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

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-standing 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 regime for studying medium-mass nuclei from Fluorine to Calcium isotopes, for first investigations with ab initio methods (i.e., “from first principles”) methods. This targets nuclei far from stability, with pinpointing key features of astrophysical processes, providing the experience and expertise of the Blue Waters staff and managed to improve scalability of our code. As a result, our system has allowed us to achieve ab initio descriptions using chiral interaction 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.

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 matrix eigenvalue problem. We have performed first-principle simulations of α and 20Ti with the aim of studying neutronless 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.

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 shed 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 16Ne, 20Ne, and 28Si 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 25Si) 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 (12Mg and 12F and 13Na) with work in progress on 32Mg and 36Mg. 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 interaction 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 12C, including the most challenging Hoyle state, the resulting state of the essential stellar triple-alpha process—this study aimed at identifying important components of the interconelium 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 α and 20Ti with the aim of studying neutronless 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 competing, 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 XSE 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


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

Figure 2: Effect on the abundance pattern from X-ray burst (XRB) nucleosynthesis simulation based on Hoyle state (α decay). Reaction rates from the BW-enabled first-principle SA-NCSM simulations of 16O are used (compared to current database, for fixed astrophysical conditions).