The UNEDF Project

Overview

A new era has dawned for nuclear structure and reaction theory. Renewed interest in the physics of nuclei is fueled by experiments at rare isotope beam facilities, which explore new regions of exotic nuclei; by astrophysical observations and simulations, which require controlled extrapolations of the nuclear equation of state; by the use of nuclei in experiments on fundamental symmetries, which rely on robust nuclear structure information; and by nuclear energy and security needs, which include predictions of reaction cross-sections and fission fragment properties. The UNEDF collaboration of nuclear theorists, applied mathematicians, and computer scientists is addressing this broad spectrum of physics through a comprehensive study of all nuclei, based on the most accurate knowledge of the strong nuclear interaction, the most reliable theoretical approaches, the most advanced algorithms, and extensive computational resources.

UNEDF stands for "Universal Nuclear Energy Density Functional." The mission of this five-year SciDAC ("Scientific Discovery through Advanced Computing") project is three-fold [1]:

- First, to find an optimal energy density functional (EDF) using all our knowledge of the nucleonic Hamiltonian and basic nuclear properties.
- Second, to apply the EDF theory and its extensions to validate the functional using all the available relevant nuclear structure and reaction data.
- Third, to apply the validated theory to properties of interest that cannot be measured, in particular the properties needed for reaction theory.

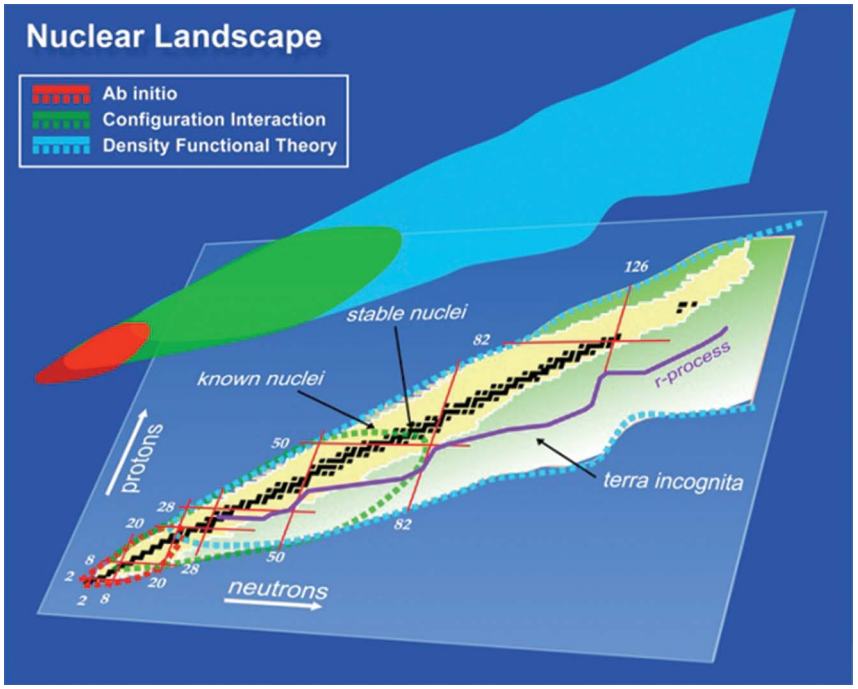

Figure 1. *Table of the nuclides and the scope of theoretical methods to describe it.*

The long-term vision is to arrive at a comprehensive and quantitative description of nuclei and their reactions. UNEDF is striving to replace phenomenological models with a well-founded microscopic theory that delivers maximum predictive power with quantified uncertainties.

By nuclear theory standards, UNEDF is large: it involves over 50 researchers from 9 universities and 7 national laboratories. Annually, it provides training to about 30 young researchers (postdocs and students). UNEDF is like a large experimental collaboration with multiple facets to its research goals.

The SciDAC model (http://www.scidac.gov) has led UNEDF members to form partnerships in which applied mathematicians and computer scientists work collaboratively with physicists to develop the required advanced algorithms and tools. At the same time, the project has catalyzed new cross-cutting physics collaborations, which include nuclear theorists around the world as international partners. The scope of the UNEDF project is large. Here we present brief snapshots that highlight the collaborative effort, the progress made, and the future

prospects; more details and references can be found at the unedf.org website.

