NUCLEAR STRUCTURE AND NUCLEAR REACTIONS

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INTRODUCTION AND CURRENT STATUS

Atomic nuclei are the essence of the visible universe. Formed in the big bang or in cataclysmic astrophysical explosions, atomic nuclei are a crucial and intriguing part of the world. The basic features of atomic nuclei were understood in terms of the nuclear shell model in the 1963 Nobel Prize winning research of Eugene Paul Wigner, Maria Goeppert-Mayer, and J. Hans de Jensen. Since then, extensive experimental programs have yielded a detailed knowledge of the nucleon-nucleon interaction. This crucial experimental information will be augmented through studies of quantum chromodynamics (QCD) (see section on Cold QCD and Nuclear Forces). More refined descriptions of nuclei and greater predictive power require understanding nuclear structure and reactions in terms of the underlying interactions. Accurate solutions of these strongly interacting quantum many-body problems will yield new insight into the structure of nuclei and the ability to calculate processes that are difficult or impossible to measure experimentally.

The structure and dynamics of atomic nuclei represent very challenging problems because, unlike the theory of electrons in atoms and molecules, naïve mean-field theories based upon the underlying interactions do not provide even a qualitative description of their structure. The nuclear interaction is strongly spin- and isospin-dependent, and finely tuned to provide a weak nuclear binding of approximately 8 MeV per nucleon, much smaller than a typical scale in QCD.

Large-scale computations have already enabled significant progress in understanding nuclei from the underlying nuclear interactions. The structure and energy levels of the lightest nuclei (consisting of up to 12 nucleons) are well reproduced with realistic two-nucleon interactions plus modest three-nucleon interactions. The same interactions provide good descriptions of electroweak form factors, transitions and response, as well as the nucleon-nucleon correlations as revealed in experiments at Thomas Jefferson National Accelerator Facility (Jefferson Laboratory) and elsewhere. The first low-energy microscopic calculations give confidence that a consistent picture of structure and dynamics is emerging. However, as nuclei with almost 300 nucleons are experimentally observed, studies of systems containing 12 nucleons are only the beginning.

Progress in large-scale nuclear calculations is only now extending to larger nuclei, where much of the promise of extreme scale computing lies. The theory of the atomic nucleus focuses on predicting and explaining rich classes of phenomena that occur in nuclei and nucleonic matter. Atomic nuclei exhibit many intriguing properties; pairing energies, for example, are a significant fraction of the Fermi energy. In heavy neutron-rich nuclei, pairing energies can be comparable to shell closure effects, a regime quite different from the most stable nuclei. The binding energies and electroweak transition rates of these nuclei are crucial to understanding the production of the heaviest elements. Understanding nuclei is also critical in exploring fundamental physics, including for example the absolute mass scale of neutrinos as to be determined in neutrinoless double beta decay.

Given its intriguing nature and importance in the birth of the universe, in astrophysical settings, in energy generation, and in industrial and medical applications, it is fundamentally important and of great practical significance that scientists have a detailed understanding of this complex quantum many-body system. The theoretical goal of increased predictive power for describing nuclear processes that occur in nature or in nuclear reactors, but cannot be measured in the laboratory with sufficient precision, drives scientists in this field to achieve detailed simulations using extreme scale computers and cutting-edge algorithms.

Three major challenges are addressed in this section: 1) a strong inter-nucleon interaction based upon—but not derivable with the necessary accuracy from—QCD; 2) the quantum many-body problem; and 3) phenomena on scales stretching over orders of magnitude in length or energy. Together, these challenges create a computationally difficult problem, and research teams have recently developed a suite of new and sophisticated computational tools capable of addressing previously unsolved problems. A driving force for these teams has been the substantial increase in computational power in the past decade. Consequently, increased computational power has, for the first time, made theories that were known for decades applicable for detailed nuclear physics investigations. The advent of extreme scale computing will enable this progress to accelerate, as shown in this report.

Scientists are on the verge of precision predictions for low-energy nuclear processes of both fundamental and practical significance such as neutron-nucleus and proton-nucleus reactions, electromagnetic transition rates, fusion of light nuclei, fission of heavy nuclei, and structure of short-lived isotopes. Scientists also aim to develop and validate novel approaches to the structure and reactions of heavier nuclei by predicting a universal nuclear energy density functional and solving density-functional theory for these systems. Building on recent successes with leadership-class computers, extreme scale computing will be critical to the advances projected over the next decade.

The following subsections highlight four important questions in nuclear structure and reactions that extreme scale computing, coupled with continued algorithmic improvements, will answer. These questions cover fundamental nuclear phenomena and span the entire chart of nuclei from the light but fundamental nucleus ^{12}C, through intermediate-mass nuclei such as ^{48}Ca, ^{76}Ge, and ^{130}Te, to the fission of the heaviest nuclei, and, finally, beyond the known nuclei at the limit of nuclear existence for the heaviest elements, and at the neutron drip line and neutron matter. The range of these questions is truly comprehensive in scope and an array of advanced techniques—which are well matched to the power of emerging extreme scale facilities—will be required. The principal benefit of this research direction will be the development of a truly predictive capability for the entire periodic table.

PRIORITY RESEARCH DIRECTIONS

Ab Initio Calculations of Light Nuclei and Their Reactions

Basic Scientific and Computational Challenges

A realistic *ab initio* approach to light nuclei with predictive power must have the capability to describe bound states, unbound resonances, and scattering states within a unified framework. Over the past decade, significant progress has been made in understanding the bound states of light nuclei starting from realistic nucleon-nucleon (NN) plus three-nucleon (NNN) interactions (Pieper and Wiringa 2001; Navrátil et al. 2000, 2007; Hagen et al. 2007b). The solution of the nuclear many-body problem is even more complex when scattering or nuclear reactions are considered. For few-nucleon systems (A=2-4), accurate methods solve the bound state and the scattering problems. However, *ab initio* calculations for scattering processes involving more than four nucleons are still the exception (Nollett et al. 2007; Quaglioni and Navrátil 2008; Hagen et al. 2007a) rather than the rule. The development of an *ab initio* theory of low-energy nuclear reactions on light nuclei is key to further refining scientists' understanding of the fundamental interactions between the constituent nucleons. At the same time, such a theory is required to make accurate predictions of nuclear astrophysics' crucial reaction rates that are difficult or even impossible to measure experimentally. This section highlights a key direction that *ab initio* methods will pursue with exascale resources.

