Hessisches Kompetenzzentrum
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Large-Scale Configuration Interaction for Ab Initio Nuclear Structure IV



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Clusters
Lichtenberg II Cluster Darmstadt

Additional Software
COCONUT

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Introduction

The primary objective of ab initio nuclear structure theory is the precise description of correlated many-nucleon systems based on fundamental principles of the strong interaction, Quantum Chromodynamics. However, realizing this goal requires overcoming the substantial complexity of the quantum many-body problem, particularly given the complex nature of nuclear interactions and the large number of possible configurations relevant for an accurate description. By leveraging the Importance-Truncated No-Core Shell Model (IT-NCSM), this project aimed to provide quasi-exact solutions to the many-body Schrödinger equation for nuclei up to mass A ≈ 25. This approach enables the comprehensive determination of key nuclear structure observables such as ground-state energies, radii, and electromagnetic moments while providing important feedback on the quality of the underlying nuclear interactions. This research project addressed the above mentioned theoretical challenges by casting the quantum many-body problem into the form of a large-scale matrix eigenvalue problem. The computational demands of this approach are immense and the resulting matrix dimensions reaches orders of magnitudes of 10^{10}. Consequently, the calculation and storage of many-body matrix elements, alongside the iterative extraction of low-lying eigenvalues and eigenvectors, constitute a significant HPC task.

Methods

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The methodological backbone of this project is the IT-NCSM developed by our group for ab initio nuclear structure studies. In standard Shell Model approaches, the full model space grows factorially, quickly becoming computationally unfeasible. The IT-NCSM overcomes this by exploiting the fact that, in the expansion of any physical eigenstate, a vast number of basis states have negligible amplitudes. By utilizing an adaptive truncation criterion based on first-order multiconfigurational perturbation theory, we selectively include only the important basis states relevant to the physics, drastically reducing the dimension of the eigenvalue problem. This approach is implemented via a sequential update scheme: Starting from a small model space, we iteratively expand the basis to larger model spaces (characterized by the truncation parameter $N_{max}\hbar\Omega$). Because states in an $(N_{max}+2)\hbar\Omega$ space are generated via limited excitations from the N_{max} space, the importance measure remains computationally efficient. A critical component is the optimized handling of three-nucleon (3N) interactions. Storing 3N matrix elements in the conventional *m*-scheme consumes prohibitive amounts of memory. To resolve this bottleneck, we utilized a storage-efficient angular-momentum and isospin-coupled format, which reduces memory requirements by up to two orders of magnitude. These elements are decoupled to the *m*-scheme on-the-fly during calculation. Finally, the Hamiltonian is represented on the importance-truncated basis, and low-lying eigenvalues are extracted using the ARPACK implementation of the Lanczos algorithm, followed by an extrapolation to the limit of a vanishing importance threshold.

Results

The project yielded significant advances in both the development of chiral interactions and the precision of ab initio nuclear structure calculations across the chart of nuclides and hypernucleides. A central achievement was the execution of large-scale NCSM calculations for semi-local momentum-space off-shell interaction families. By testing 15 interaction variants on ^{16}O, ^{24}O, and ^{40}Ca, we successfully identified regions of the off-shell parameter space that provide stable binding, while ruling out combinations that result in weakly bound or unbound systems near reaction thresholds. In the domain of hypernuclear physics, we successfully extended the natural orbital basis to hypernuclei. Applying this method to helium, lithium, and beryllium isotopes, we demonstrated that this optimized basis offers superior convergence compared to the harmonic oscillator basis. This enabled the detailed identification of layered nucleon and hyperon halo structures in light hypernuclei through the analysis of one-body densities and mass radii. Furthermore, we achieved high-precision predictions for nuclear charge and matter radii, specifically within the Boron isotopic chain. By investigating radius differences, we reduced model-dependence and obtained results that could hint at a proton halo in ^{8}B. Finally, a major methodological breakthrough was the development of so-called transcoder neural networks. Unlike previous extrapolation schemes, these networks leverage correlations between energies, radii, and electromagnetic

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moments. This framework allowed for precise, uncertainty-quantified predictions of electric dipole moments and the magnetic octupole transition strength in ^{10}B.

Discussion

The results obtained in this project highlight the increasing predictive power of ab initio methods when combined with advanced computational optimizations and machine learning. The study of the SMSOS interaction family revealed that while chiral interactions are robust, the significant variation in binding energies across off-shell choices points to the necessity of additional constraints, likely from three-body scattering data, to fix off-shell Low-Energy Constants in a controlled manner. The successful application of natural orbitals to hypernuclei addresses a long-standing challenge in converging the wave functions of loosely bound, halo-like systems. This establishes natural orbitals as a standard tool for future hypernuclear campaigns, significantly extending the reach of the NCSM to heavier hypernuclei without prohibitive computational costs. Similarly, the work on Boron radii demonstrates that analyzing isotope-dependent radius differences is a powerful strategy to suppress correlated uncertainties, providing direct and precise inputs for experimental isotope-shift measurements. Looking forward, the transcoder neural network framework developed represents a paradigm shift for extracting observables that are typically slow to converge, such as electromagnetic moments. Future work will focus on generalizing this framework to a more rigorous application to electromagnetic transition strengths and extending the natural-orbital IT-NCSM approach to medium-mass hypernuclei. Combined with the refined interaction parameters identified in this project, these tools lay the groundwork for a comprehensive ab initio description of complex nuclear phenomena.

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