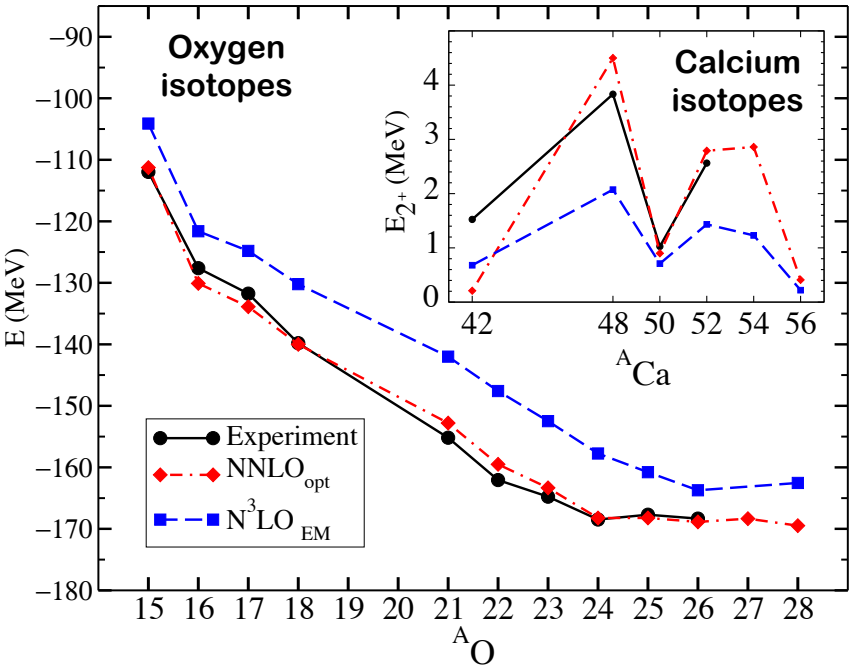
Streamlining the nuclear force

Objectives

- Apply state-of-the-art optimization methods for wide range of calibration problems in nuclear physics for scalable codes spanning ab initio to density functional theory approaches
- Optimization of nuclear interaction from chiral effective field theory at next-to-next-to leading order using the optimization tool POUNDERS in the phase-shift analysis
- Provide uncertainty quantification for nuclear structure modeling

Impact

- Nucleon-nucleon and three-nucleon interactions are key input in *ab initio* nuclear structure computations
- A decade of work has focused on hand-tuned potentials at next-to-next-to-next-to-leading order
- Computationally expensive three-nucleon forces are believed to play a pivotal role in description of nuclei and nuclear matter



Accomplishments

- The derivative-free, nonlinear least squares solver POUNDERS in TAO was used to systematically optimize potentials based solely on two-nucleon forces
- The optimization of the low-energy constants of the new interaction NNLO$_{op}$ yields a χ^2/datum of about one for laboratory scattering energies below 125 MeV. The new interaction yields very good agreement with binding energies and radii for A=3,4 nuclei.
- Less pain and more gain: NNLO$_{opt}$ captures key aspects of nuclear structure without resorting to three-nucleon forces.

Caption: The ground-state energies of oxygen isotopes obtained in coupled cluster method with the NNLO$_{opt}$ interaction obtained in this work and the previous interaction N^{3}LO$_{EM}$ compared with experiment. The inset shows the first 2$^+$ state in selected calcium isotopes.

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Reference: A. Ekström et al., Phys. Rev. Lett 110, 192502 (2013)

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