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

Allocation: NSF PRAC/171.5 Knh
PI: Jerry Draayer[1]
Co-PIs: K. D. Launey[1], T. Dytrych[1,2]
Collaborators: R. Baker[1], G. Sargsyan[1], A. Mercenne[1], D. Langr[3], M. Kocourek[3]

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

EXECUTIVE SUMMARY

The Blue Waters (BW) system has enabled modeling of nuclear wave functions with unprecedented accuracy for light- and medium-mass nuclei. This is key to addressing two of the 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 at Michigan State University. Breakthrough theoretical advances [1,2] along with the development of novel highly scalable algorithms [3,4] and coupled with the BW 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 with collective and cluster substructures, 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 owing to a dual challenge: the nonperturbative nature of QCD in the low-energy regime and the complexity of many-particle nuclei. Because short-lived nuclei are currently difficult or impossible to access by experiment but are 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 knowledge at the frontiers of multiple branches of physics, including astrophysics, neutrino physics, and applied physics.

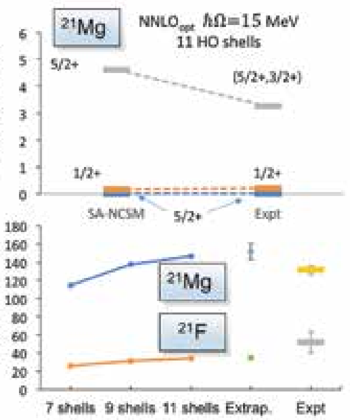

Figure 1: First-ever **ab initio** descriptions of collective features in magnesium (Mg) isotopes. SA–NCSM calculations are performed for ultralarge model spaces using chiral potentials and compared to experiment: (upper panel) energy of the three lowest excitations of 21Mg and (lower panel) transition probabilities from the first excited state to the ground state.

METHODS & CODES

The research team has 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 ultralarge model spaces encountered by standard *ab initio* approaches. These theoretical advances [2,6,7], coupled with the computational power of the Blue Waters system, have allowed the team to reach medium-mass nuclei that are inaccessible experimentally and to other *ab initio* methods.

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 have had the unique opportunity to work with supercomputers and massively parallel programming environments. The following list describes the results and their impact:

- While enhanced deformation and cluster substructures are difficult to describe from first principles, the SA–NCSM and the BW system have allowed the first *ab initio* descriptions of deformed nuclei using chiral interactions [2,6,7]. The team has continued to study emergent deformation and clustering in nuclei, from first principles, for Mg isotopes and their mirror nuclei. In addition to calculations for ^{21}Mg and ^{21}F, ^{22}Mg and ^{22}Ne, new results are now available for ^{23}Mg and ^{23}Na, and the challenging ^{28}Mg (Fig. 1). For ^{28}Mg, new observations have revealed an anomaly in a specific type of collective transition, which has been explained by the SA–NCSM model as shape mixing.
- For neutrino experiments, it is important to reduce uncertainties related to the response of the detector nuclei to the neutrino. Response functions are now feasible for intermediate-mass nuclei, such as ^{40}Ar, the next-generation detector ingredient. As an illustration, BW has allowed the team to carry forward large-scale *ab initio* calculations for the response for ^{20}Ne (Fig. 2). Such calculations are important for studies of nuclear compressibility, which in turn inform the equation of state for neutron stars. In addition, various peaks in the response function can provide further insight into clustering substructures and collective degrees of freedom.
- *Ab initio* modeling of open-shell intermediate-mass nuclei is now feasible, and these, in turn, are used to study nuclei on the path of the X-ray burst nucleosynthesis, key to further understanding the origin and production of heavy elements. For example, *ab initio* calculations for ^{20}Ne, and especially the negative parity states (Fig. 2), as well as for ^{15}O, are used to calculate alpha decay probabilities, which enter as a critical input into reaction rates for (α,p) and proton capture reactions. Indeed, the alpha-induced reaction for ^{15}O is currently not well understood but has been suggested to have the largest effect on nucleosynthesis simulations. This *ab initio* modeling is important for providing accurate predictions for deformed and, in the future, heavy nuclei of interest to understand the r-process nucleosynthesis, one of the most challenging problems in astrophysics today.

WHY BLUE WATERS

Currently, only the BW system provides resources required for these *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 Blue Waters' capabilities, and with the help of the BW staff, the research team managed to improve scalability and performance of its code. As a result, the team's largest production runs efficiently utilized 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 terabytes 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.

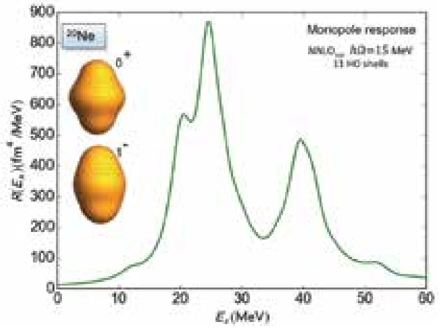

Figure 2: The first *ab initio* response of the deformed ^{20}Ne to an external probe vs. the energy transfer, revealing a clear evidence (the highest peak) for a giant monopole resonance and informing nuclear compressibility. Other emergent features detected within the SA–NCSM model are also shown: enhanced collectivity (0^+) and clustering (1^-).

PUBLICATIONS & DATA SETS

D. Langr, T. Dytrych, K. D. Launey, and J. P. Draayer, "Accelerating many-nucleon basis generation for high performance computing enabled *ab initio* nuclear structure studies," *Int. J. High Perform. Comp. Appl.*, vol. 33, no. 3, pp. 522–533, 2019, doi: 10.1177/1094342019838314.

D. Langr, T. Dytrych, J. P. Draayer, K. D. Launey, and P. Tvrdík, "Efficient algorithm for representations of U(3) in U(N)," *Comput. Phys. Commun.*, 2019, doi: 10.1016/j.cpc.2019.05.018.

F. Knapp, T. Dytrych, D. Langr, and T. Oberhuber, "Importance basis truncation in the symmetry-adapted no-core shell model," *Act. Phys. Pol. B*, vol. 50, pp. 541–547, 2019, doi: 10.5506/APhysPolB.50.541.

R.B. Baker *et al.*, "Benchmark calculations of electromagnetic sum rules with symmetry-adapted basis and hyperspherical harmonics," *Phys. Rev. C*, to be submitted, 2019.

G. Sargsyan et al., "Emergent collectivity in Mg isotopes from first principles," in preparation, 2019.

P. Ruotsalainen *et al.*, "Isospin symmetry in *B(E2)* values: Coulomb excitation study of ^{21}Mg," Phys. Rev. C, vol. 99, p. 051301 (R), 2019, doi: 10.1103/*PhysRevC*.99.051301.

M. Burrows et al., "*Ab initio* folding potentials for nucleon-nucleus scattering based on NCSM one-body densities," Phys. Rev. C, vol. 99, p. 044603, 2019, doi: 10.1103/*PhysRevC*.99.044603.

J. Henderson *et al.*, "Testing microscopically derived descriptions of nuclear collectivity: Coulomb excitation of ^{22}Mg," *Phys. Lett. B*, vol. 782, p. 468, 2018, doi: 10.1016/j.physletb.2018.05.064.

M. Burrows *et al.*, "*Ab initio* translationally invariant non-local one-body densities from a no-core shell-model theory," Phys. Rev. C, vol. 97, p. 024325, 2018, doi: 10.1103/physrevc.97.024325.