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

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EXECUTIVE SUMMARY

The Blue Waters system enables us to achieve large-scale modeling of light- and medium-mass nuclei, including short-lived nuclei not yet accessible to experiment but key to understanding astrophysical processes, which are the focus of current and next-generation rare isotope experimental facilities. The scale of computational challenges inherent in the modeling of such intricate quantum many-body systems makes the Blue Waters resources essential for addressing long-lasting questions of importance to nuclear theory and experiment, as well as to astrophysics. Breakthrough theoretical advances [1,2] coupled with the Blue Waters cutting-edge computational power have opened a new region, the intermediate-mass nuclei from Fluorine to Calcium isotopes, for first investigations with *ab initio* (i.e., "from first principles") methods. This targets nuclei far from stability, while pinpointing key features of astrophysical processes, probing fundamental symmetries in nature, as well as supporting current and upcoming experiments at radioactive beam facilities.

RESEARCH CHALLENGE

One of the quintessential open problems in contemporary physics is to design a comprehensive many-body theory for modeling and predicting nuclear structure and reactions starting from internucleon 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 highly intensive endeavor due to dual challenges: namely, the nonperturbative nature of QCD in the low-energy regime and the complexity of many-particle nuclei. As short-lived nuclei, currently inaccessible to experiment, are often found 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 have a tremendous impact on advancing our knowledge at the frontiers of multiple branches of physics such as astrophysics, neutrino physics, and applied physics.

METHODS & CODES

We have developed an innovative *ab initio* nuclear structure approach, dubbed the symmetry-adapted no-core shell model (SA-NCSM) [1], with concomitant computer code "LSU3shell" [3–4], 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 the Blue Waters system, allow us to reach medium-mass nuclei that are inaccessible experimentally and to other *ab initio* methods [2,5] (see Fig. 1).

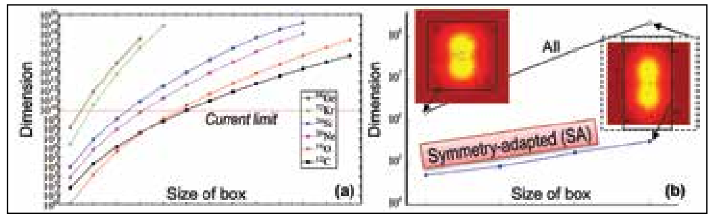

Figure 1: Nuclear model space: (a) Explosive growth with increasing particle number and the space ("box") in which particles reside (the largest dimension currently attainable is shown by the red horizontal line) and (b) tamed dimensions in the SA framework using symmetries known to dominate the dynamics.

RESULTS & IMPACT

The nuclei of interest represent a considerable challenge requiring computational power of nearly the entire Blue Waters (BW) machine and its system memory. Two graduate students have carried forward these studies and had the unique opportunity to work with supercomputers and massively parallel programming environments. The following list describes the results and their impact:

- We have provided the first *ab initio* description of the open-shell ^{19}Ne, ^{20}Ne, ^{24}Ne and ^{24}Si nuclei [2]. Such nuclei in the intermediate-mass region are key to further understanding the production of heavy elements, and especially X-ray burst nucleosynthesis. Of special interest are short-lived nuclei (such as ^{24}Si) that are difficult or impossible to study experimentally (see Fig. 2).
- We have studied emergent phenomena from first principle in Mg isotopes and their mirror nuclei (^{21}Mg and ^{21}F, ^{22}Mg and ^{22}Ne, with work in progress on ^{23}Mg and ^{24}Mg). While enhanced deformation and cluster substructures are difficult to describe from first principles, the BW system has allowed us to achieve *ab initio* descriptions using chiral internucleon interactions [5]. This is important for providing accurate predictions for deformed and, in the future, heavy nuclei of interest to understanding the r-process nucleosynthesis.
- Another study has focused on ^{12}C, including the most challenging Hoyle state, the resulting state of the essential stellar triple-alpha process—the study aimed at identifying important components of the internucleon interaction. A remarkable finding reveals that only a few components of the interaction can account for most of the physics, including binding energies and collectivity.
- We have performed first-principle simulations of ^{48}Ca and ^{48}Ti with the aim of studying neutrinoless double-beta decay for these heavy nuclear systems. The goal is to reduce large uncertainties in the nuclear structure matrix elements, which will, in turn, allow us to determine the neutrino type from planned experiments at the Deep Underground Neutrino Experiment.