Reactions That Made Us: Triple-Alpha Process and $^{12}C(\alpha,\gamma)^{16}O$

Extreme scale computing will enable the first precise calculation of $2\alpha(\alpha, \gamma)^{12}C$ and $^{12}C(\alpha,\gamma)^{16}O$ rates for stellar burning (see Figure 9); these reactions are critical building blocks to life, and their importance is highlighted by the fact that a quantitative understanding of them is a 2010 U.S. Department of Energy milestone (DOE 2007). The thermonuclear reaction rates of alpha-capture on ^{8}Be (2α-resonance) and ^{12}C during the stellar helium burning (see Figure 9 for a schematic depiction) determine the carbon-to-oxygen ratio with broad consequences for the production of all elements made in subsequent burning stages of carbon, neon, oxygen, and silicon. These rates also determine the sizes of the iron cores formed in Type II supernovae (Brown et al. 2001; Woosley et al. 2002), and thus the ultimate fate of the collapsed remnant into either a neutron star or a black hole. Therefore, the ability to accurately model stellar evolution and nucleosynthesis is highly dependent on a detailed knowledge of these two reactions, which is currently far from sufficient.

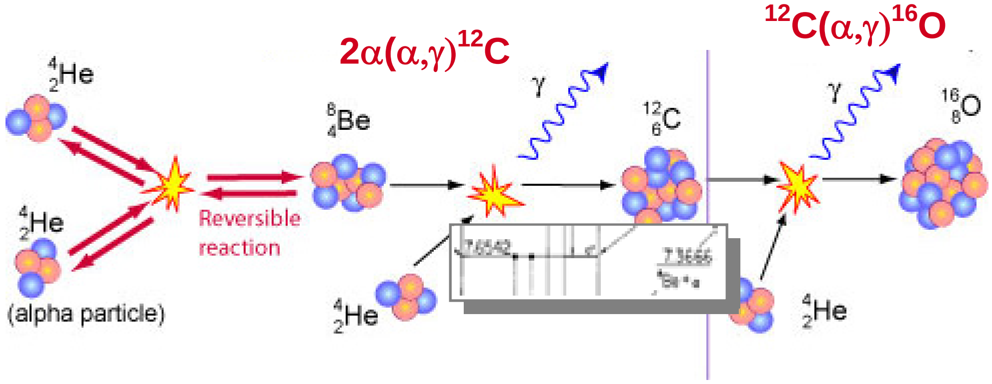


Figure 9. A schematic view of the ^{12}C and ^{16}O production by alpha burning. The $^{8}Be+\alpha$ reaction proceeds dominantly through the 7.65 MeV triple-alpha resonance in ^{12}C (the Hoyle state). Both sub- and above-threshold ^{16}O resonances play a role in the $^{12}C(\alpha,\gamma)^{16}O$ capture reaction. Image courtesy of Commonwealth Scientific and Industrial Research Organisation (CSIRO).

Experimental measurement of these reaction rates at energies relevant for astrophysics (at approximately 300 keV in the center of mass) is impossible with existing techniques because of their extremely small cross-sections. Because of the influence of alpha-cluster resonances in ^{12}C and ^{16}O, theoretical extrapolations of measurements performed at higher energies to the relevant low-energy region have large uncertainties (for recent measurements, see Assuncão et al. 2006). Presently, all realistic theoretical models fail to describe the alpha-cluster states, and no fundamental theory of these reactions exists. Yet, a fundamental theory is needed to determine the rate of the $^{12}C(\alpha,\gamma)^{16}O$ reaction to at least 10% accuracy to fix the subsequent burning stages.

These calculations can be performed by using several independent *ab initio* methods, which will permit results verification and allow for systematic uncertainties to be determined. The methods are as follows: 1) the Green's Function Monte Carlo (GFMC) approach generalized for scattering; 2) the *ab initio* no-core shell model (NCSM) extended by the resonating group method (RGM); and 3) the coupled cluster method. The calculations can proceed in several phases with increasing complexity, and a general picture of the computational requirements for these calculations is shown in Figure 10.

The first phase focuses on the Hoyle state in ^{12}C. This is an alpha-cluster-dominated, 0^+ excited state lying just above the $^8Be+\alpha$ threshold and is responsible for the dramatic speedup in the ^{12}C production rate. The calculation of this state will be the first exact description of an alpha-cluster state. It can be achieved with 10% accuracy of the excitation energy within 3 years using the current petaflop machines, and with 5% accuracy in 10 years using improved Hamiltonians. Calculations of alpha-capture on ^8Be will be performed within the next 5 years. Calculations for ^{16}O, and in particular of the alpha-cluster resonances that impact the $^{12}C(\alpha,\gamma)^{16}O$ reaction, will follow. Finally, the $^{12}C(\alpha,\gamma)^{16}O$ calculations will be completed within a 10-year time frame.

Scientists can reliably estimate the increase in computer resources needed to address the 16O nucleus with GFMC. Presently, the GFMC calculation of the 12C ground state requires approximately 400 peta operations. The Hoyle state will require tens of calculations of the same size. The number of operations will increase by a factor of approximately 1200 for 16O, with the growth provided by the available computing resources increasing from the petascale to the extreme scale.

Currently, it is becoming feasible to calculate, within the NCSM/RGM framework, low-energy nucleon-^{12}C or nucleon-^{16}O scattering with soft NN forces using approximately 1000 cores on present-day machines. The computational demand increases dramatically (a factor of approximately 10^6) with increasing size of the projectile (from a single nucleon to an alpha particle) and by including the NNN interaction. Therefore, this is clearly a problem requiring the extreme scale computation level.

The ground state of ^{16}O can presently be computed within the coupled-cluster method. Here, the inclusion of NNN forces is challenging, and estimates put its computational expense at the petascale. The computation of excited states is an order of magnitude more computationally expensive than this because of the proximity of the scattering continuum; it will be based on a Gamow basis consisting of bound, resonant, and scattering states. The lowest-lying excited 0^+ state in ^{16}O is an alpha-particle excitation and requires the inclusion of four-particle, four-hole cluster configurations. The computational resources required for the calculation of this state are estimated to be at a scale of tens to hundreds of peta-operations and can be performed on current and next-generation machines (up to 20-petaflop machines).

Because of the growth of the number of cores by a factor of approximately 1000, it will not be easy to use an extreme scale computer for these calculations. The present ability in GFMC was obtained by splitting the work on one Monte Carlo configuration among tens of cores (previously just one core was used). For ^{16}O, the work will have to be shared at an even finer level; many cores will have to work on the computation of one wave function and, because of memory limitations, operations involving wave functions stored on different nodes will be necessary.

