The nuclear structure and low-energy reactions (NSLER) collaboration

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Abstract. The long-term vision of the Nuclear Structure and Low-Energy Reactions (NSLER) collaboration is to arrive at a comprehensive and unified description of nuclei and their reactions that is grounded in the interactions between the constituent nucleons. For this purpose, we will develop a universal energy density functional for nuclei and replace current phenomenological models of nuclear structure and reactions with a well-founded microscopic theory that will deliver maximum predictive power with minimal uncertainties that are well quantified. Nuclear structure and reactions play an essential role in the science to be investigated at rare isotope facilities, and in nuclear physics applications to the Science-Based Stockpile Stewardship Program, next-generation reactors, and threat reduction. We anticipate an expansion of the computational techniques and methods we currently employ, and developments of new treatments, to take advantage of petascale architectures and demonstrate the capability of the leadership class machines to deliver new science heretofore impossible.

1. The physics of nuclei: NSLER vision and background

Our long-term vision is to arrive at a comprehensive and unified description of nuclei and their reactions that is grounded in the fundamental interactions between the constituent nucleons. We seek to replace current phenomenological models of nuclear structure and reactions with a well-founded microscopic theory that delivers maximum predictive power with uncertainties that are well quantified.

Six years from now, new nuclear facilities will be churning out experimental data on short-lived nuclei. RIBF at RIKEN in Japan, SPIRAL-II, and GSI-FAIR will all be well on the way to either completion or full schedules of runs. The U.S. will also have an enhanced program established to continue research associated with the physics of nuclei. These facilities are trying to answer the basic questions concerning how protons and neutrons make stable nuclei and rare isotopes, and how simple patterns arise in complex nuclei. Today’s experimental facilities are paving the way with exciting results concerning the nature of nuclear closed shells when the neutron-to-proton ratio is high, the behavior of light nuclei near the drip lines where neutron skins can develop and binding becomes very weak, and the masses and lifetimes of very neutron-rich and unstable nuclei. Such results also impact our understanding of element production in the Universe, and also impact application-oriented needs in national security and energy production.

Nuclear theory, during the same time frame, faces the continuing challenges of developments that enable answers to the question(s): “Given a lump of nuclear material, what are its properties, where did it come from, and how does it interact?” We seek a unified framework for the description of nuclei and nuclear reaction processes that allows for accurate predictions and quantifiable error estimates for those predictions. Important in this pursuit is the understanding that we will not be able to measure every nuclear property that may be important even with the most sophisticated future experimental
facilities. For example, neutron cross sections on highly radioactive species may be important in the design of next-generation reactors or in various astrophysical nucleosynthetic processes, but their actual measurement may be difficult to impossible.

The need to develop better theory and computational techniques for the description of nuclear structure and reaction cross sections for various applications has been pointed out in several high-level documents including the Nuclear Science Advisory Committee (NSAC) 2004 Report: A Vision for Nuclear Theory; the NSAC 2005 Report: Guidance for Implementing the 2002 Long-Range Plan; and the DOE Path to Sustainable Nuclear Energy (2005), which points to the need for cross sections in planning for the advanced reactor technology. Theoretical challenges facing the ‘physics of nuclei’ community were outlined in the RIA Theory Blue Book [1] written in 2005 by a large part of the community.

The nuclear many-body problem represents unique challenges and yet entails significant similarities with other fields of science. We use techniques to solve the many-body problem that are used in other quantum systems (for example, Green’s function Monte Carlo, Hamiltonian diagonalization, coupled-cluster theory, nuclear density functional theory and extensions to it). All of these methods focus on solutions of a problem filled with difficulty and yet at the same time, in some instances, possessing rather astonishing simplicity. The nuclear quantum many-body problem has the unique feature of being driven by a Hamiltonian that is characteristically short-ranged, with many active operators (spin, angular momentum, isospin, tensor,...). In contrast to atoms and molecules, the nuclear interaction self-binds protons and neutrons in the nucleus and a real three-body force is present among nucleons. Furthermore, the nuclear interaction is not completely understood, but can be parameterized in a systematic way. Research in Effective Field Theory [2] has enabled us to make connections with the underlying QCD symmetries. Indeed, recent progress enabled the community to describe certain nuclear properties through mass 12 in an ab-initio many-body framework based on such interactions [3] or their more phenomenological cousins [4]. The future holds the promise of using these ab-initio results to guide us to the appropriate choice of density functional to be used in calculations of heavy nuclei.