Forging New Connections

The playing field for UNEDF is the nuclear landscape of Figure 1. The sizable area marked "terra incognita," which is populated by unstable isotopes with large neutron fractions, is of particular interest. Above the table of nuclides are shown three broad classes of theoretical methods, which are also used in atomic and condensed matter physics. The bulk of the nuclides are covered by Density Functional Theory (DFT), which provides the theoretical underpinning and computational framework for building a nuclear EDF. By enhancing and exploiting the overlaps with *ab initio* and configuration interaction (CI) approaches, we are constructing and validating a universal EDF informed by microscopic interactions as well as experimental data.

The UNEDF components and paths between them are shown in the UNEDF strategy diagram in Figure 2. New interconnections and collaborative efforts within and across the boundaries have become indispensible. By necessity the developments have largely occurred in parallel; in subsequent sections we give examples of the interplay as UNEDF has worked to fulfill its mission.

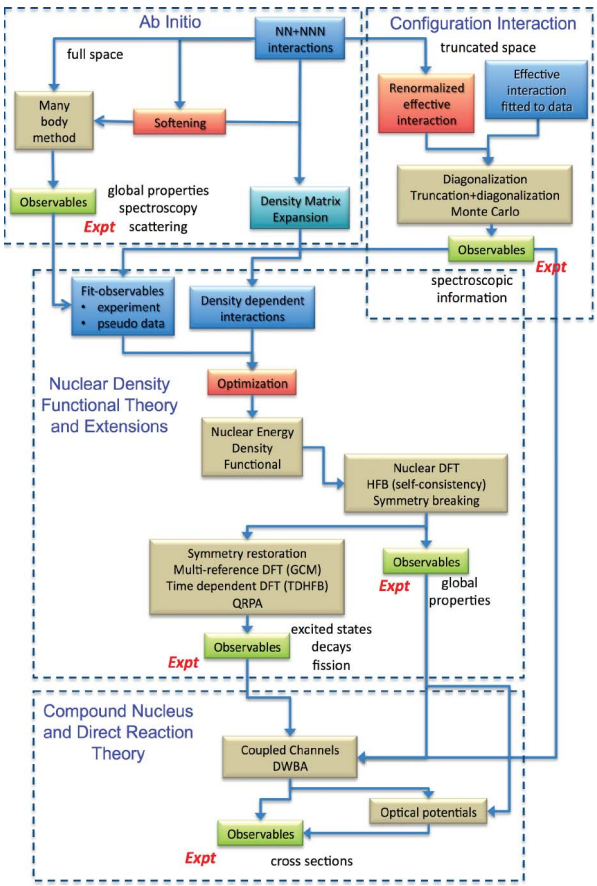

Figure 2. *UNEDF project scope and various active interconnections.*

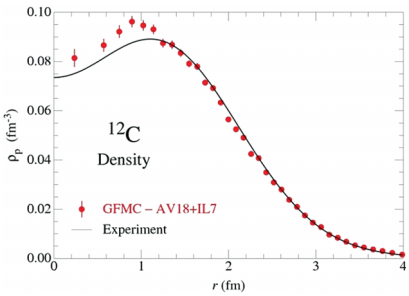

Figure 3. *Carbon-12 density calculated with GFMC using the ADLB library [2].*

Enhancing *ab initio* Structure Calculations

Direct connections of the EDF to microscopic nuclear interactions require improving the scope and accuracy of *ab initio* methods. Major advances in *ab initio* nuclear structure calculations under UNEDF have focused on improving the effective use of high performance computing—especially the efficient scaling to very large numbers of parallel processors.

A prime example of UNEDF synergy has been the development of the Asynchronous Dynamic Load Balancing (ADLB) software library by using Green's Function Monte Carlo (GFMC) calculations as a test bed. Load balancing means ensuring that every parallel processor is used effectively; it is essential to optimal scaling. The ADLB library has enabled GFMC to run efficiently on over 100,000 core processors [2].

A major test case is the ^{12}C energy and proton density (Figure 3), which is also a proof of principle whether a microscopic nuclear Hamiltonian calibrated to few-body nuclei can successfully predict the energy and

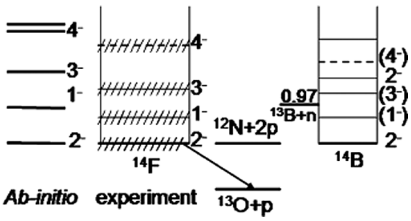

Figure 4. *Theoretical ("ab-initio") spectrum from NCFC compared to experimental results for ^{14}F [6].*

density distribution of larger nuclei. Unlike quantum chemistry, where the Coulomb interaction is firmly established, the input nuclear Hamiltonian must be tested and improved as needed even as the nuclear DFT itself is developed. The GFMC/ADLB combination predicts the ^{12}C experimental energy and radius to within 1%, which is a compelling validation [2]. The next targets are excited states in ^{12}C, including the famous Hoyle state.