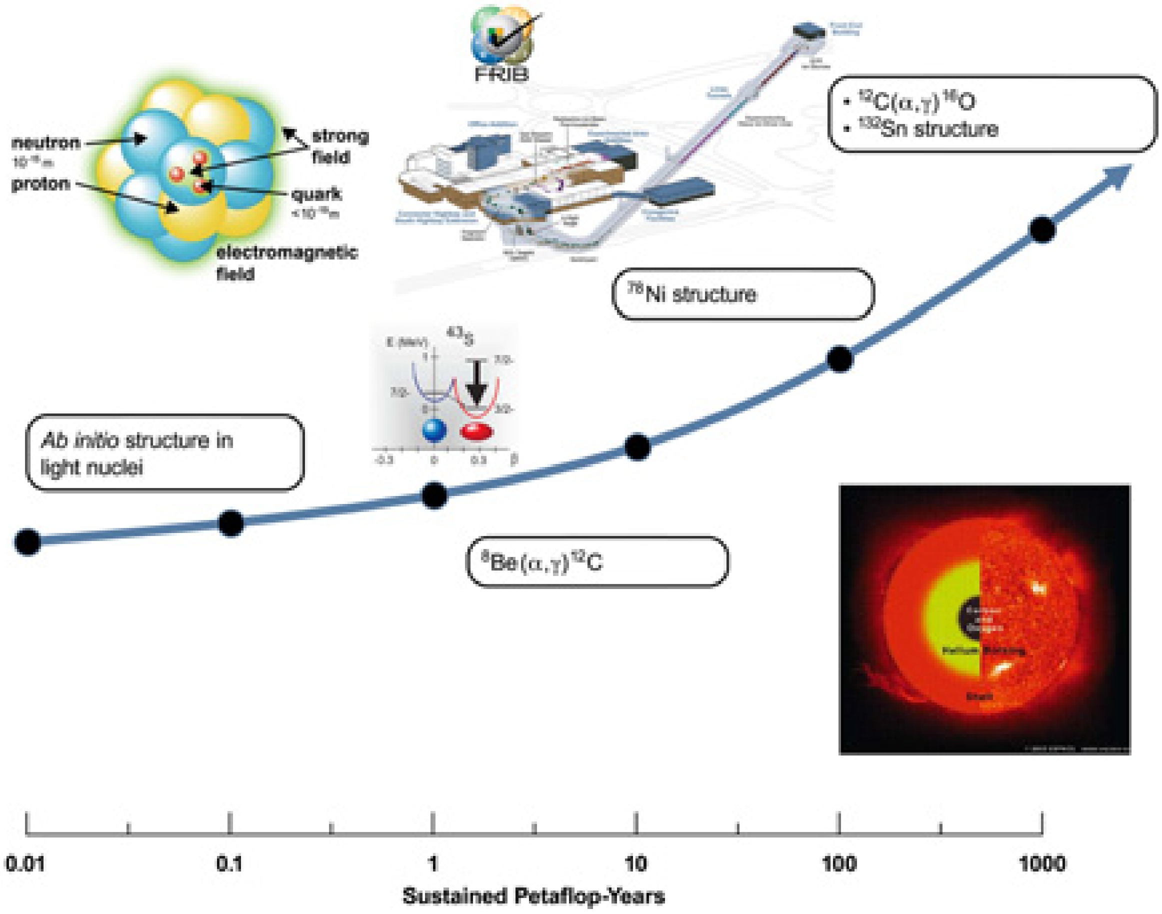


Figure 10. Anticipated highlights for the priority research direction "Reactions That Made Us." Top-middle image courtesy of Michigan State University. Remainder of image courtesy of James P. Vary (Iowa State University).

In the NCSM/RGM, the matrix elements for hundreds of density operators must be calculated. These calculations are both central processing unit and memory intensive. Calculations are presently completed using message-passing interface (MPI) with distribution of the memory allocation. For example, in the calculation of matrix elements of the density operators, the cores are divided into groups, each of which is responsible for computing matrix elements of a subset of operators. This type of parallelization will need to be optimized and propagated to a finer level of distribution among clusters of computing cores in extreme scale machines as the complexity of the task grows rapidly with the mass of the target nucleus, the mass of the projectile (alpha particle), and presence of the NNN force.

Scientific Outcomes and Impacts

The primary outcome of this effort will be a comprehensive understanding of the mechanism behind these two key reactions, and the ability to model the chemical evolution of the universe. Success will permit an accurate determination of the reaction rates at low energies relevant to stellar burning, which are currently limited by large experimental uncertainties. In particular, the uncertainty in the ^{12}C(α,γ)^{16}O reaction rate is currently about 40% (Angulo et al. 1999). By achieving this research goal, scientists will enhance the predictive power of stellar modeling. At the same time, scientists will develop *ab initio* tools to describe the structure of weakly bound nuclei that will be studied at the Facility for Rare Isotope Beams (FRIB) at

Michigan State University. Verification of model predictions by experiments at FRIB will provide necessary checks on the theoretical approaches and the underlying two- and three-body forces used. One computational outcome will be the development of a library for distributing shared-memory work to subsets of nodes within a massively parallel machine.

A successful completion of this program will provide essential input for modeling of stellar evolution and element production. It will provide a firm basis for extrapolating future experimental results. It will guide and be validated by light exotic nuclei studies at FRIB and other exotic beams facilities. Finally, scientists will understand how ^{12}C and ^{16}O, elements critical for life, are produced in nature.

Weak Nuclear Structure—Nuclei as Laboratories for Neutrino Physics

Basic Scientific and Computational Challenges

The neutrino is one of the most elusive particles in the universe and yet one of the most influential. The mass and interaction of the neutrino with other matter are less than a millionth of an electron's—yet neutrinos power spectacular core-collapse supernovae that seed the universe with heavy elements. The fact that neutrinos even *have* a mass is one of the great discoveries of the past 10 years. If the neutrino is its own antiparticle—a so-called Majorana particle—then physics beyond the current standard model of elementary particles must be invoked with consequences impinging upon the matter and antimatter imbalance in the early universe. While the ^{12}C$(\alpha,\gamma)^{16}$O reactions reveal how life can exist, a Majorana neutrino may reveal how matter itself came to exist. However, stringent upper-limits on the existence of neutrino Majorana mass contributions would force scientists to look to other explanations for the fundamental matter-antimatter asymmetry that is observed in the universe today. For recent reviews of current knowledge of neutrino properties, see Avignone et al. (2008), Camilleri et al. (2008), and Haxton (2008).

The primary venue for discerning the fundamental properties of neutrinos is atomic nuclei. A number of experiments are being planned worldwide to determine their properties, but interpreting the results of those experiments will require reliable calculations of nuclear structure and of the interaction between neutrinos and nuclei. Two broad classes of experiments are relevant here, and because of the difficulty in obtaining constraints needed to calibrate these experiments, both require sophisticated theory to be interpreted. As a check on the calculations, as well as a determination of the systematic uncertainty in the theory, scientists will use competing methods to compute the reaction and decay rates.

The first method consists of long-baseline experiments to measure neutrino flavor oscillations, which are sensitive to the differences in neutrino masses, as well as neutrino flavor-mixing angles. Detectors used in these experiments are based on target nuclei such as carbon and oxygen, and it is crucial to understand the neutrino-induced response of these nuclei to fully exploit measurements. At lower energies, neutrino cross-sections on these nuclei also play an important role in late-stage stellar evolution, as well as driving gravitational-collapse supernovae and the creation of heavy elements in supernovae. Reliable calculations require accurate treatment of the strong interaction and a realistic representation of the weak interaction currents. At low energies, the neutrinos couple with nuclei predominantly through so-called "allowed" operators, which are simple, easily calibrated, and cross-checked through experimentation. However, at higher energies—including those relevant to the detectors—scientists also need "forbidden" current operators, which are much more difficult to compare directly to the experiment.

