1. DOE award DE-SC0005248; Louisiana State University, Baton Rouge, LA
2. "*Ab Initio* Nuclear Structure and Reaction Calculations for Rare Isotopes", PI: J.P. Draayer
3. Final Report – 07/01/10 - 06/30/14
4. Participating National Laboratory: Los Alamos National Laboratory

5. Abstract. We have developed a novel *ab initio* symmetry-adapted no-core shell model (SA-NCSM), which has opened the intermediate-mass region for *ab initio* investigations, thereby providing an opportunity for first-principle symmetry-guided applications to nuclear structure [DLD+13b] and reactions [DHL+14] for nuclear isotopes from the lightest p-shell systems to intermediate-mass nuclei. This includes short-lived proton-rich nuclei on the path of X-ray burst nucleosynthesis and rare neutron-rich isotopes to be produced by the Facility for Rare Isotope Beams (FRIB). We have provided *ab initio* descriptions of high accuracy for low-lying (including collectivity-driven) states of isotopes of Li, He, Be, C, O, Ne, Mg, Al, and Si, and studied related strong- and weak-interaction driven reactions that are important, in astrophysics, for further understanding stellar evolution, X-ray bursts and triggering of s, p, and rp processes, and in applied physics, for electron and neutrino-nucleus scattering experiments as well as for fusion ignition at the National Ignition Facility (NIF).

6. Project accomplishments. During this project, in accordance with our proposed Project Timetable, the SA-NCSM has been further developed and its highly-scalable computer code has been optimized for efficient use of modern high performance computer (HPC) resources. With the development of the SA-NCSM model, and with the help of HPC resources provided by Blue Waters, National Energy Research Scientific Computing Center (NERSC), and Louisiana Optical Network Initiative (LONI) and Louisiana State University's Center for Computation & Technology (CCT), we have performed first-principle nuclear structure calculations for isotopes, such as ^{6}Li, ^{6,8,10}He, ^{8,12}Be, ^{12,14}C and ^{16,18}O, with a focus on cluster and collectivity-driven states, together with heavier nuclei, ^{19,20,22,24,32}Ne, ^{20,22,24}Mg, ^{23}Al, and ^{24}Si. These *ab initio* nuclear structure calculations have supplied energies, electromagnetic transitions, radii, and one-body density matrix elements, which have been used in reaction studies of interest to national labs carried forward in collaboration with co-PI Anna Hayes at Los Alamos National Lab. The following list outlines the project accomplishments.

- **Development and optimization of the SA-NCSM.** The symmetry-adapted no-core shell model code has been developed and further optimized for efficient use of modern HPC resources [DLD+13b, LSDD14]. It has been already shown to scale to tens of thousands of processors. This is vital for applications to heavier nuclei and larger model spaces. The key component of the SA-NCSM is that it tremendously reduces the model space, that grows exponentially with the number of particles and the space in which they reside (Fig. 1a), to only physically relevant subspaces of low-spin/high-deformation configurations and hence, ultra-large model spaces become solvable. During the last year of the project, we have started the implementation of two-body density matrix elements (TBDME).

  The current stable version of the SA-NCSM code, `LSU3shell`, and its documentation are publicly available at the git repository hosted at *SourceForge*, `sourceforge.net/projects/lsu3shell`. The stable version of the code allows for calculations of matrix elements of one- and two-body operators (straightforwardly extensible to three-body operators), as well as of transition matrix elements (for computations of point-particle root-mean-square radii, electric quadruple moments, E2 and M1 transition rates [DLD+13b, DML+14]), and of one-body density matrix elements (OBDME) to be used as an input to reaction calculations.

- **Expanding the reach of *ab initio* (first-principle) nuclear structure approaches.** *We have provided ab initio calculations for light nuclei and up through mass number ~ 30 (p- and sd-shell nuclei) with impact to astrophysics, ν physics, and studies at NIF, for collectivity-driven nuclear states exemplified by the challenging Hoyle state, as well as for neutron-rich nuclei to be studied at FRIB.* In particular, we have carried forward:

  (1) *Ab initio* calculations for Li, He, B, Be, C, O isotopes of the p shell [DLD+13b, HLK+14], which has established the existence of a novel approximate symmetry in nuclei and confirmed the efficacy of the SA-NCSM symmetry-guided concept (Fig. 1c) – *ab initio* descriptions of light isotopes are essential for electron- and neutrino-scattering and NIF-related experiments;

