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Project Abstract: Atomic nuclei are strongly interacting, quantum many-body systems displaying fascinating properties. They exhibit emergent phenomena characteristic of large complex systems while at the same time being laboratories of most fundamental laws of nature. The goal of the NUCLEI project is to use advanced applied mathematics, computer science, and physics to accurately describe the atomic nucleus in its entirety. In this proposal, we will build on previous successes to treat a wide range of nuclei and study their electroweak transitions and reactions important in both terrestrial experiments and astrophysical environments. We will employ advanced quantum many-body methods, ranging from ab initio methods such as the nuclear shell model, coupled cluster, in-medium similarity renormalization group, and quantum Monte Carlo, to the density functional methods used to treat complex nuclei and inhomogeneous nucleonic matter. We will develop advanced applied mathematics and computer science to allow the resulting algorithms to perform efficiently on the fastest available computers, optimize the input interactions and operators, and provide reliable uncertainty quantification of the results. The input interactions and currents developed by us will interface with the multinucleon lattice QCD results as these become available. Such a coupling is critical for providing complete understanding of nuclei and their reactions rooted in the theory of strong interactions; in the long term, this will result in unifying the fields of nuclei and hadrons. Our computational studies will impact experimental programs, including existing low-energy nuclear physics facilities, the future Facility for Rare Isotope Beams, Jefferson Laboratory, and neutrino experiments.

Final Report

Summary: This Report summarizes the accomplishments of NUCLEI researchers at The University of Tennessee, Knoxville (UTK) and those supported via subcontracts at the University of North Carolina at Chapel Hill (UNC) and Iowa State University (ISU). Dr. Jon Engel and Dr. James Vary are the Co-Principal Investigators at UNC and ISU, respectively.

The SciDAC-4 NUCLEI collaboration had the goal to advance the computation of atomic nuclei and to make reliable predictions including uncertainty estimates for observables of interest. These goals were achieved by developing improved nuclear interactions and currents that are input to the computations, and by advancing the algorithms and techniques used for computing nuclear observables of interest. The computed results advanced our understanding of how nuclei work; they helped to guide and interpret experiments at existing low-energy nuclear physics facilities, the Facility for Rare Isotope Beams, Jefferson Laboratory, and neutrino experiments. In addition, predictions were made that await confrontation with experimental results. The results have been published in many papers, see https://www.osti.gov/search/semantic:DE-SC0018223. The main achievements are described in what follows.

Nuclear interactions: The NUCLEI researchers helped developing semi-local interactions based on effective field theories of quantum chromodynamics, the basic theory of the strong nuclear force. They also adjusted parameters of nuclear interactions that include the Delta isobar as a degree of freedom for a more accurate description of the binding energies of nuclei. The resulting interactions and currents were the starting point of many computations that helped to interpret and guide experiments.

Neutron skins: Heavy nuclei contain more neutrons than protons and a neutron skin is formed at their surface. The thickness of this skin contains information that helps to constrain the mass-radius relationship of neutron stars. NUCLEI researchers computed the neutron-skin thickness in the heavy nucleus ^{208}Pb and showed that consistency with data from nucleon-nucleon scattering does not permit thick skins. The theoretical results is smaller, and more precise, than a recent extraction via parity-violating electron scattering at Jefferson Lab. The dipole polarizability is strongly correlated with the neutron-skin thickness. For these reasons, NUCLEI researchers also computed dipole polarizabilities of nuclei such as ^{40}Ca and found agreement with available data.

Optical potentials and nucleon-nucleus scattering: The scattering of nucleons off atomic nuclei can be described using so-called optical potentials. Based on accurate nuclear interactions and ground-state densities, one can construct such potentials in a parameter-free way and thereby tie nucleon-nucleus scattering back to the properties of the strong nuclear force. NUCLEI researchers constructed optical potentials for the description of elastic nucleon-nucleus scattering. This is an important first step towards the inclusion of inelastic effects. Progress in this direction is relevant because many experiments probe the structure of nuclei by scattering nucleons off them.

Beta decays: Most nuclei created in the laboratory are short-lived and decay via the weak interaction. This is beta decay. A long-standing problem was that computed beta decays in nuclei were faster than what one would expect from the beta-decay of the neutron. NUCLEI researchers showed that two-body currents, i.e. beta decays that happen while a decaying nucleon is interacting with other nucleons in the nucleus, slow down beta decay. The accurate computation of this process solved a 50-year puzzle. Based on these insights, NUCLEI researchers computed beta-decay half-lives for nuclei across the nuclear chart.

Charge radii: Nuclear charge radii can be measured very precisely and this helps to test nuclear theory. NUCLEI researchers computed charge radii for several isotopic chains of nuclei and compared to measurements. Theory differed from experiment particularly in nuclei with where neutrons exceed the "magic" number 28. This difference points to deficiencies in the employed interactions and/or methods and therefore continues to be useful to further refine and improve these.

Neutrinoless double beta decay: Neutrinoless double beta decay is a hypothetical decay that violates the conservation of lepton number. If observed, this decay would point to physics beyond the standard model and give us insight into the nature of the neutrino. Experiments world-wide are searching for this decay. A nuclear matrix element links the lifetime of this decay, if observed, to the neutrino-mass scale. So far, nuclear theorists do not agree on the size of this matrix element, and the differences are factors of two-to-three. NUCLEI researchers computed this matrix element from first principles in ^{48}Ca and found that it is smaller than expected from other computations. This nucleus has a simple-enough structure to make this computation feasible; however, it is too rare to use as a detector. Nevertheless, the computation with uncertainty estimates was a first step and experimentally relevant nuclei can now be targeted.