Predictions for Proton-Dripping Fluorine-14

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Overview: Predicting properties of nuclei, before they are measured experimentally, constitutes a major challenge for theoretical nuclear physics. It also provides important input for planning experiments and analyzing results. Using *ab initio* nuclear theory, a first-principles approach, the Jaguar facility at ORNL (INCITE award), the Franklin facility at NERSC, with dramatically improved algorithms and codes (UNEDF and TOPS awards under SciDAC), we have successfully solved the quantum many-body problem for yet-to-be-observed Fluourine-14. We predict the mass of this nucleus, its low-lying excited states, and its proton emission energy to more stable Oxygen-13. All states are found to be unbound resonances that decay by proton emission ("proton dripping") to produce lighter and more stable nuclei. They will be appear as resonances associated with the formation of Fluourine-14 in the collision of a radioactive Oxygen-13 beam with a hydrogen target, a reaction planned for the first Fluourine-14 observation.

Significance:
Nuclei constitute 99% of the visible matter in the universe and a detailed theoretical understanding of their properties is of fundamental importance for nuclear astrophysics and for practical applications: developing new energy sources, such as fusion reactors, or improving other energy sources, such as nuclear reactors. Progress in these important applications is hampered by a lack of knowledge of nuclei in regions that are hard to access by direct experimental measurements. For this reason, we need a robust nuclear theory with verifiable predictive power to calculate those properties, their structure and reaction cross sections. To achieve this goal, we have developed state-of-the-art theory, based on first principles, along with advanced algorithms and codes that run efficiently on massively parallel computers to produce precision results. To test the current status of these advances, we challenged ourselves to produce predictions for an unstable nucleus, Flourine-14, that has yet to be observed in an experiment. Experiments currently underway at the DOE-supported Cyclotron Institute, Texas A&M University, use our results for preparation and analysis. Comparison with experiment will then provide the ultimate test of the predictive power of the theory and calibrate where we stand on achieving the long-term goal of simulating nuclear properties for systems relevant to energy generation.

Impact:
This multi-faceted research effort directly impacts DOE's science and computing missions with longer-term implications for DOE's energy mission. The primary impacts include development and testing of new nuclear interactions along with a computational quantum many-body framework having, in aggregate, a robust predictive power. One key science goal is the determination of the strong interaction, especially in extreme domains of the nuclear environment such as systems with a high ratio of protons to neutrons. This work underpins that effort since our predictions for Fluorine-14, when compared with forthcoming experimental results, will reveal the role of the elusive three-nucleon interaction in regions not easily accessible by other means and validate the nuclear structure simulation algorithms and methods.

Resources and approaches:
We have developed leading-edge theory, algorithms and codes to carry out this investigation. The bulk of the work involves the calculation of eigenvalues and eigenvectors of a large sparse matrix and requires the distribution of workload evenly over more than 30,000 compute cores. This technological achievement is noteworthy itself and is having an impact of code library developments. We used DOE's Jaguar facility for the largest production runs along with NERSC facilities for other runs production runs and development/testing.

Collaboration:
These results emerged from a request by Texas A&M experimentalists and from a multi-institution collaboration (Iowa State University, Moscow State University, Ames Laboratory, Lawrence Berkeley National Laboratory). Our progress benefited greatly from additional collaborations in closely aligned research areas with scientists in other DOE-sponsored groups: Lawrence Livermore National Laboratory

(Navratil, Ormand), Ohio State University (Furnstahl), Michigan State University (Bogner), and Oak Ridge National Laboratory (Dean, Nam).

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Future:
We motivate continued development of the *ab initio* nuclear many-body theory, to improve the theory of the underlying strong two-nucleon and three-nucleon interactions, and to develop additional methods for applications to reactions that are costly or impossible to access experimentally. These future efforts will also help in the efficient and productive use of DOE's experimental facilities, such as FRIB.

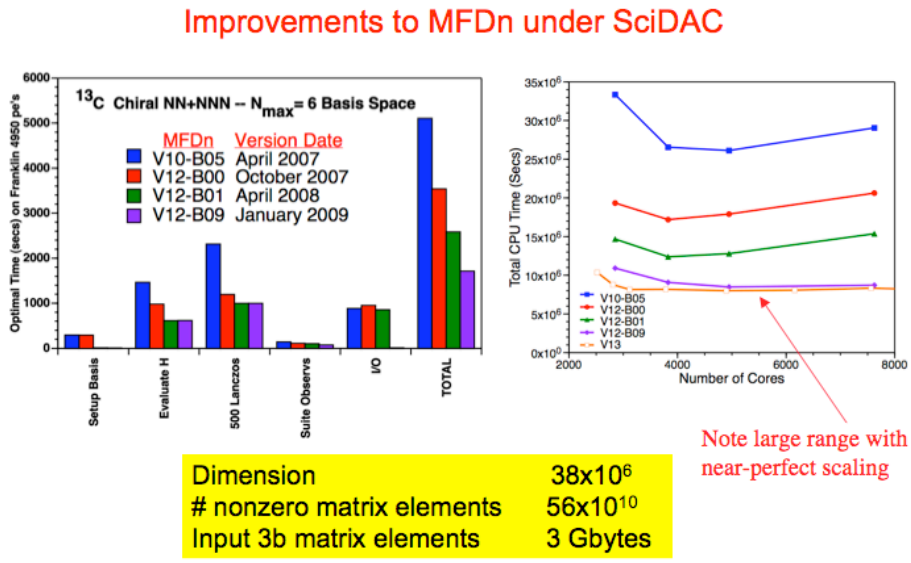

Figure 1. Measures of algorithm and code performance improvements gained with UNEDF and TOPS support. A standard test case is run with versions of the code MFDn developed over time from an initial (pre-SciDAC) version in April 2007 up through a recent version, V13. Total wallclock time is reduced by about a factor of 3 (left panel) and scaling performance is significantly improved (right panel).