COLLABORATIVE RESEARCH: ADVANCING FIRST-PRINCIPLE SYMMETRY-GUIDED NUCLEAR MODELING FOR STUDIES OF NUCLEOSYNTHESIS AND FUNDAMENTAL SYMMETRIES IN NATURE

Allocation: NSF PRAC/3,430 Knh
PIs: J.P. Draayer[1], W.M. Tang[2]
Co-PIs: K.D. Launey[1], T. Dytrych[1,3], B. Wang[2]
Collaborators: D. Langr[4], M. Kocourek[4], T. Oberhuber[4], R. Baker[1], G. Sargsyan[1], A. Mercenne[1]

[1]Louisiana State University
[2]Princeton University
[3]Czech Academy of Sciences
[4]Czech Technical University

EXECUTIVE SUMMARY

The objective of this project is to provide nuclear wave functions of unprecedented accuracy by combining the cutting-edge computational power of the Blue Waters (BW) system with advanced techniques of nuclear structure calculations. This enables large-scale modeling of light- and intermediate-mass nuclei along with, for the first time, medium-mass nuclei. This is key to addressing the two most challenging questions in physics today; namely, the origin of elements and whether the neutrino is its own antiparticle. The work also supports and informs current and projected experimental efforts at state-of-the art radioactive beam facilities, including the upcoming Facility for Rare Isotope Beams. Breakthrough theoretical advances [1,2], coupled with BW's cutting-edge computational power, have opened a new region—the intermediate-mass nuclei from fluorine to calcium isotopes—for first investigations with *ab initio* ("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 a dual challenge; namely, the nonperturbative nature of QCD in the low-energy regime and the complexity of many-particle nuclei. Because short-lived nuclei, currently inaccessible to experiment, are often found to be key to understanding processes in extreme environments ranging from stellar explosions to the interior of nuclear reactors, first-principle nuclear models that hold predictive capabilities will have 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" [3–5], 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 BW system, allow us to reach medium-mass nuclei that are inaccessible experimentally and to other *ab initio* methods (see Fig. 1) [2,6].

RESULTS & IMPACT

The nuclei of interest represent a considerable challenge requiring computational power of nearly the entire 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:

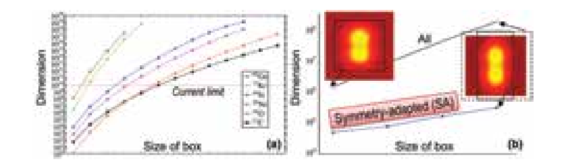

Figure 1: Nuclear model space—(a) Explosive growth with increasing particle number and the space (box) in which particles reside (the largest dimension currently attainable is shown by the red horizontal line); and (b) tamed dimensions in the SA framework using symmetries known to dominate the dynamics.

- We have provided the first *ab initio* description of the open-shell intermediate-mass nuclei, such as ^{19}Ne, ^{20}Ne, ^{24}Ne and ^{24}Si [2], with *ab initio* wave functions to be provided as input to our *ab initio* reaction code under development. Such nuclei, along with (α,p) and proton capture reactions, are key to further understanding the production of heavy elements, and especially the X-ray burst nucleosynthesis. Of special interest are short-lived nuclei (such as ^{24}Si) that are difficult, and often impossible, to study experimentally.
- We have studied emergent deformation and clustering in nuclei, from first principles, for 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 the first *ab initio* descriptions of deformed nuclei using chiral internucleon interactions [6]. This is important for providing accurate predictions for deformed and, in the future, heavy nuclei of interest to understanding the r process nucleosynthesis, one of the most challenging problems in astrophysics today.
- 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 DUNE (Deep Underground Neutrino Experiment), which represents one of the most fundamental problems in physics today (see Fig. 2).

Large investments have been made in new generations of radioactive beam facilities to enable important discoveries in nuclear science. These calculations, enabled by the BW system, aim to make significant contributions in this area, supporting and informing current and upcoming experiments at these facilities. 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's PAID program, may have wider impact, as multiphysics simulations in the areas of nuclear energy and national security have similar needs.

WHY BLUE WATERS

Currently, only the BW system provides resources required for the *ab initio* studies of medium-mass isotopes with cutting-edge accuracy. To illustrate the level of complexity, applications to medium-mass nuclei require more than hundreds of exabytes of memory to store the Hamiltonian matrix. In order to capitalize on advances feasible with the SA–NCSM and BW capabilities, with the help of the BW staff, we managed to improve scalability and performance of our code. As a result, our largest production runs utilized efficiently 715,712 concurrent threads running on 22,366 Cray XE6 compute nodes to solve the nuclear eigenvalue problem with a memory footprint of up to 750 TB of data. Clearly, the BW system represents a unique computational platform that already plays a crucial role in advancing *ab initio* nuclear theory toward new domains.

PUBLICATIONS & DATA SETS

Draayer, J.P., et al., Untangling simple patterns in intricate atomic nuclei. *Walter Greiner Memorial Volume*, World Scientific Publishing Co. (2018).

Langr, D., T. Dytrych, K.D. Launey, and J.P. Draayer, Accelerating Many-Nucleon Basis Generation for High Performance Computing Enabled Ab Initio Nuclear Structure Studies. *Intl. J. High Performance Computing Applications*, submitted (2018).

Pan, F., X. Ding, K.D. Launey, and J.P. Draayer, A simple procedure for construction of the orthonormal basis vectors of irreducible representations of O(5) in the OT(3) ⊗ON(2)basis. *Nucl. Phys. A*, 974 (2018), p. 85.

Pan, F., et al., Exact solution of mean-field plus an extended T= 1 nuclear pairing Hamiltonian in the seniority-zero symmetric subspace. *Physics Letters B*, 780 (2018), p. 1.

Burrows, M., et al., *Ab initio* translationally invariant nonlocal one-body densities from no-core shell-model theory. *Phys. Rev. C*, 97 (2018), p. 024325.

Launey, K.D., et al., *Ab initio* Picture of Nuclei: Shapes, Rotations, and Vibrations from Chiral Potentials. *Bulg. J. Phys.*, 44 (2017), p. 345.

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 (2017), p. 044312.

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

Draayer, J., et al., No-core Symplectic Model: Exploiting Hidden Symmetry in Atomic Nuclei. *Journal of Physics: Conference Series*, 1st ed., 863 (2017), p. 012008.

Dreyfuss, A.C., et al., Simple Patterns in Nuclei. *Proceedings of the 6th International Conference on Fission and properties of neutron-rich nuclei* (Sanibel Island, Fla., 2017).

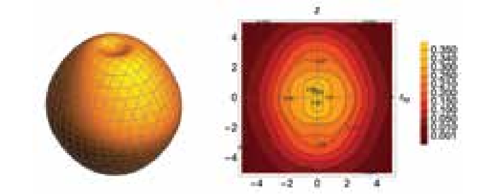

Figure 2: First *ab initio* simulations of the medium-mass ^{48}Ti nucleus of importance to studies of the neutrinoless double-beta decay, with a view toward reducing large uncertainties in the nuclear structure matrix elements. This will, in turn, allow us to determine if the neutrino is its own antiparticle.