For atomic nuclei, three's a crowd
Enabling microscopic calculations of nuclei

Main contact for this slide:

Richard Furnstahl, Ohio State University (furnstahl.1@osu.edu) (614) 292-4830

References:

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"Similarity Renormalization Group for nucleon-nucleon interactions", S.K. Bogner, R.J. Furnstahl, and R.J. Perry, Phys. Rev. C 75, 061001 (2007).

The Team:

This collaboration involves Eric Anderson, Richard Furnstahl, Robert Perry (Ohio State University); Eric Jurgenson (OSU now LLNL); Petr Navratil (LLNL); Scott Bogner (Michigan State University); Achim Schwenk (TRIUMF). It is supported by UNEDF grants DE-FC02-09ER41586 and DE-FC02-0741457, DOE contract DC-AC52-07NA27344 and NSF grant PHY-0653312.

About the graphics:

Top-right: Because celestial bodies can deform from tidal forces, the gravitational force on the earth from the sun and moon is not just the net force from considering them as isolated pairs. The additional interaction is a three-body force. An analogous situation holds for interacting nucleons, because protons and neutrons are composite. This force is important for nuclear binding energies (about 1 MeV out of 8 MeV for the triton) and has important spin-isospin dependences. Unfortunately, including three-body forces is computationally expensive, which restricts the size of systems that can be calculated.
Center-left: The computational cost can be greatly reduced by using the Similarity Renormalization Group (SRG) to soften the forces. The figure shows the SRG evolution of the two-body force represented as a matrix in momentum variables. The large short-range repulsion (manifested as red regions) is driven toward zero (non-green) values away from the diagonal, which means high energy is decoupled from low energy and can be neglected. At the same time, the initial three-body force between nucleons must also evolve. Until recently, this was an unsolved technical challenge.
Bottom-right: The black curve shows the convergence of the ground-state energy of Helium-4 as a function of the Hamiltonian matrix size that is diagonalized. The actual dimension of the matrix grows very rapidly with the plotted size Nmax and only lower values are feasible in larger nuclei. The Hamiltonian here includes a chiral effective field theory two-body (NN) potential plus a corresponding three-

body (NNN) potential. The red curve shows the convergence using the newly evolved three-body force. The softening of the interaction greatly accelerates the convergence and even a small matrix gives a reasonable approximation.

What was accomplished:
The Similarity Renormalization Group method was extended to few-body forces by using the harmonic oscillator basis technology from the No-Core Shell Model (NCSM). To produce the interaction used here, twenty million coupled differential equations were solved. This is not a large-scale computational problem in itself, but these interactions now become inputs to NCSM and coupled cluster (CC) calculations that reach to the petascale and beyond.

The impact this accomplishment will have on science, computing, energy, or the environment:
Understanding nuclear structure and reactions from microscopic forces is a key component of several DOE milestones for nuclear physics. The development of these interactions is a key step toward making calculations of larger nuclei feasible using methods that expand the nuclear wave function in a basis (e.g., NCSM and CC).

Resources and approaches (facilities, computing resources, software, innovative approaches, etc.) used:
The development are funded through the SciDAC-2 UNEDF project. This was the first application of SRG flow equations to nuclear physics problems.

What future efforts associated with and/or motivated by this accomplishment are proposed and why?
This work is an important step towards the long-term goal of a microscopic description of nuclei. In the near term, we will extend the tests of the softened interactions to Lithium isotopes. In collaboration with other members of the UNEDF collaboration we will explore heavier nuclei with NCSM and CC calculations, and there will be applications to reactions through the NCSM plus resonating group method (RGM).