Configuration interaction *ab initio* methods use basis expansions and require the (partial) diagonalization of extremely large matrices. These are known by various names according to details of the implementation, including No-Core Shell Model (NCSM) and No-Core Full Configuration (NCFC) methods (see accompanying article by Barrett, Navratil, and Vary). Improvements by applied mathematicians working with nuclear theorists on eigensolvers, data structures, and new combinatorial algorithms have resulted in substantial performance gains for CI codes such as MFDn, allowing efficient scaling to large numbers of processors [3].

An example of what this scaling enables is the recent prediction of the ^{14}F mass and excitation spectrum in advance of the experimental measurements, which meant solving a Hamiltonian matrix of dimension 2 billion using 30,000 cores [4] (Figure 4). The predictions and measurement agree within the combined experimental and theoretical uncertainties (not shown). Another recent application involving many UNEDF members is an explanation of the anomalously long lifetime of ^{14}C by identifying the critical role of the three-nucleon (NNN) force in its beta decay [5]. We can look forward to many such confrontations of theory and experimental data from rare isotope facilities.

CI codes used within the UNEDF project apply both fully microscopic and phenomenological shell model approaches, and use different algorithms. But common computational issues are leading UNEDF scientists to develop the Leadership Class Configuration Interaction (LCCI) framework to unify, preserve, and disseminate valuable CI codes and resources. This will provide a user-friendly environment for researchers to download and run state-of-the-art CI codes needed for theoretical predictions as well as experimental analysis.

To make *ab initio* methods more convergent, it can be advantageous to "soften" the initial Hamiltonian by decoupling low-momentum and high-momentum parts. Renormalization group (RG) methods achieve this decoupling by evolving interactions in small steps. The resulting two-nucleon (NN) potentials are very convergent but the initial NNN interaction is also changed. Until recently a consistent NNN evolution had not been achieved. But a UNEDF collaboration successfully combined Similarity RG (SRG) evolution methods with NCSM technology. Figure 5 illustrates the improved convergence with the evolved three-body force [7]. These SRG interactions are now being applied to larger nuclei and in reaction calculations.

The interactions used in the ^{14}C calculations and the SRG evolutions are systematically constructed (outside of UNEDF) using chiral effective field theory (EFT). UNEDF members have demonstrated that the coupled-cluster (CC) *ab initio* method can be used to accurately calculate closed-shell medium-mass nuclei such as ^{40,48}C with chiral EFT two-body interactions (or RG-softened versions) as well as proton halo nuclei like ^{19}F [8]. The CC formalism has been extended to include NNN forces and their inclusion in calculations of the heavier nuclei will break new barriers. A recent development is the first in-medium SRG diagonalization of closed-shell nuclei such as ^{40}C with accuracy comparable to CC results [9].

Microscopic Inputs to a Nuclear EDF

As implied by the diagram in Figure 2, multiple inputs and constraints are being used to build a universal nuclear EDF. The foundation is

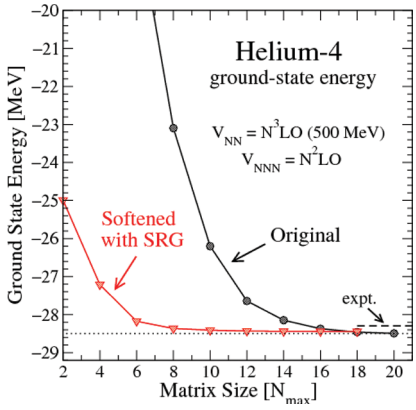

Figure 5. *Improved convergence in helium-4 using Similarity Renormalization Group (SRG) interactions, including an evolved NNN force [7].*

provided by EDF's of the Skyrme type, whose phenomenological successes have been extensively benchmarked as part of the UNEDF project. *Ab initio* approaches can provide "control-data" to constrain more general functionals as well as to directly motivate novel density and momentum dependences.