Large investments have been made in new generations of radioactive beam facilities to enable important discoveries in nuclear science. While the above-mentioned applications focus on specific important questions, the concurrent new developments and dramatic improvements of the LSU3shell computer code, carried forward as part of the BW PAID program, may have wider impact, as multi-physics simulations in the areas of nuclear energy and national security have similar needs.

WHY BLUE WATERS

The *ab initio* nuclear structure studies represent an extremely computing-intensive endeavor. To illustrate the level of complexity, applications to medium-mass nuclei require in excess of hundreds of exabytes of memory to store the Hamiltonian 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 HPC systems. Currently, only the BW system provides resources required for the *ab initio* SA-NCSM studies of medium-mass isotopes. In order to capitalize on this opportunity, we drew from the experience and expertise of the Blue Waters staff and managed to improve scalability of our code. As a result, our largest production runs efficiently utilized 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, the BW system represents a unique computational platform that already plays a crucial role in advancing *ab initio* nuclear theory.

PUBLICATIONS AND DATA SETS

Dreyfuss, A. C., et al., Understanding emergent collectivity and clustering in nuclei from a symmetry-based no-core shell-model perspective, *Phys. Rev. C*, 95:4 (2017), 044312, DOI: 10.1103/PhysRevC.95.044312.

Draayer, J. P., T. Dytrych, and K. D. Launey, Symmetry-adapted no-core shell model—the *ab initio* picture of nuclear collectivity. in *Emergent Phenomena in Atomic Nuclei from Large-scale Modeling: A Symmetry-guided Perspective*, in press (2017); ISBN: 978-981-3146-04-4.

Launey, K.D., et al., Symmetry-guided large-scale shell-model theory. *Prog. Part. Nucl. Phys.*, 89 (2016), p. 101, DOI: 10.1016/j.ppnp.2016.02.001.

Dytrych, T., et al., Efficacy of the SU(3) scheme for *ab initio* large-scale calculations beyond the lightest nuclei, *Comput. Phys. Commun.*, 207 (2016), p. 202.

Draayer, J. P., et al., No-Core Symplectic Model—Exploiting Hidden Symmetry in Atomic Nuclei, accepted, *Journal of Physics: Conference Series* (2016).

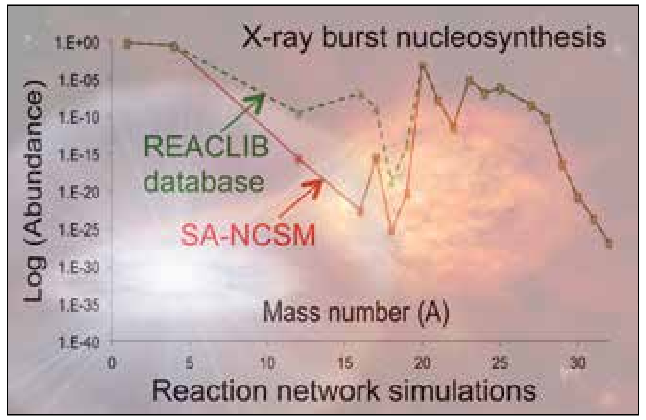

Figure 2: Effect on the abundance pattern from X-ray burst (XRB) nucleosynthesis simulations (based on Hix's Xnet) when reaction rates from the BW-enabled first-principle SA-NCSM simulations of ^{20}Ne are used (compared to current database, for fixed astrophysical conditions).