We carried out large-scale modeling of light and medium-mass nuclei. This included 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 to modeling such intricate quantum many-body systems makes Blue Waters essential for addressing long-lasting challenges in nuclear theory and experiment, as well as astrophysics.

A breakthrough theoretical advance [1] coupled with the Blue Waters cutting-edge computational power opened a new region, the intermediate-mass nuclei from fluorine to argon isotopes, for first investigations with ab initio methods. This breakthrough (i.e. “from ab initio for first investigations with open-shell isotopes in the intermediate-mass region”) makes the problem highly compute-intensive, it also empowers ab initio models with a universal character essential for modeling the co-existence of diverse nuclear substructures and predictive capabilities vital for descriptions of nuclear species far from the valley of stability. Because such nuclei are often key to understanding processes in extreme environments, from stellar explosions to the interior of nuclear reactors, first-principles nuclear models have had and will have a tremendous impact on advancing the frontiers of multiple branches of physics such as astrophysics, neutrino physics, and applied physics. While the ab initio nuclear structure approaches for light nuclei have achieved remarkable progress, computational challenges hindered applications to heavier systems.

We developed an innovative ab initio nuclear structure approach (with concomitant computer code named LSU3shell), dubbed the symmetry-adapted no-core shell model (SA-NCSM) [1], that embraces the first-principles concept and capitalizes on exact as well as approximate symmetries of nuclei [2]. The ab initio SA-NCSM solves the time-independent Schrödinger equation as a Hamiltonian matrix eigenvalue problem using many-nucleon basis states organized according to definite shape deformation and total intrinsic spin. The main advantage of this basis stems from the fact that it is designed for the description of low-lying nuclear dynamics, thereby supporting the exclusion of configurations that contribute very little to nuclear states of interest [3,4]. The theory provides an opportunity for first-principles-guided applications, from quark/gluon considerations to nuclear structure and reactions for rare isotopes beyond the lightest “s-” and “p-shell” systems (hydrogen to carbon isotopes) [5–8]. This approach significantly reduces the dimensionality (i.e. size) of the model space from those encountered when using ultra-large basis spaces of standard ab initio approaches.

These theoretical advances coupled with the power of Blue Waters allowed us to advance an ab initio large-scale nuclear modeling initiative that proffered cutting-edge predictive capabilities for determining the structure of nuclear systems, including rare isotopes up through medium-mass nuclei that are inaccessible experimentally and fall far beyond the reach of other ab initio methods. Our aim is to provide nuclear structure information of unprecedented quality and scope that will further understanding of fundamental symmetries in nature that are lost in massive datasets or require exascale architectures, and to extract essential information for astrophysics (e.g., nucleosynthesis and stellar explosions), neutrino physics, and energy-related applied physics problems.

These points describe results and projected studies:

• We studied electron scattering off 6Li (a fluorine radioisotope) [9]. These are examples of open-shell isotopes in the intermediate-mass region, with complexity far beyond the reach of complementary ab initio methods. Following this success, we will target neon, magnesium, and silicon isotopes, especially those close to the limits of stability (at proton and neutron drip lines), providing important input to nuclear reaction studies. Such reactions in the intermediate-mass region are key to further understanding phenomena like X-ray burst nucleosynthesis or the neon-sodium and magnesium-aluminium cycles.

• We studied electron scattering off 20Ne (an isotope of neon) and 18F nuclei (a fluorine radioisotope) [9]. These are examples of open-shell isotopes in the intermediate-mass region, with complexity far beyond the reach of complementary ab initio methods. Following this success, we will target neon, magnesium, and silicon isotopes, especially those close to the limits of stability (at proton and neutron drip lines), providing important input to nuclear reaction studies. Such reactions in the intermediate-mass region are key to further understanding phenomena like X-ray burst nucleosynthesis or the neon-sodium and magnesium-aluminium cycles.

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The freely-moving deformable liquid droplets are fully resolved in time and 3D space, and all the scales of the turbulent motion are simultaneously resolved down to the smallest relevant length and time scales. Our direct numerical simulations (DNSs) solve the unsteady 3D Navier–Stokes and continuity equations throughout the whole computational domain, including the interior of the liquid droplet. The droplet surface motion and deformation are captured accurately by using the level set method (LSM). The discontinuous density and viscosity are smoothed out across the interface by means of the continuous surface force (CSF) approach. A variable density projection method is used to impose the incompressibility constraint. So far we focused on validating our numerical solution method. We compared our simulation results of an initially spherical liquid water droplet settling in stagnant air, under the effect of gravity and surface tension, with available experimental data. We monitored the shape changes, the terminal velocity, and the conservation of both mass and momentum. Once this validation is completed we will simulate the motion of a number of liquid droplets in isotropic turbulence. This will allow us to examine the dispersion statistics of the droplets and their effects on the carrier flow turbulence (two-way coupling).

**WHY BLUE WATERS?**

DNS of turbulent flow is very demanding in terms of computational power and memory. The computational grids need to be fine enough to resolve the smallest flow structures accurately; this requirement becomes more and more stringent as the Reynolds number, based on the Taylor microscale, increases. In addition, we seek an accurate time history of the flow in order to compute time-dependent statistics, thus limiting the time-step size (time interval) for advancing the solution in time. For example, DNS of single-phase isotropic turbulence at Reynolds number 300 requires a grid of 2,0483 mesh points, and about 12 hours on 65,536 processors to cover seven large eddy turnover times. The demand for computational power is even larger if a multiphase flow (e.g., liquid droplets in air) is considered; the standard projection method for incompressible flows must be replaced by a variable-density projection method. The latter results in a variable-coefficients Poisson’s equation that is not solvable by means of a fast Fourier transform, thus requiring an iterative solver. We use the multigrid-preconditioned conjugate gradient solver provided by the PETSc library. Given the requirements outlined above, Blue Waters is a necessary tool for our research.