Ab initio calculations can be used to test candidate EDF's even for systems not available in the laboratory. Current functionals are least constrained in their isovector dependence, so a system of neutron drops would be ideal, but the neutrons would not be self-bound. However, DFT says that the functional should work with a theoretical external potential, which can be used to "trap" neutrons and adjust their density profiles. UNEDF calculations applying GFMC (up to 16 neutrons) and Auxiliary Field Diffusion Monte Carlo (AFDMC, up to 54 neutrons) methods to generate such control-data are being used to probe deficiencies of conventional EDF parameterizations and to improve them. In Figure 6 such a comparison for radii is shown for the original SLy4 functional and an adjusted version [10]. The neutron drop results are validated by also calculating with NCFC and with other Hamiltonians.

A parallel effort uses trapped neutron systems as well, but tests *ab initio* DFT methods against full calculations based on the same Hamiltonian. A hybrid approach uses chiral EFT for the long-distance (pion range) NN and NNN interactions that can be translated into novel density dependences through a revitalized incarnation of the density matrix expansion. These new functionals are being optimized and tested using the extensively developed EDF infrastructure [11].

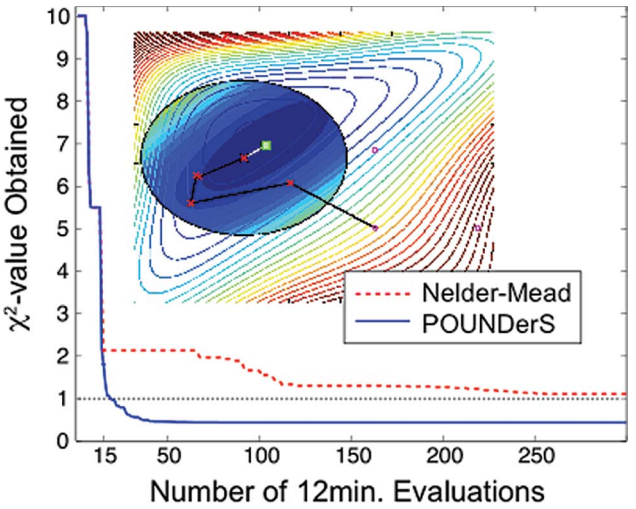

Figure 7. *Greatly improved converg-ence is seen with the novel optimi-zation algorithm POUNDerS [13].*

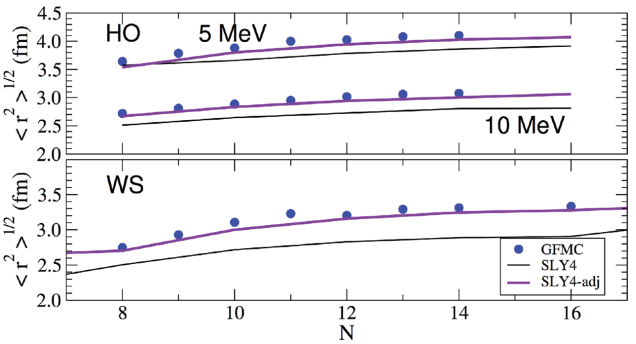

Figure 6. *GFMC calculations of the radii of N neutrons in harmonic oscillator (HO) and Woods-Saxon (WS) traps, which are used to adjust the SLy4 Skyrme functional [10].*

Enhancing and Extending DFT Infrastructure

Much effort in the UNEDF project has been devoted to developing and improving the algorithmic and computational infrastructure needed to optimize candidate EDF's and to apply symmetry restoration required for accurate calculations of self-bound nuclei. Performance optimization of DFT-solver codes has enabled large-scale mass table calculations on 9,060 processors for 840,000 configurations in 9,000 nuclei in a 12-hour run. The MADNESS (Multiresolution ADaptive NumErical Scientific Simulation) framework is an example of applying state-of-the-art applied mathematics technology to create a DFT solver with an adaptive pseudo-spectral method [12].

