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# *Precision Nuclear Structure Calculations with the In-Medium Similarity Renormalization Group*



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## Introduction

The structure of nuclei gives fundamental insight into strong interactions between nucleons, beyond-standard-model physics, and astrophysical processes in neutron-rich environments. A systematic theoretical description of nuclei based on inter-nucleon interactions has become possible over the past two decades. Such calculations are able to make predictions for observables difficult to measure experimentally and for nuclei currently not able to be studied at rare-isotope beam facilities. Moreover, these calculations are systematically improvable, allowing us to reach high precision and quantify theoretical uncertainties. However, the many-body methods employed, while scaling polynomially in the number of particles, still require supercomputers to evaluate the large-scale transformations of data to describe the system (many-body operators). Especially state-ofthe-art methods reaching higher precision require considerable computational resources.

## Methods

The main methods employed in this project are chiral effective field theory for nuclear forces and the in-medium similarity renormalization group to solve the many-body problem. Chiral effective field theory provides a general expansion of nuclear forces with free parameters to be fixed to data. In this project, uncertainties in these free parameters were accounted for using a Bayesian history matching prescription to generate potentially valid sets of parameter values. These each define a nuclear



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potential and can be fed into many-body calculations to assess input uncertainties in many-body calculations. The in-medium similarity renormalization group (IMSRG) is a many-body method that generates an approximate unitary transformation of the many-body Hamiltonian, which gives us the ground-state wavefunction and ground-state properties like the mass and radius of the nucleus. The method relies on a truncation in the many-body operators included, giving the IMSRG(2) approximation at the two-body level and the more refined IMSRG(3) approximation at the three-body level.

## Results

We used the IMSRG(2) to predict moments of charge density distributions in Yb isotopes, being used for pioneering laser-spectroscopy studies. A key feature of this study was the assessment of correlations across isotopes, as we studied $^{168}$Yb through $^{176}$Yb. This required many repeated many-body solutions. We used the IMSRG(3) to predict the differential charge radius from $^{12}$C to $^{13}$C with many-body uncertainties quantified. $^{12}$C is a particularly challenging nucleus to describe, with strong signatures of cluster structures. The improved many-body solution offered by the IMSRG(3) was essential here. We used the IMSRG(3) to compute excitation energies in neutron-rich Ca isotopes. A long-standing challenge of the IMSRG(2) has been the inability to quantitatively predict the first excited-state energy in $^{48}$Ca correctly, which is an indicator of the closed-shell structure of the nucleus. The IMSRG(3) allows us to assess many-body uncertainties and give a more precise prediction.

## Discussion

Our calculations of the structure of Yb isotopes are being used to understand precision isotope-shift measurements. Specifically, our calculations of higher moments of the charge distribution are novel in microscopic calculations. While a comparison with experimental data is still outstanding, we found that our precision calculations of $^{12}$C give important corrections over standard calculations. These will play a key role in assessing uncertainties and for a robust comparison with the alloptical measurement of the $^{12}$C–$^{13}$C radius difference. We found that high precision calculations of the excitation energy of $^{48}$Ca were able to bring in important corrections, bringing the predicted value into better agreement with experiment. The calculations here are especially expensive, and work still needs to be done to scale the numerical implementation to many MPI ranks. A key goal for upcoming studies is to employ a distributed IMSRG solver, capable of storing three-body matrix elements (a key bottleneck) distributed across many nodes. This will enable unprecedented calculations reaching high precision in medium-mass and heavy nuclei. Developments to this end were also performed using the project on Lichtenberg.



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## Publications

Matthias Heinz, Diagrammatic resummations for the in-medium similarity renormalization group, ESNT Workshop “Automated tools for many-body theory,” France, June 5-8, 2023

Matthias Heinz, Precision nuclear structure with the in-medium similarity renormalization group, Yonsei University Physics Seminar, South Korea, May 23, 2023

Matthias Heinz, Improved ab initio nuclear structure for medium-mass and heavy nuclei, Arbeitstreffen Kernphysik 2023, Germany, February 23 - March 2, 2023

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