  (2) First calculations for sd-shell nuclei, such as Ne, Mg, Al, and Si isotopes (Fig. 1b), including the proton-rich ^{24}Si of importance to further understanding X-ray bursts and the neutron-rich ^{32}Ne close to the region targeted by projected experiments at FRIB [DDLL12, LDD+13a, DDL+13, LDD+13b];

  (3) *Ab initio* calculations for ^{12}C and collectivity-driven states [DML+14] – a systematic benchmark study that has shown that considerably reduced SA-NCSM spaces yield very accurate binding energies, excitation

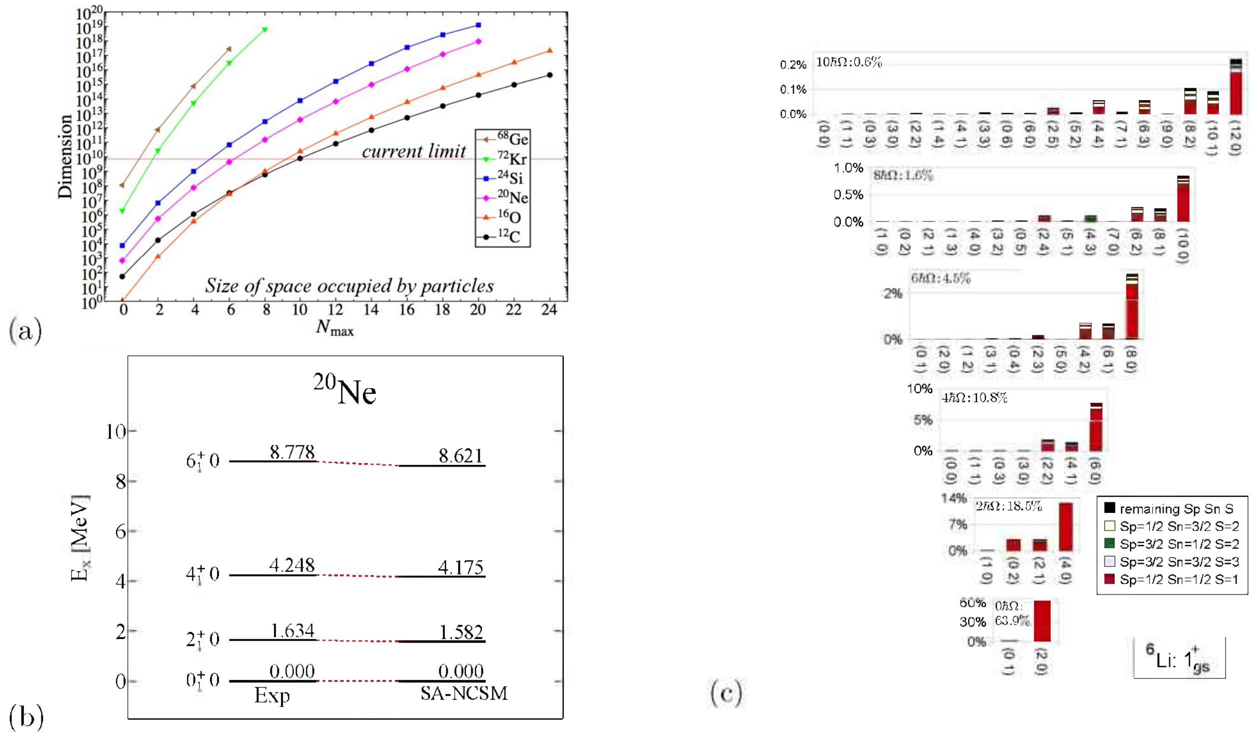


Figure 1: (a) Explosive growth of the nuclear model space (red line shows the current limit on best-in-class supercomputers). (b) First-ever *ab initio* SA-NCSM calculations for intermediate-mass nuclei in a challenging model space of 13 oscillator shells (inaccessible by conventional *ab initio* models). Figure taken from [DLD$^+$14]. (c) Discovery, unveiled by the *ab initio* SA-NCSM, of a simple orderly pattern in low-lying nuclear states that favors configurations of large deformation (clustering to the right) and low spin (red bars). Figure from [DLD$^+$13b].

energies, point-nucleon matter rms radii, electromagnetic moments and transition probabilities;

(4) Fully microscopic no-core symplectic shell-model (NCSpM) calculations for the Hoyle state of ^{12}C and its rotational band states (Fig. 2a), which continue to foster debate in experimental and theoretical studies, as well as for Be (Fig. 2b), C, Ne, Mg, Al, and Si isotopes – key to understanding the physics that is foremost responsible for cluster substructures and enhanced collectivity [DLD$^+$13a, TFL$^+$14, FTL$^+$14, LDD$^+$13b].