The second experimental methodology consists of neutrinoless double-beta decay (0ν ββ decay) measurements (Vogel 2007). These decays can only occur if the neutrino is its own antiparticle; if so, a neutrino can be emitted and reabsorbed within the same nucleus. If these decays do occur, the lifetime is inversely proportional to the mass of the neutrino and the nuclear matrix element. Unlike 2ν ββ decay, which can be largely calibrated by comparison to ordinary beta decay, the operator responsible for the 0ν ββ-decay nuclear matrix element is neither theoretically simple nor easily constrained by other experiments. Among the specific target nuclei are ^{48}Ca, ^{76}Ge, and ^{130}Te.

The fundamental challenge is to create a computer model of the structure of a nucleus, and then compute the nuclear coupling to neutrinos. Starting from fundamental measurements of NN interactions and using rigorous mathematical methods, effective interactions suitable for use on petascale and extreme scale computers, as well as the weak current operators that describe the interactions of neutrinos with nucleons, will be developed. This will be a significant computational project. A general illustration of the computational requirements for these calculations is provided in Figure 11.

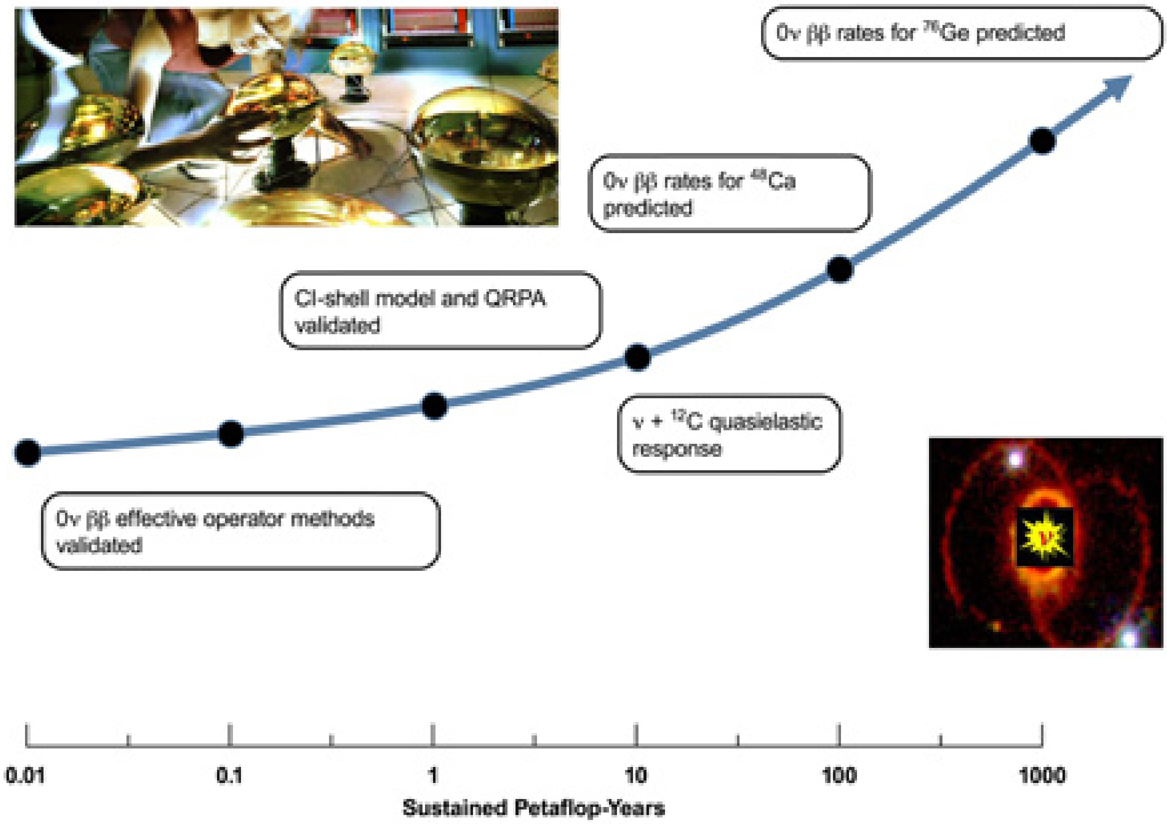


Figure 11. Anticipated highlights for priority research direction “Nuclei as Neutrino Physics Laboratories.” Image courtesy of James P. Vary (Iowa State University).

Two main techniques will need to be extended to use extreme scale computing facilities: quantum Monte Carlo (QMC), primarily for the ν-nucleus cross-sections and configuration-interaction shell model (CI-SM) for the 0ν ββ-decay nuclear matrix element and subsequent lifetime. These have complementary strengths and weaknesses. QMC techniques can use “bare” NN and NNN interactions taken directly from experiment, but QMC cannot yet tackle the heavy nuclei, such as ^{76}Ge or ^{130}Te, relevant to 0ν ββ decay. CI-SM is the technique of choice for detailed spectra and can use arbitrary forms of interactions, not just local potentials—but to fit the problem even on an extreme scale machine, the NN interaction must be renormalized. A third technique, quasi-particle random-phase approximation (QRPA), makes computationally much more modest demands and is thus widely used, but is a more severe approximation.

Each of these techniques faces challenges to be scaled to extreme scale computers. QMC techniques must have actions that are now confined to a single computing core distributed over multiple computing cores. CI-SM will require finding the lowest part of the spectrum of a very large matrix, with dimensions on the order of 1-10 trillion; although the matrix is very sparse, storing the nonzero elements will require petabytes of memory. Furthermore, CI-SM requires vector operations that must communicate across the entire machine. Finally, for CI-SM, scientists must renormalize the experimentally determined NN interaction; this in itself will be a computationally intensive problem because one needs to evaluate the induced NNN interactions in large-basis spaces.

Scientific Outcomes and Impacts

If the neutrino is its own antiparticle, the resulting 0ν ββ-decay lifetime of various nuclei will depend sensitively on the absolute mass of the neutrino. The goal is to compute the 0ν ββ-decay lifetime for nuclei relevant to planned experiments with theoretical uncertainty to 30-50%, cross-checked using competing methods. Accurate estimates of the expected lifetime could affect design of experiments requiring expensive isotopically enriched materials. If a 0ν ββ-decay lifetime is actually measured, these calculations will enable the extraction of the neutrino mass.

Long-baseline oscillation experiments measure the difference between neutrino masses as well as other parameters of the neutrino mass matrix. To correctly interpret the experiments, the ν-nucleus cross-sections will be required to be computed with uncertainties that are less than approximately 20%.

