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

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. As short-lived nuclei, currently inaccessible to experiment, are often found to be 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 had and will have a tremendous impact on advancing our knowledge at the frontiers of multiple branches of physics. This project uses ab initio (“from first principles”) theory to find a solution to this problem.

Methods & Codes
The team has developed an innovative ab initio nuclear structure approach, dubbed the symmetry-adapted no-core shell model (SA-NCSM), simulated using the computer code “LSU3shell”, which 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. These theoretical advances, coupled with the computational power of the Blue Waters system, allow them to reach medium-mass nuclei that are inaccessible experimentally and to other ab initio methods.

Why Blue Waters
Currently, only the Blue Waters system provides the resources required for ab initio studies of medium-mass isotopes with high accuracy. To illustrate the level of complexity, applications to medium-mass nuclei require hundreds of exabytes of memory to store the Hamiltonian matrix. The team’s current 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.

Results & Impact
• Provided the first ab initio description of the open-shell $^{19}$Ne, $^{20}$Ne, $^{24}$Ne and $^{24}$Si nuclei, with impact on X-ray burst nucleosynthesis and difficult-to-study short-lived nuclei (such as $^{24}$Si)
• First principles studies of emergent phenomena in Mg isotopes and their mirror nuclei to provide predictions for deformed and heavy nuclei
• Performed $^{48}$Ca and $^{48}$Ti studies that impact neutrino experiments which will be conducted at DUNE (Deep Underground Neutrino Experiment) [Ne – Neon, Si – Silicon, Mg – Magnesium, Ca – Calcium, Ti – Titanium]