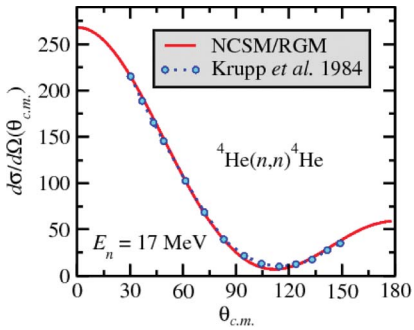

Figure 8. *Calculated [14] NCSM/RGM cross-section for 17 MeV neutrons on ^{4}He compared to experiment.*

Another example is the optimization algorithm POUNDerS, developed by a UNEDF team of applied mathematicians, which yields dramatic computational savings over alternative optimization methods, as seen in Figure 7. Using the UNEDF Experimental Database and the optimized solver HFBTHO, the Skyrme SLy4 functional was re-optimized using the derivative-free POUNDerS algorithm. The resulting parameterization UNEDF0 sets a solid baseline of nuclear ground-state properties to compare with future functionals [13]. New hybrid functionals with microscopic input from chiral EFT [11] are being optimized using this approach.

A New Era for Reaction Theory

One of the principal aims of the UNEDF project is to calculate reliable reaction cross-sections for astrophysics, nuclear energy, and national security, for which extensions of standard phenomenology is insufficient. The interplay of structure and reactions is essential for a successful description of exotic nuclei as well. Such interplay is characteristic of the *ab initio* no-core shell model/resonating-group method (NCSM/RGM), which treats bound and scattering states within a unified framework using fundamental interactions between all nucleons. A quantitative proof-of-principle calculation of this approach is shown in Figure 8 [14]. A wide range of applications is now possible including ^{3}H(d,n)^{4}He fusion, the ^{7}Be(p,γ)^{8}B reaction important for solar neutrino physics, and many more to come.

Neutron reactions on heavier nuclei are being modeled using DFT results to predict not just bound states, but also scattering states for nucleons. Microscopic calculations of reaction cross-sections for nucleon-nucleus scattering have been performed by coupling the elastic channel to all particle-hole excitations in the target, and also with one-nucleon pickup channels. Target excitations were described in a random-phase (QRPA) framework using a Skyrme functional and the resulting transition potentials were used in large coupled-channel calculations. As illustrated in Figure 9, the calculated reaction cross-sections agree very well with experimental data, and also with predictions of global optical potentials where data are not available. For the first time, the observed absorption in the reaction cross-section can be accounted for by explicit channel coupling [15].

Another important capability for reactions is the calculation of level densities. A new proton-neutron algorithm for the parallel JMoments code was recently designed and implemented, which improved its scalability to tens of thousands of cores, and increased its overall performance by a factor of more than 10,000. This development opens the door to calculating accurate nuclear level densities and reaction rates for a large class of nuclei [16].

Cold Atoms as a Testing Ground

UNEDF theorists have made important contributions to the study of strongly coupled superfluid systems such as ultracold Fermi atoms, which show many similarities to the cold nuclear matter found in the crust of neutron stars. Cold atoms make excellent laboratories for testing and improving the computational methods to be used for nuclei; indeed, GFMC and AFDMC calculations from UNEDF scientists have set the standard for numerical results of the unitary gas at zero temperature.

Cold atom systems allow predictions of superfluid DFT that are testable against experiment. An example is shown in Figure 10, where a nuclear DFT code adapted to the antisymmetric superfluid local density approximation (ASLDA) [17] is applied to strongly interacting spin-imbalanced atomic gases in extremely elongated traps. Families of Larkin-Ovchinnikov (LO) states with prominent transversal oscillations of the pairing potential are predicted, as indicated by the radial alignment of

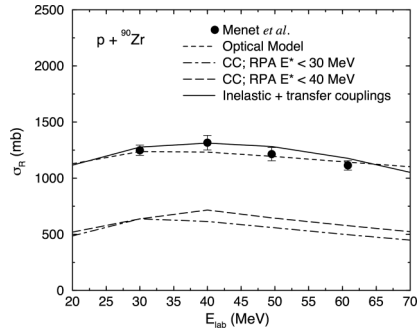

Figure 9. *Calculated reaction cross-sections for protons on ^{90}Zr as a function of incident energy compared to data. The solid line is the full calculation while the dashed curve is from the global optical potential [15].*

nodes, coexisting with a superfluid state having a smooth pairing potential [18].

A recent major UNEDF achievement is the full implementation of the time-dependent superfluid local density approximation (TDSLDA) on a 3D spatial lattice [16]. Unlike many past approaches, matrix operations are not needed and the size of the basis set it can handle is 2–3 orders of magnitude larger than previous methods, with an implementation that can use 97% of the Jaguar supercomputer at Oak Ridge National Lab. These codes are being used to simulate the unitary gas (e.g., vortex formation) [16] and a heavy nucleus under the action of various external fields. While still exploratory, these first-time simulations of this kind for fermion superfluids serve as proof of principle for an eventual treatment of fission.