CI-SM can also compute neutrino cross-sections that can provide a cross-check of the QMC and QRPA calculations. As part of this computational project, calculations will be compared using several different methods, usually with the same starting point, from which a systematic uncertainty associated with the calculation can be estimated. One important issue for CI-SM is renormalization, not only of the interaction between nucleons but also between neutrinos and nucleons. Rigorous renormalization methods exist and must be applied consistently to the interaction and the neutrino coupling. Comparisons with results from QMC, where more direct models of the current can be employed, will provide crucial validations.

Currently, significant experimental effort and funds are being invested to answer the above questions, but the experimental results cannot be persuasively evaluated without significant theoretical effort. With extreme scale computing, theoretical studies will provide a basis for reliable interpretation of experiments that explore the properties of neutrinos.

Microscopic Description of Nuclear Fission

Basic Scientific and Computational Challenges

Current understanding of nuclear fission, a fundamental nuclear decay, is still incomplete because of the complexity of the process. Nuclear fission has many societal applications ranging from power generation to national security. In addition, it also plays a role in the synthesis of nuclei in the r-process. Yet, to date, scientists have no microscopic understanding of this complex phenomenon and are unable to make reliable and accurate predictions of fission half-lives, cross-sections, or the distribution of fission products. The ongoing (2009) Scientific Discovery through Advanced Computing Program (SciDAC)-2 Universal Nuclear Energy Density Functional project (Bertsch et al. 2007) and petascale computing resources are opening the way for a comprehensive microscopic description of static properties of atomic nuclei and the fission process.

A promising starting point to obtain a predictive model of nuclear fission is the density functional theory (DFT); see the Nuclear Fission Extreme Scale Computing sidebar. This theory provides the justification for an energy-functional approach to explaining and predicting nuclear structure across the complete table of the nuclides. The accurate nuclear energy functionals currently in use are purely phenomenological and have parameters that are fit to only a subset of nuclear properties. Petascale computing resources and improvements in DFT codes made available through the Universal Nuclear Energy Density Functional project (Bertsch et al. 2007) are opening avenues to the comprehensive microscopic description of complex nuclear phenomena in general, particularly in nuclear fission. Several approaches, each entailing a number of serious computational challenges, can be applied to the description of nuclear fission and will be pursued in this program. The adiabatic approach requires as a first step the determination of the potential energy surface (PES) in a multidimensional space of collective coordinates, which comes from constrained Hartree-Fock-Bogoliubov (HFB) calculations (Warda et al. 2002; Staszczak et al. 2005).

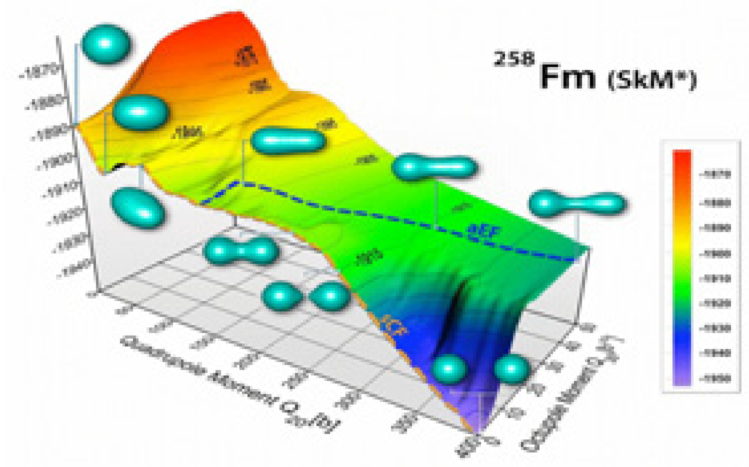
Including all relevant degrees of freedom to obtain a realistic and precise PES is a particularly challenging task. Compounding this issue is the need to evaluate the inertia tensor (Giannoni and Quentin 1980; Warda et al. 2002; Goutte et al. 2005). For this program to succeed, it will be critical to develop suitable algorithms to improve the efficiency of constrained calculations. The imaginary-time HFB (Levit 1980; Arve et al. 1987; Puddu and Negele 1987; Skalski 2008) approach relies on the computation of the full spectrum of dense complex matrices with dimensions that can reach millions. Not all of these matrices are Hermitian. Solving eigenvalue problems of that scale will require an enormous amount of memory, which will create a major bottleneck in the calculations. Heterogeneity in future computer architectures (e.g., use of graphical processing units) will pose another complication. New approaches will therefore be needed to overcome the memory bottleneck in these extreme scale calculations. A general illustration of the computational requirements for these calculations is provided in Figure 12.

Nuclear Fission and Extreme Scale Computing

The United States generates 19% of its electrical power with nuclear power plants; in Europe this figure is 30%. Nuclear power plants produce energy from the fissioning of heavy nuclei. This nuclear fission occurs spontaneously (without an external cause) or when the nuclei are hit by neutrons generated by other fissioning nuclei (induced fission). These are complex processes that are not well understood. This lack of precise knowledge leads to nuclear power plants being built or operated with additional costly safety margins. In principle, increased knowledge of the yields will offer the opportunity to increase, with confidence, the power ratings of existing nuclear reactors and will allow improved design of future reactors.

This situation presents a unique opportunity for nuclear theory to achieve, with the help of extreme scale computers, unprecedented predictive power for both spontaneous and induced fission. The yields under a variety of complex environmental conditions will be investigated in great detail to determine optimum operating conditions. This optimization will account for safety, cost, and efficiency factors at an unprecedented level of accuracy.

The figure below shows an energy surface of the fissioning nucleus ^{258}Fm using one of the currently available approximations. This energy surface determines the fission pathway and the eventual fission energy yield. It is the complexity of this surface—with competing pathways indicated by the dashed lines and superimposed shapes—that makes the problem as challenging as it is, as the yields depend sensitively on subtle differences in the texture of the energy surface. Thus, the predicted dominant fission pathway (the orange dashed line) may not be correct. A more reliable theoretical approach, enabled by extreme scale computers, is needed to make predictions accurate enough to be useful for improved nuclear reactor designs.



Potential energy surface of ^{258}Fm computed with a standard phenomenological energy-density functional. The fission path follows the line of lowest energy while corrections, such as thermal fluctuations and correlations, lead to alternative nearby paths. The blue figures indicate the shapes taken during fission along different paths. Image courtesy of A. Staszczak, A. Baran, J. Dobaczewski, and W. Nazarewicz (Oak Ridge National Laboratory).

