 BGL hours per year for this part of the project.

The HFB codes require very little memory (about 100Mbytes for a single processor). Therefore, we suggest that this part of the project should be performed on the IBM Blue Gene at ANL. As is the case with the SMMC code, we believe that these calculations should perform at least as well as on Seaborg. We therefore request 100,000 BGL hours per year for this part of the project.

Thus, while the pull-down menu on question 5 asked for one particular machine, we believe this project's time should be split across several platforms. We have used Seaborg as the major platform requested, although clearly, the XT3, and BGL will also be extremely useful for the project.

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