NEXT GENERATION WORK

Next generation Track-1 systems in the coming years will enable us to carry out more systematic analyses on a larger class of materials. Our initial work shows that simulations of larger sized systems are important. Also, more systematic studies will enable us to carry out big data assessments of correlated many-body wave functions, towards the idea of "correlated electron genomics."

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COLLABORATIVE RESEARCH: INNOVATIVE *AB INITIO* SYMMETRY-ADAPTED NO-CORE SHELL MODEL FOR ADVANCING FUNDAMENTAL PHYSICS AND ASTROPHYSICS

Allocation: NSF PRAC/3.00 Mnh
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EXECUTIVE SUMMARY

We use Blue Waters to carry out large-scale modeling of light and medium-mass nuclei, including short-lived nuclei not yet accessible to experiment but critical to understanding astrophysical processes, which are the focus of current and next-generation rare isotope experimental facilities. The scale of computational challenges inherent to modeling such intricate quantum many-body systems makes the utilization of Blue Waters resources essential for addressing long-lasting challenges of importance to nuclear theory and experiment, as well as astrophysics. **Breakthrough** theoretical advances [1] coupled with Blue Waters' **cutting-edge** computational power have opened a new region, the intermediate-mass nuclei from fluorine (F) to calcium (Ca) isotopes, for **first** investigations with *ab initio* methods. This breakthrough fundamentally advances our understanding of nucleosynthesis, as nuclear energy spectra and reaction rates for many short-lived nuclei involved in nucleosynthesis are **not yet accessible by experiment or reliably measured** for the astrophysically relevant energy regime.

INTRODUCTION

One of the quintessential open challenges in contemporary physics is to design a comprehensive many-body theory for modeling and predicting nuclear structure and reactions starting from inter-nucleon forces that are consistent with the underlying theory of Quantum Chromodynamics (QCD). The ultimate goal of *ab initio* theory is to find a solution to this problem, which is a computationally-intensive endeavor due to a dual challenge, namely, the non-perturbative nature of QCD in the low-energy regime and the complexity of many-particle nuclei. Short-lived nuclei, currently **inaccessible to experiment**, are key to understanding processes in extreme environments. From stellar explosions to the interior of nuclear reactors, first-principle nuclear models that hold predictive capabilities have been and will be demonstrating a tremendous impact on advancing our knowledge at the frontiers of astrophysics, neutrino physics, and applied physics.

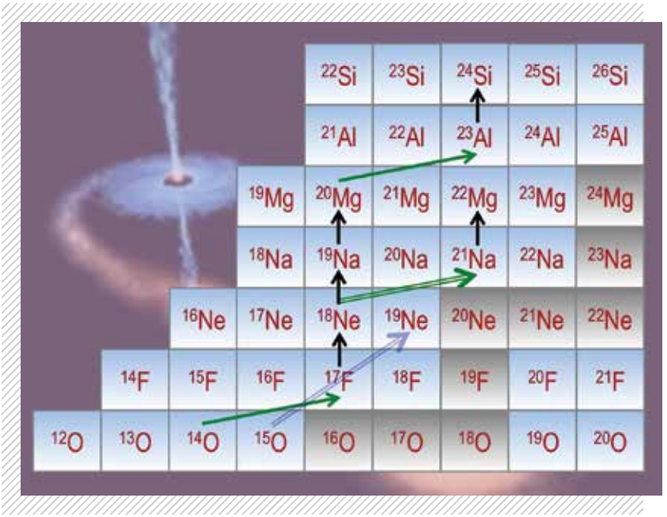

FIGURE 1: Nuclear region of interest to X-ray burst nucleosynthesis—it is now opened up for *ab initio* investigations by the unique capabilities of our SA-NCSM symmetry-guided concept and Blue Waters.

METHODS & RESULTS

We have developed an innovative *ab initio* nuclear structure approach, symmetry-adapted no-core shell model (SA-NCSM) [1], with concomitant computer code dubbed *LSU3shell* [2], that embraces the first-principles concept and capitalizes on a new symmetry of the nucleus. The *ab initio* SA-NCSM solves the time-independent Schrödinger equation as a Hamiltonian matrix eigenvalue problem. The main computational task is to evaluate a large symmetric Hamiltonian matrix and to obtain the lowest-lying eigenvectors that correspond to the experimental regime. Accuracy is based on the degree of convergence, which is linked to the size of the model space that can be achieved. The SA-NCSM utilizes physically relevant model space of significantly reduced dimensionality compared to ultra-large model spaces encountered by standard *ab initio* approaches. These theoretical advances coupled with the computational power of Blue Waters allow us to reach medium-mass nuclei that are inaccessible experimentally and fall far beyond the limits of other *ab initio* methods. The nuclei of interest represent a considerable challenge requiring computational power of near full-capacity of Blue Waters and its system memory. The following list describes the results and projected studies:

- We have provided the **first** *ab initio* description of the open-shell ^{20}Ne and ^{18}F nuclei. Following this success, we target Ne, Mg, and Si isotopes of importance to nuclear reaction studies. Such reactions in the intermediate-mass region are key to further understanding phenomena like X-ray burst nucleosynthesis and the Ne-Na and Mg-Al cycles.
- Work in progress focuses on one of the most challenging problems in nuclear physics today: achieving an *ab initio* description of the so-called Hoyle state in ^{12}C, the resulting state of the essential stellar triple-alpha process, key to modeling nucleosynthesis and stellar explosions. We have also calculated important low-lying states in ^{12}C, including negative-parity states and giant monopole and quadrupole resonances.
- We have studied ^{10}He (the focus of current experimental proposals), with impact on experimental techniques around the neutron-drip line that involve halo nuclei. Further calculations in even larger model spaces, only feasible with Blue Waters, will be key to resolving the observed inconsistency among several experimental results.

