NUCLEI at Leadership-Class

The NUCLEI (NUclear Computational Low-Energy Initiative) SciDAC project

- Is a collaboration of nuclear physicists, applied mathematicians and computer scientists using high-performance computing to explore the nuclear landscape.
- Provides results critical to nuclear science and nuclear astrophysics, and to nuclear applications in energy and national security.
- Addresses physics topics including nuclear interactions and their uncertainties, ab initio studies of light nuclei and their reactions and of nucleonic matter and its astrophysical properties.
- Fundamentally advances the studies of neutron-rich nuclei and the fission of heavy nuclei, and the key nuclear physics issues in neutron stars and tests of fundamental symmetries.

To continue to push scientific frontiers in low-energy nuclear physics, NUCLEI application teams work to effectively utilize high-performance computing resources. NUCLEI project members have utilized computing resources at the OLCF and ALCF through the INCITE program since 2008.

Structure of the Exotic Halo Nucleus $^4$He

The no-core shell model combined with the resonating-group method (NCSM_RGM) was used on Titan to present the first ab initio calculation of the continuum spectrum of $^4$He as a $4\pi e^++n$ system starting from a nucleon-nucleon (NN) interaction that describes two-nucleon properties with high accuracy.

Comparison of the energy spectrum from recent measurements at G4AC, consistency with the presence of the second low-lying negative $2^-$ resonance obtained for the first time in this experiment. Additional resonances states emerge in these calculations in the $2^-$ and $1^+$ channels near the second $2^-$ resonance and in the $0^+$ at slightly higher energy. There was no evidence of low-lying resonances in the $0^+$ and $1^+$ channels.

Ab Initio Extreme Neutron Matter

The Hamiltonian matrix evaluation and diagonalization code MFDn ("Many-Fermion Dynamics – nuclear") solves the nuclear problem with the no-core shell model. It can be used to predict properties of neutron-rich systems which relate to exotic nuclei and nuclear astrophysics and to guide future experiments at DOE-sponsored rare isotope production facilities.

Spontaneous Fission Lifetimes

Spontaneous fission is a magnificent example of a motion during which the nucleus evolves in a multidimensional space of complex shapes, going through regions that are forbidden by classical mechanics. HFODD, a nuclear Density Functional Theory code, uses Titan to investigate the dynamical evolution of the heavy nucleus fermium-264 from its ground state to its symmetric split into two $^{132}$ nuclei.

Dynamic and static paths for spontaneous fission of $^{264}$Fm in the $50$-plane of elongation ($Q_5$) andinity ($Q_2$) obtained by minimizing the collective action integral. It is shown that the fusion pathway connects the slightly deformed ground-state of $^{260}$Fm with the $^{150}$Yb+$^{114}$Xe pre-scission configuration through a family of elongated rotational shapes, thus bypassing the axial saddle (fission barrier).

Streamlining the Nuclear Force

The computationally expensive three-nucleon force (3NF) play an important role in the description of nuclei and nuclear matter. Using state-of-the-art optimization methods to construct a high-precision potential andNUCCOR on Titan, NUCLEI members showed that key aspects of atomic nuclei, such as the characteristics of "magic" nuclei, can be understood with two-nucleon forces alone. In light of this, the role of 3NFs needs to be revisited.

- The derivative-free, nonlinear least squares solver POWDERERS in TAO was used to systematically optimize potentials from chiral effective field theory up to next leading order in the phase-shift analysis based solely on two-nucleon forces.
- The optimization of the low-energy constants of the new interaction NW0 (input) through ab initio Hartree-Fock calculations of the $\alpha$ decay, which is the main part of the current experiment. The inset shows the first $2^+$ state in the $\alpha$ decay.