As in other fields of science, the nuclear quantum many-body problem requires significant computational expertise in order to generate new and exciting science. The NSLER collaboration plans to build a national capability to calculate nuclear structure and low-energy cross sections, and assess their uncertainties. This capability requires a multi-pronged program of theoretical, algorithmic, and computational developments that will utilize leadership-class computation to solve several long-standing fundamental problems in nuclear physics, and will deliver cross section information that is more accurate than is currently available. The NSLER collaboration entails both improving the predictive power of nuclear calculations by connecting microscopic effective interactions to the basic nuclear interactions, and assessing quantitative error estimates of the results. We also anticipate an expansion of the computational techniques and methods we currently employ, and developments of new treatments, to utilize petascale architectures for new scientific discoveries in this area.

During the past 10 years, the nuclear theory community has been pursuing developments of sophisticated computational techniques to investigate properties of nuclei based only on the underlying nuclear forces. These developments have led to a new understanding of light nuclei using ab-initio many-body methods and heavier nuclei using self-consistent mean-field techniques. Furthermore, the first steps have been taken to understand nuclear reactions using ab-initio techniques. This collaboration will focus on significantly expanding both our many-body and density functional methods to calculate nuclear cross sections for a variety of nuclei across the chart of nuclei. We have targets of opportunity that are relevant to DOE missions. Light nuclear cross sections are important in NIF and NNSA-related work; cross sections of drip-line nuclei will shed light on their structure and dynamics relevant to exotic nuclei research; neutron-induced reactions on a wide variety of targets are important to the Stockpile Stewardship Program and advanced reactor technology programs. Indeed, if we are to close the fuel cycle in advanced reactor technology, we will need to understand neutron cross sections, nuclear decay, and fission on many nuclei ranging from light to heavy systems. Calculation of neutron cross sections requires a detailed knowledge of nuclear properties, and our collaboration will ad-
dress this issue. Theoretical error estimates for our cross sections will be relevant to covariance studies for network evaluations.

In order to meet the overarching goal of a consistent theoretical framework from which one can calculate nuclear properties, we have developed a roadmap with five basic components. These components are shown in Figure 1. We plan to i) calculate light nuclear structure and reaction information using realistic nuclear potentials (this is represented by the top two ellipses within the diagram); ii) use the information we learn in the first step to guide us in our development of a universal energy density functional that will describe medium-mass and heavy nuclei within the context of nuclear density functional theory and its extensions (represented by the third and fourth ellipse within the diagram); iii) incorporate new density functional information into reaction cross section calculations including the building of density functional motivated optical potentials and level densities (represented by the bottom ellipse), iv) integrate mathematical algorithms with science applications for optimal performance; and v) deliver to the community open-source software for the calculation of nuclear cross sections relevant to the various DOE missions. Verification of different methods with each other and validation with experimental data will play an important role in our efforts. We believe that within this approach it should be possible not only to calculate exciting new science in light to medium-mass nuclear systems, but because of the strong link from ab initio calculations to the development of the energy-density functional for DFT (and also using input from effective field theory), we should be able to formulate a universal energy density functional appropriate for nuclear structure and reaction calculations across the periodic table. This is the stated goal of NSLER and will be a primary focus.

2. The physics of nuclei: Present computational status

Virtually all microscopic theories for nuclear processes represent a substantial computational challenge, and the past decade has seen the exploitation of emerging computational capabilities to make spectacular progress in a fundamental description of the structure of nuclei. Confidence in our ability to accurately calculate nuclear structure and dynamics has increased dramatically over the past ten years due to advances in theory, algorithms, and the historic advances in computational power. In particular, first-principles approaches to light nuclei - Green’s Function Monte Carlo (GFMC) [5], No-core Shell Model (NCSM) [6], and Coupled Cluster (CC) [7] theory - have yielded important information about nuclei, including uncovering the role played by the three-nucleon interaction.

A GFMC calculation of the $^{12}$C ground state with a realistic two- and three-nucleon interaction requires approximately 55,000 node hours on the Bassi machine at NERSC. The code presently runs at 1.46 Gflops/processor or 19% of peak on Bassi, but only at 9% of peak on Blue Gene Light. GFMC is essentially a branching random walk with large sparse linear algebra calculations on each node. Parallel efficiencies are typically greater than 95% up to 2,048 processors for calculations up to $A = 10$. However, the parallel efficiency for $^{12}$C is 70% of linear speedup on only 256 and 384 processors due to the relatively large granularity (in both memory and CPU time) of the current parallelization scheme.

The NCSM is an ab initio configuration-interaction (CI) approach based on effective interactions derived from realistic two- and three-nucleon interactions. Calculations with three-body effective interactions with basis dimensions approaching $4 \times 10^7$ have been performed using approximately 3500
processors on THUNDER at LLNL. The largest of these calculations typically require on the order of 30 PFlop.