Quality Control in UNEDF

Integral to the UNEDF project is the verification of methods and codes, the estimation of uncertainties, and assessment. Methods to verify and validate include the cross-checking of different theoretical methods and codes (e.g., GFMC vs. AFDMC vs. NCFC), the use of multiple DFT solvers with benchmarking, and the confrontation of *ab initio* functionals with *ab initio* structure using the same Hamiltonian. Uncertainty quantification follows using tools for correlation analysis to estimate errors and significance. A new way to estimate theory error bars is to use multiple RG-evolved Hamiltonians and examine the cutoff dependence of calculated observables.

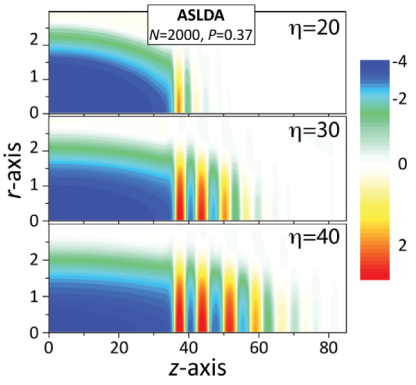

Figure 10. *Pairing potential of polarized Fermi gas in an extremely elongated trap with different aspect ratios [18] calculated using nuclear codes developed for fission.*

The UNEDF assessment component has required the development and application of statistical tools. Particularly important for potential experiments is the analysis of experimental data significance. For example, the sensitivity of two optimized functionals to particular data is shown in Figure 11 [13]. Statistical tools are used to deliver uncertainty quantification and error analysis for theoretical studies as well as for the assessment of new experimental data. Such technologies are virtually unknown in the low-energy nuclear theory community at present, but are essential as new theories and computational tools are applied to entirely new nuclear systems and to conditions that are not accessible to experiment.

Outlook

These brief highlights represent only part of the development within the UNEDF project and new results are appearing steadily. Please visit unedf.org to find further summaries, updates, and references. While UNEDF is in the final year of its 5-year term, its impact will be ongoing. Indeed, UNEDF has created

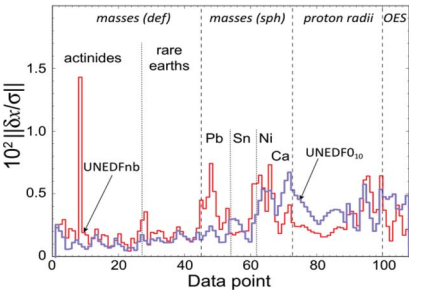

Figure 11. *The sensitivity of candidate EDF fits to particular data can be assessed. See Ref. [13] for details.*

infrastructure and interconnections that are only just beginning to be fully exploited. An important spin-off for the future has been the training of young scientists in the new developments of low-energy nuclear theory.

The worldwide impact of the UNEDF collaboration, which is unique in the field of low-energy nuclear physics in its scope, size, and structure, was evident at the 2010 INPC meeting in Vancouver, where UNEDF highlights were quoted in several plenary talks. While based and funded in the United States, UNEDF collaborates closely with foreign efforts and individual scientists sharing similar fundamental science goals. Such collaborations include joint software developments and benchmarking, and representatives of international collaborating projects attend the UNEDF annual meetings. These UNEDF activities have had positive leveraging effects on our foreign partners, including the joint UNEDF-JUSTIPEN and UNEDF-FIDIPRO efforts and a new initiative involving low-energy nuclear theory in France, FUSTIPEN.

High performance computing provides answers to questions that neither experiment nor analytic theory can address; hence, it becomes a third leg supporting the field of nuclear physics. A series of meetings on extreme scale computing in 2009 identified several major research thrusts that have a strong foundation in UNEDF achievements [20]. These include pathways to a quantitative microscopic description of fission, computing properties of nuclei that determine the r-process nucleosynthesis path in stars, computing properties of nuclei used in double-beta decay experiments and neutrino-nucleus cross-sections for modeling supernova explosions, and computing the triple-alpha process that produces ^{12}C, the nucleus at the core of organic chemistry and thus life forms. The future prospects are bright!

Acknowledgments

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