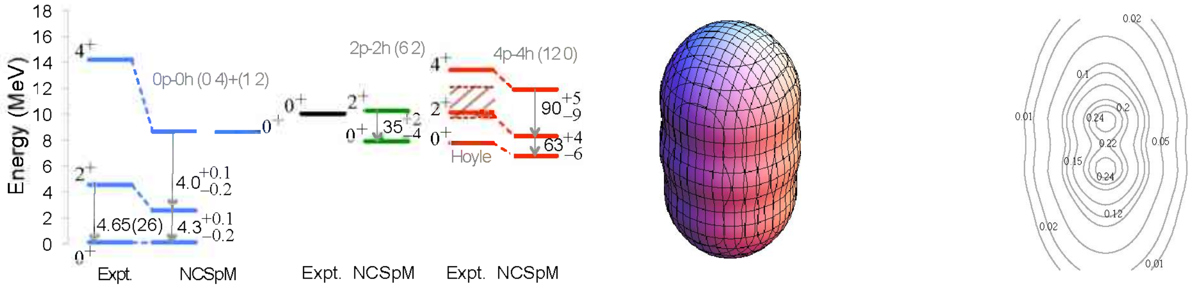
- **Strong- and weak-interaction driven reactions for light and intermediate-mass ($\lesssim$ 30) nuclei.** *SA-NCSM advances in ab initio descriptions of intermediate-mass nuclei and states of enhanced collectivity have also enabled reaction calculations, including electron and neutrino scattering of importance to neutrino experiments, as well as astrophysical proton-capture reactions for intermediate-mass nuclei dominated by a few isolated resonances.* In particular, under this award, we have provided:

  (1) Electron scattering charge form factors for ^{6}Li and ^{12}C (with wavefunctions calculated in the *ab initio* SA-NCSM), which, in turn, determine weak interaction cross sections [DHL$^+$14] – the outcome is important, as it provides a direct probe of the magnitude and structure of the challenging higher-shell components in the wavefunctions, as well as confirms the SA-NCSM efficacy in the high-momentum regime (Fig. 3a) and the results of earlier work of both PI's [Hay92, RD92, ED99];

  (2) The excited 15.11-MeV 1^+ state in ^{12}C in the *ab initio* SA-NCSM needed for neutrino-Carbon cross sections of importance to neutrino experiments, including the noteworthy MiniBooNE, T2K, and DUSEL;

  (3) *Ab initio* SA-NCSM calculations for selected states in Be, C, O, and F isotopes for reactions of interest to NIF – e.g., ^{9}Be$(t,p)^{11}$Be and ^{18}O$(t,n)^{20}$F with cross sections that cannot be measured experimentally but can only be determined theoretically, and ^{9}Be$(n,p)^9$Li, shown by Hayes and collaborators to be essential for successful fusion burn diagnostics [HJS$^+$06];

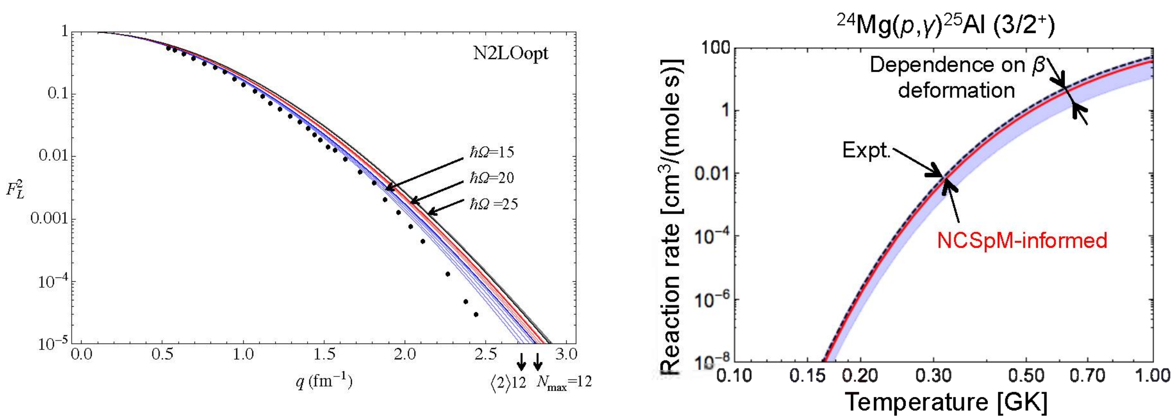
  (4) *Ab initio* SA-NCSM OBDMEs for reaction rates of interest to astrophysics, including (p,γ) reactions for