The nuclear CCSD codes are written in Fortran90 with MPI and MPI-I/O. The largest calculation we have attempted so far for $^{40}$Ca in a model space of seven shells involves 2 million unknowns using 1024 processors of Seaborg at NERSC (with 4 processors per node for computations at 400 MFlop/s/processor). The total computation on this type of run is 7.2 peta-operations.

We are unable to use ab-initio techniques for all nuclei, and we turn to nuclear DFT for calculations [8] of global low-energy nuclear properties and reaction information. The NSLER collaboration will use information from ab-initio nuclear studies to develop a universal nuclear energy-density functional that provides predictive power for nuclear properties in heavy nuclei.

Recently, we performed a full DFT mass table evaluation for even-even nuclei. Such global calculations require approximately 40 peta-operations to complete and were performed on 200 processors of an IBM Power-3. These calculations did not restore the broken symmetries present in the DFT, and they did not consider all nuclei. Future progress will involve algorithmic developments that enable symmetry restoration and nuclei with odd numbers of protons and/or neutrons. We estimate a factor of 1,000 increase in computational needs in order to accomplish this task.

We will also use the energy density functional to develop neutron-nucleus scattering potentials (‘optical potentials’). These will be augmented by correlation information that comes into such scattering problems. Initial work using complex basis states in shell-model diagonalization codes [6] shows promise for expansions to calculations of doorway states and other inputs that will enable improvements of these nuclear optical potentials used in cross-section calculations and coupled-channel reactions calculations. In the following, we briefly describe the NSLER computational portfolio.

3. Computational challenges of NSLER

Our physics goals can be realized only with a close cooperation between the physics and computer science collaborators. The issues range from algorithmic – finding the optimal methodology – to optimization on current architectures, to producing the scalable codes appropriate for petascale computers. All production codes will be open source and freely available.

Imminently available computational capabilities, extending to the petascale, provide unprecedented opportunities for breakthrough scientific achievements in nuclear theory. Versions of the codes already exist that together will enable a unified theory of nuclear structure and reactions, nearly all of them are already parallel, and some of them already scale to thousands of processors. All of them, however, require major investment in order to reach the petascale. The necessary investment is in the form of analysis, software libraries, implementation of modern algorithms, and in some cases new computer science research inspired by this particular family of application codes.

We have assembled a world-class team of experienced computer scientists and applied mathematicians to carry out this work. In many cases, they have already worked with the target code bases and identified targets of opportunity. In other cases, they will apply general measurement and analysis techniques to discover and address barriers to petascale computation. The planned work falls into three broad categories: performance analysis and code improvements (benchmarking, tuning, load balancing); applied mathematics (quadrature schemes, optimization, higher-order singular value decomposition, and eigensolvers); and application frameworks (COMPUNET). The paragraphs below provide the essence of the needed computational improvements.

Performance Analysis and Code Improvements. We will carry out performance evaluations of all the existing codes using well-established tools such as TAU and others developed as part of the PERC SciDAC Center. We will look at new algorithms for the operations in the coupled-cluster and DFT applications. We will analyze the existing NC SM algorithms (REDSTICK and MFD) and develop optimal serial and parallel NCSM algorithms. We will develop an asynchronous, dynamic, multi-threaded load-balancing library to enable finer-grained parallelism than is currently possible in the GFMC code, necessary for moving this code and others into the petascale regime.

Applied Mathematics. We will develop scalable quadrature methods for use with the many-body calculations and nuclear DFT. We will apply TAO (Toolkit for Advanced Optimization) to the fitting
problems generated by the application of a non-linear model. We will apply modern automatic differentiation software to obtaining the derivative information for the Skyrme energy functional. We will investigate the application of higher-order singular value decomposition to the 6-D tensors that arise in coupled-cluster and density functional theory. We will develop new specialized eignen solvers for application to the No-Core Shell Model, and analyze current implementations of the Lanczos algorithm to see if they can be adapted to the extremely large and sparse eigenvalue problems in many-body interactions.

Application Frameworks. We will develop a framework for the integration of our application codes (and others) into a “Computational Nuclear Environment” that can be used by other communities (experimentalists, NP, NNSA, and nuclear energy) to calculate relevant cross-section information. This work will rely on technology developed in the CCA (Common Component Architecture) SciDAC project. We will also develop a web portal for education and non-expert access to this application.

One can see from the above that a number of theoretical, computational, and algorithmic advances will be required to fulfill the goals of the NSLER collaboration. We look forward to working towards those goals through the SciDAC program.

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