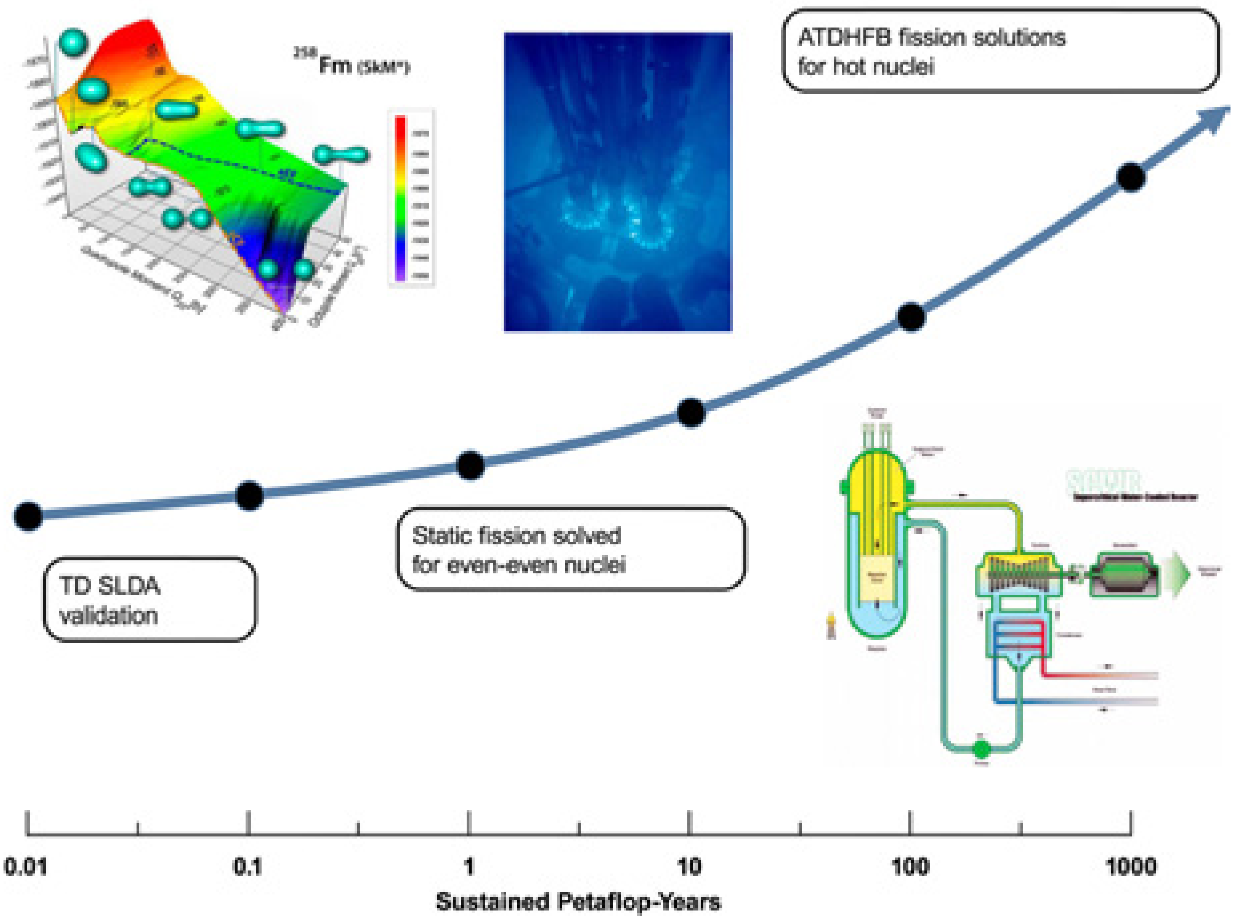


Figure 12. Anticipated highlights for priority research direction “Microscopic Description of Nuclear Fission.” Top-left image courtesy of A. Staszczak, A. Baran, J. Dobaczewski, and W. Nazarewicz (Oak Ridge National Laboratory). Remainder of image courtesy of James P. Vary (Iowa State University).

Fission half-lives are extremely sensitive to the details of the underlying PES and the collective mass tensor. This requires extending the current program of energy density functional development to an unprecedented level of precision because phenomenological energy functionals provide essentially a qualitative description. Novel functionals will typically involve 10-30 parameters to be determined through the global minimization of a large number of observables. Constraining effectively each term of the energy functional requires performing symmetry-unrestricted HFB calculations and possibly adopting techniques beyond the mean-field methods. The dimensionality of the problem, combined with the necessity to reach the global minimum, will probably require massive global optimization algorithms. The phenomenon of fission will be investigated with various microscopic approaches. A first step from current capabilities is to follow the adiabatic time-dependent Hartree-Fock-Bogoliubov (ATDHFB) theory.

At least four degrees of freedom—elongation, mass asymmetry, necking, and triaxiality—must be considered. To attain sufficient mesh refinement, it will be necessary to compute of the order of 100,000-plus constrained HFB calculations for every nucleus.

Two nonadiabatic approaches will also be explored. The first is the instanton method, which relies on determining periodic trajectories for the imaginary time HFB equations. Finding the bounce solutions (periodic instantons) is a difficult numerical challenge. The second approach, applicable in the context of induced fission where the explicit time propagation can be conducted, is a stochastic extension of the time-dependent superfluid local density approximation (TD-SLDA) of DFT. The appeal of this approach, equivalent to the many-body Schrödinger equation, is that two-body and higher correlations become accessible, and dissipation is naturally incorporated into the theoretical description. TD-SLDA has been successfully implemented on current leadership-class super computers, specifically on the Cray XT4 Jaguar at Oak Ridge National Laboratory. A stochastic realization of TD-SLDA will require sufficiently large ensembles of size from thousands to millions of realizations.

Nonadiabatic approaches to spontaneous and induced fission will allow the prediction of the mass and excitation energy distribution of the fission fragments, half-lives, and cross-sections. Beyond the scission point, the emerging fragments start accelerating, and the binding energy of the mother nucleus is converted partially into the kinetic energy of the fragments. At the same time, because strong dissipative processes become increasingly more important, a significant part of the energy is converted into the internal excitation energy of the fragments. The stochastic approach to the time-dependent fission dynamics will allow scientists to calculate these dissipative processes microscopically and predict the nuclear viscosity.

One of the implementation difficulties of stochastic TD-SLDA is the large local memory demand per MPI process and the limited random-access memory/core. Current state-of-the-art calculations prescribe a single MPI process per node so that all the memory in a node is aggregated into a larger, addressable local memory. This approach leaves the other processor cores idle or requires lightweight thread level control within the MPI process to use these cores. Scientists anticipate the need to increase the size of the Hilbert spaces, which will exacerbate this memory-aggregation problem or force the computations out of core—effectively stalling productivity even in the single determinant problems. Programming techniques that go beyond single-node memory aggregation will be refined or developed to satisfy this need. Such developments will also need to include the implicit/explicit use of the extra processor cores.

Scientific Outcomes and Impacts

The computational approach to fission envisioned here, combined with experiments, will provide a predictive framework that may lead to improved nuclear reactor design (AFC 2006). In the area of national security, developing a theoretical description of fission aligns with the goals of the National Nuclear Security Administration Stockpile Stewardship Program, which entails an accurate and complete modeling of the behavior and performance of devices in the nation’s aging nuclear weapons stockpile. Improving the accuracy of that description is central to the continuing process of certifying both the safety and the reliability of the stockpile without resumption of nuclear testing and to reduce the threat from nuclear proliferation.