(a) (b)

Figure 2: (a) ^{12}C energy spectrum (left) together with the Hoyle-state matter-density profile (right) calculated by the fully microscopic no-core symplectic shell model (NCSpM) in the ultra-large model space of 22 oscillator shells and compared to experiment ("Expt."). $B(E2)$ transition rates are in W.u. units. Figure taken from [DLD$^+$13a]. (b) NCSpM matter-density profile of the ^{8}Be ground state.

the short-lived ^{20}Mg, ^{24}Si, ^{28}S and ^{32}Ar that are expected to tremendously affect the light curve for X-ray bursts. Reactions rates for several resonances for ^{22}Mg$(p,\gamma)^{23}$Al, ^{24}Mg$(p,\gamma)^{25}$Al (Fig. 3b), and ^{18}O$(p,\gamma)^{19}$F are studied using R-matrix coupled-channel method and deformation β derived in the NCSpM [ULR$^+$14].



(a) (b)

Figure 3: (a) Longitudinal electron scattering form factors for the ^{6}Li ground state calculated for SA-NCSM selected model spaces (thickness of curves) of 14 oscillator shells, compared to experiment (dots). Figure taken from [DHL$^+$14]. (b) Reaction rate for the 419-keV $3/2^+$ resonance in ^{24}Mg+p using the β deformation calculated in the fully microscopic NCSpM (red, solid) compared to experiment (black, dashed). The deformation dependence is also shown (blue shade). Figure taken from [ULR$^+$14].

The collaboration with LANL, started as a result of this award, is continuing with a focus on neutrino scattering cross sections for C, O, and Ar (ingredient nuclei in neutrino-experiment detectors), with the aim to reduce uncertainties that will become dominant in neutrino experiment data analysis with larger dataset statistics.

7. Publications and Theses

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11. Kristina D. Launey, Alison C. Dreyfuss, Jerry P. Draayer, Tomas Dytrych, and Robert Baker, (Proc. of the 3rd Intl. Workshop on "State of the Art in Nuclear Cluster Physics" (SOTANCP3), May 26-30, 2014, Yokohama, Japan), to be published in J. Phys.: Conf. Ser..
12. J. P. Draayer, T. Dytrych, K. D. Launey, A. C. Dreyfuss, and D. Langr, (Proc. of the 11th Intl. Spring Seminar On Nuclear Physics, May 12-16, 2014, Ischia), to be published in J. Phys.: Conf. Ser..
13. Jerry P. Draayer, Tomas Dytrych, Kristina D. Launey, Alison C. Dreyfuss, and Daniel Langr, (Proc. of the XXXVII Symposium on Nuclear Physics, January 6-9, 2014, Cocoyoc, Mexico), to be published in J. Phys.: Conf. Ser..
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8. People working on the project (graduate students, postdocs, and visitors)

Kristina D. Launey – senior research associate; full support (2011-2013)
Neelam Upadhyay – postdoctoral scholar; full support (2013-2014)
Nikola Nikolov – postdoctoral scholar; full support (2012)
Xin Guan – graduate student; full support (2012)
Alison Dreyfuss, Anthony Risolio, Brian Harvie – students, supported by NSF (REU at Dept. of Phys. & Astron.)

9. Updated current and pending support (other)

1. Agency / Program: SURA (Southeastern Universities Research Association)
   Title: Research Support; Period: 01/01/02-continuing; PD/PI: Jerry P. Draayer
   Award: Annually $50,000 (2002-2007); $65,000 (2008-present); Support: Part-time postdoc Dytrych & Launey, Students, Other
2. Agency / Program: LSU (Louisiana State University)
   Title: Buyout / Rebate; Period: 01/01/02-continuing; PD/PI: Jerry P. Draayer
   Award: Annually, half of PD/PI's annual salary (Currently $75,000); Support: Part-time postdoc, Students, Other
3. Agency / Program: NSF
   Title: Next-generation ab initio symmetry-adapted no-core shell model and its impact on nucleosynthesis; Period: 2013-2015; PD/PI: Jerry P. Draayer; Co-PI: Tomas Dytrych & Kristina D Launey;
   Award: Allocations of resources on the Blue Waters system for *ab initio* SA-NCSM large-scale computations, which can effectively exploit the petascale computing capabilities offered by Blue Waters.

10. Cost status– Approved budget: $450,000. Actual costs incurred by the date of the report: $450,000.

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