NEXT-GENERATION *AB INITIO* SYMMETRY-ADAPTED NO-CORE SHELL MODEL AND ITS IMPACT ON NUCLEOSYNTHESIS

Allocation: GLCPC/0.5 Mnh
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EXECUTIVE SUMMARY:

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 foci 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* (i.e. "from first principles") methods. This breakthrough fundamentally advances our understanding of nucleosynthesis, as nuclear energy spectra and reaction rates for many short-lived nuclei involved in nucleosynthesis are not yet accessible by experiment or reliably measured for the astrophysically relevant energy regime.

INTRODUCTION

One of the quintessential open problems in contemporary physics research is to design a comprehensive many-body theory for modeling and predicting nuclear structure and processes starting from inter-nucleon forces that are consistent with the underlying theory of quantum chromodynamics (QCD). The ultimate goal of *ab initio* nuclear theory is to establish a bridge from the properties of many-nucleon systems down to the fundamental blocks—namely, nuclear potentials that are tied to the underlying principles of QCD. While this bridge 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.

METHODS & RESULTS

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.

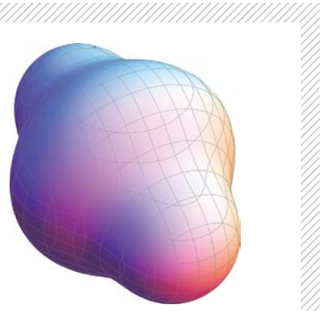

FIGURE 1: First *ab initio* results for the ^{20}Ne ground state, only feasible with the capabilities of the SA-NCSM symmetry-guided concept and the Blue Waters system.

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 provided the first *ab initio* description of ^{20}Ne (an isotope of neon) and ^{18}F 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-aluminum cycles.
- We studied electron scattering off ^{6}Li (a lithium isotope) with wave functions calculated in the *ab initio* SA-NCSM [10]. Results show the efficacy of the SA-NCSM model space selection, for the first time, toward reproducing the low- and high-momentum components of the ^{6}Li ground-state density. This finding is crucial for planned studies of neutrino scattering off ^{12}C (a carbon isotope) and ^{16}O (an oxygen isotope).
- A work-in-progress focuses on one of the most challenging problems in nuclear physics: achieving an *ab initio* nuclear modeling of the first excited 0^+ state (the so-called Hoyle state) in ^{12}C, the resulting state of the essential stellar triple-alpha process. Knowing the structure of low-lying states of ^{12}C is key to modeling nucleosynthesis and stellar explosions.

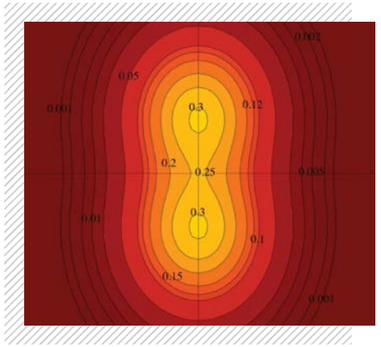

FIGURE 2: Density profile of the challenging ^{8}Be ground state from first principles, revealing two alpha subclusters. Results are obtained in the SA-NCSM utilizing only a small fraction of a large-scale model space.

WHY BLUE WATERS?

The *ab initio* nuclear structure studies are extremely compute-intensive and at the forefront of physics research. The state-of-the-art techniques of computational group theory in the SA-NCSM approach dramatically reduce the size of the problem and the associated memory requirement to hundreds of terabytes and petabytes at the cost of a major increase in computing intensity. Numerical investigations of the intermediate-mass region of the periodic table with the SA-NCSM approach are beyond the scale of available academic HPC systems.

Currently, only Blue Waters provides resources required for the *ab initio* SA-NCSM studies of medium-mass isotopes with cutting-edge accuracy. The largest production runs ran 717,600 concurrent threads on 22,425 Cray XE6 compute nodes. The next generation of Track-1 system will dramatically improve accuracy and predictive power of first-principles nuclear structure modeling while extending its reach towards even heavier isotopes.

PUBLICATIONS

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DIRECT SIMULATION OF DISPERSED LIQUID DROPLETS IN ISOTROPIC TURBULENCE

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EXECUTIVE SUMMARY:

The objective of our research is to enhance understanding of the two-way interactions between liquid droplets and a turbulent flow by performing direct numerical simulations (DNS). The freely moving deformable liquid droplets are fully resolved in three spatial dimensions and time and all the scales of the turbulent motion are simultaneously resolved down to the smallest relevant length and time scales. Our DNS 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. Discontinuous density and viscosity are smoothed out across the interface by means of the continuous surface force approach. A variable-density projection method imposes the incompressibility constraint.

INTRODUCTION

The two-way interactions between liquid droplets and turbulent flows are important in nature and engineering applications, for example cloud formation and burning of liquid fuel in internal combustion (reciprocating and jet) engines and rockets. Understanding the physical details of the vaporization and mixing processes in a turbulent flow is an essential prerequisite to understanding the chemical reaction and the eventual control/optimization of energy conversion.

METHODS & RESULTS

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 constrain.

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 flows 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 $2{,}048^3$ 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.

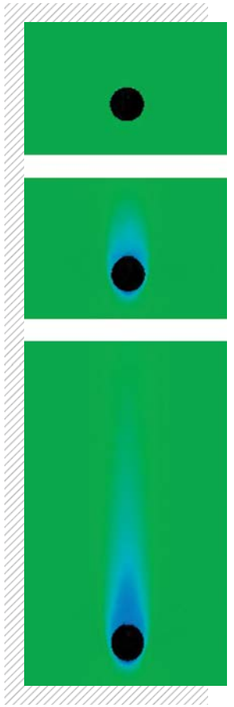

FIGURE 1: A liquid water droplet with initial diameter 0.6 mm is falling in stagnant air under the effect of gravity (=10 times gravity). The droplet's initial spherical shape changes with time due to the effects of acceleration, surface tension, and drag forces. Time (a) 0.0s; (b) 0.001 s; (c) 0.005 s. The velocity contours in the wake region are shown in blue.