Of all the various nuclear decay processes, nuclear fission—important in the r-process nucleosynthesis, in the modeling of reactions relevant to the advanced fuel cycle for next generation reactors, and in the context of national security—is among the most difficult to tackle. It is a quantum many-body tunneling problem whose typical time-scale changes by orders of magnitude when adding just a few nucleons. The microscopic theory of nuclear fission, rooted in internucleon interactions, still provides a particularly difficult challenge.

The ultimate outcome of the nuclear fission project is a treatment of many-body dynamics that will have wide impacts in nuclear physics and beyond. The computational framework developed in the context of fission will be applied to the variety of phenomena associated with the large amplitude collective motion in nuclei and nuclear matter, molecules, nanostructures, and solids.

Physics of Extreme Neutron-Rich Nuclei and Matter

Basic Scientific and Computational Challenges

Understanding neutron-rich nuclei is vital to discovering the origin of heavy elements (NAP 2003) and defining the properties of neutron-star crusts (Ravenhall et al. 1983). About half of the elements from iron to uranium are produced via successive steps consisting of neutron capture followed by beta decay (the r-process). The structure of neutron-rich nuclei determines the radiative capture cross-sections and beta-decay rates that are critical inputs to r-process nucleosynthesis calculations. The regions around the supposed doubly magic nuclei ^{60}Ca, ^{78}Ni, and ^{132}Sn are of particular interest as they could be waiting points in the r-process. The existence and location of shell closures affect the r-process path as illustrated in Figure 13, where the r-process path is schematically drawn assuming shell closures at the traditional magic numbers. The dynamic and static properties of neutron star crusts determine neutron-star cooling and gravity wave emissions from neutron star mergers.

Unfortunately, present understanding of neutron-rich nuclei is very limited, and extrapolations based on current theoretical models are not reliable. First, the extreme isospin of neutron-rich nuclei magnifies unconstrained properties of the effective nuclear interaction. Second, the proximity of the neutron drip line dramatically increases the number of relevant many-body configurations, including the continuum, and makes accurate computations impossible at the present time. In the coming decade, progress towards the most neutron-rich nuclei will be made with both theory and experiment. The future FRIB at Michigan State University will provide experimental data for selected nuclei along the r-process path. These data will calibrate and validate theoretical methods which, with the advent of exascale computing facilities, will enable accurate theoretical predictions for extremely neutron-rich nuclei (see Figure 13).

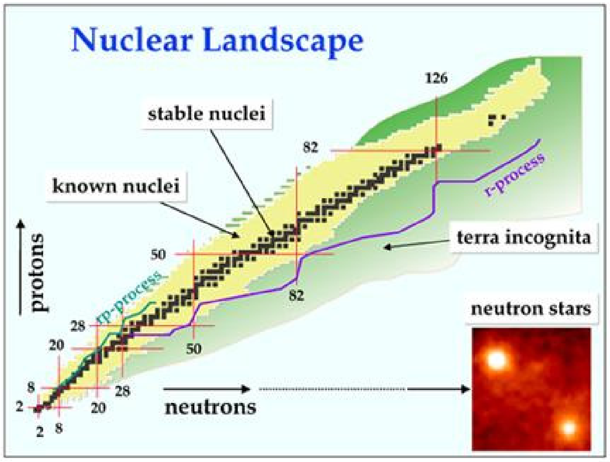


Figure 13. The chart of atomic nuclei displays the speculated r-process path of rapid neutron capture across neutron-rich nuclei. The structure of extremely neutron-rich nuclei is essential input to understand the origin of heavy elements as well as the cooling properties of and the gravity wave emission from neutron star crusts. Image courtesy of James P. Vary (Iowa State University).

The *ab initio* nuclear-structure program aims at building nuclei starting with nucleon degrees of freedom and their mutual interactions. Extending this program to neutron-rich nuclei in the ^{60}Ca, ^{78}Ni, and ^{132}Sn regions and towards the neutron drip lines poses great theoretical and computational challenges. A general picture of the computational requirements for these calculations is illustrated in Figure 14.

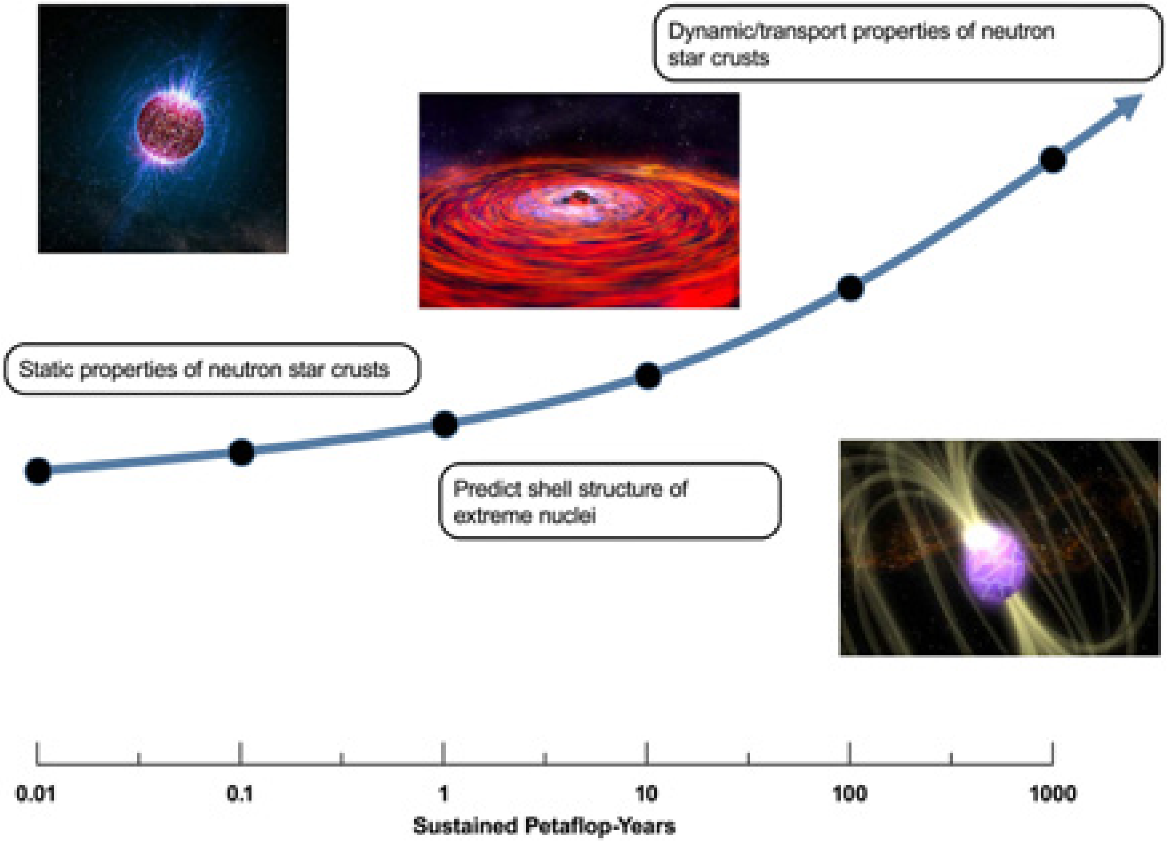


Figure 14. Anticipated highlights for priority research direction "Physics of Extreme Neutron-Rich Nuclei and Matter." Image courtesy of James P. Vary (Iowa State University).