WHY BLUE WATERS

Ab initio nuclear structure studies represent an extremely computing-intensive endeavor. To illustrate the level of complexity, applications to medium-mass nuclei require over hundreds of exabytes of memory to store the Hamiltonian

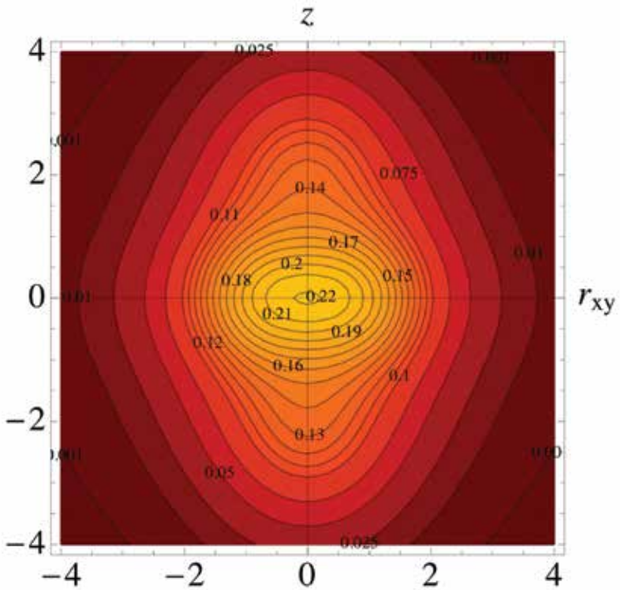

FIGURE 2: Density profile of the challenging ^{10}He ground-state resonance from first principles, revealing a surprising intrinsic structure.

matrix. The SA-NCSM drastically reduces the size of the problem and the associated memory requirement down to hundreds of terabytes and petabytes, but this comes at the cost of a major increase in computing intensity. As a result, SA-NCSM investigations of the intermediate-mass region are beyond the scale of available academic high-performance computing systems. Currently, only Blue Waters provides resources required for the *ab initio* SA-NCSM studies of medium-mass isotopes with cutting-edge accuracy. To capitalize on this opportunity, we drew from the experience and expertise of the Blue Waters staff and managed to improve the scalability of our code. As a result, our largest production runs utilized efficiently 717,600 concurrent threads running on **22,425 Cray XE6 compute nodes** to solve the nuclear eigenvalue problem with Hamiltonian matrices that occupy up to 400 TB of memory. Clearly, Blue Waters represents a unique computational platform that already plays a crucial role in advancing *ab initio* nuclear theory toward new domains.

NEXT GENERATION WORK

The major increase in computational power provided by the second generation of Track-1 system, along with emergent algorithms designed to take advantage of modern massively parallel architectures, will enable *ab initio* theories to start providing information of unprecedented quality for probing fundamental symmetries and physics beyond the standard model. Furthermore, increased computational resources will allow the SA-NCSM framework to address even heavier nuclear systems. For example, addressing neutrinoless double beta decay for ^{48}Ca should become feasible at a level that will reduce large uncertainties in the nuclear structure matrix elements and allows one to determine the neutrino type from planned experiments, which represents one of the most fundamental problems in physics today.

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NANOSCALE MECHANICS OF DEFORMATION IN HIGH-CAPACITY LITHIUM-ION BATTERIES

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EXECUTIVE SUMMARY

Silicon (Si) is one of the most promising electrode materials for high-performance lithium (Li) ion batteries because it has an order of magnitude higher specific capacity compared to conventional graphite electrodes. However, Si electrodes crack massively during Li insertion since they expand by 300% when fully-lithiated; they also delaminate from the current collector after many charge cycles. We have conducted large-scale parallel molecular dynamics simulations and density functional theory calculations on Blue Waters to uncover the underlying mechanisms for cracking and delamination of the Si electrode during charge cycling; these mechanisms are in excellent agreement with experiments. Blue Waters resources were needed because of the computational scale of the problem and the many computational runs needed to cover the entire parameter space. Our results have provided rich insights into the design and engineering of damage tolerant electrode materials for high-capacity Li-ion batteries.

INTRODUCTION

Lithium ion batteries are high-energy-dense systems that store energy by insertion of Li ions into solid electrodes. Silicon is one of the most promising electrode materials for high-performance Li-ion batteries since it possesses the highest known specific capacity of 4200 mAh/g, which is an order of magnitude greater than conventional graphite electrodes. During lithiation, the Si electrodes form Li_xSi compounds and undergo huge volume expansion of about 300% since one Si atom can theoretically bond with a maximum of x = 3.75 Li atoms. When attached to a metal current collector, such as copper (Cu), the massive and inhomogeneous