Closed-shell nuclei and their neighbors are of particular interest for both experimental and theoretical research because they form the pillars of understanding and modeling for atomic nuclei.

The effective nuclear Hamiltonian, including the isospin dependence of the effective nuclear two- and many-body forces, is under intense investigation and will become far more precise in the next 3 years. These interactions will be employed with state-of-the-art nuclear-structure tools such as configuration interaction (Lisetskiy et al. 2004), the coupled-cluster method (Hagen et al. 2008), the nuclear density-functional theory (Bertsch et al. 2007), and Monte Carlo techniques (Chang et al. 2004) to calculate the properties of closed-shell nuclei and their neighbors. Of particular interest are the regions around the neutron-rich nuclei ^{78}Ni and ^{132}Sn. These calculations will predict the evolution of shell structure and will explore the drip line and the limits of nucleonic matter. For the understanding of neutron star crusts, the transport properties of systems composed of extremely neutron-rich nuclei and a surrounding neutron gas must be computed.

Calculations of nuclei in the ^{78}Ni region and of static properties of matter in the crust of a neutron star require a facility with tens of petaflop-years of capacity, while computations of nuclei in the ^{132}Sn region and transport properties of crust matter require a facility with hundreds of petaflop-years capacity. Scientists assume the program will be balanced such that investments in computational hardware and software are matched with investments in theory and personnel.

Scientific Outcomes and Impacts

Calculations of nuclei in the ^{78}Ni region and of static properties of matter in the crust of a neutron star require a facility with tens of petaflop-years of capacity, while computations of nuclei in the ^{132}Sn region and transport properties of crust matter require a facility with hundreds of petaflop-years capacity. Scientists assume the program will be balanced such that investments in computational hardware and software are matched with investments in theory and personnel.

These extreme scale computations will allow scientists to determine the limits of nuclear stability—that is, how many neutrons or protons can be bound in a given nucleus. This theoretical effort will have a major impact upon the experimental program to search for these limits at research facilities such as the FRIB. The combination will allow scientists to model some of the most exotic environments in astrophysics, and understand and model the chemical evolution of the universe.

In the crust of neutron stars, neutron-rich nuclei coexist with a surrounding gas of neutrons; the structure and dynamic properties of this unusual matter will be calculated using advanced Monte Carlo methods. In turn, it will be possible to interpret the wealth of astronomical data obtained from visual, x-ray, and gamma-ray telescopes. This will allow scientists to infer details of the nature of these sites and the processes (such as potentially gravitational wave emission) that occur there. The major computational challenge in these efforts is to develop and implement scalable algorithms for the strongly interacting inhomogeneous quantum many-body problem.

An important complement to the work described here will be the experimental program conducted at the FRIB (NRC 2006). The theoretical and computational tools envisioned above will provide an essential framework to interpret FRIB experimental data and will eventually guide the future experimental program. In turn, FRIB data will be essential to verify *ab initio* calculations and calibrate the nuclear many-body Hamiltonian.

Computations of neutron star matter, when combined with observations, will provide information about nucleonic matter at supernuclear densities. The interpretation of observations of isolated, cooling neutron stars require an accurate microscopic understanding of superfluidity and neutrino emission processes in neutron-rich matter. Similarly, observations of gravity waves with the advanced Laser Interferometer Gravitational-Wave Observatory and future detectors will, when combined with a realistic description of the neutron star matter, allow scientists to infer the mass and radius of a neutron star. Combined observations of multiple neutron stars will produce definitive constraints on the equation of the state of the densest matter in the universe.

CONCLUSIONS

Nuclear structure and reaction calculations have consistently made use of available state-of-the-art computers. With steady improvements in nuclear models enabled by computing advances, scientists have reached the ability to make precise predictions of the properties of light nuclei. Extreme scale computing resources will enable such calculations across the periodic table. Besides increasing current understanding of fundamental nuclear physics, these calculations will be of great benefit to other areas including astrophysics, nuclear reactor design, and stockpile stewardship. Progress will rely on continuing a balanced research program, as recent examples illustrate:

- Nuclear physics has benefited from access to the most powerful computers available through grants of time at major computing facilities. The Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program is an excellent example.

- Collaboration between nuclear physicists, applied mathematicians, and computer scientists have proven exceptionally fruitful under the Scientific Discovery through Advanced Computing program. There are many formidable obstacles to the efficient use of extreme scale computers.

Table 2 provides an outline of the milestones for the work described in this section. Provided that the computational resources become available for research in nuclear structure and nuclear reactions at the anticipated scales, the forefront research that will be conducted are provided as milestones.

Table 2. Milestones for Nuclear Structure and Nuclear Reactions

Scale	**Milestone**
>1 Petaflop-year	• Static description of fission for cold even-even nuclei in limited deformation spaces • Time-dependent SLDA • Compute effective transition operators for $0\nu\ \beta\beta$ decay using same method as effective interaction • Side-by-side comparison of $0\nu\ \beta\beta$ decay in CI-shell model and QRPA using same model space/Hamiltonian • Hoyle state in ^{12}C
>20 Petaflop-years	• ATDHFB description of fission in large deformation space • Partial implementation of stochastic TD-SLDA (reduced ensemble) • Moments of quasi-elastic response for ν-^{12}C • Calculations of $0\nu\ \beta\beta$ decay in ^{48}Ca • Tests of current operator; compare methods against experiments • Scattering and capture of $\alpha + {}^{8}$Be • ^{78}Ni structure • Static properties of neutron star crust
>100 Petaflop-years	• ATDHFB description of fission in hot nuclei • Full implementation of stochastic TD-SLDA • Moments of quasi-elastic response for ν-^{16}O • Initial estimates of π-production cross-sections in ν-^{12}C and ν-^{16}O • Converged excitation spectrum of ^{16}O
>1 Exaflop-year	• Complete microscopic description of nuclear fission for odd nuclei such as ^{235}U • Scattering and capture of $\alpha + {}^{8}$Be • ^{132}Sn structure • Calculations of $0\nu\ \beta\beta$ decay in ^{76}Ge • Dynamic/transport properties of neutron star crust