NUCLEI advances through INCITE

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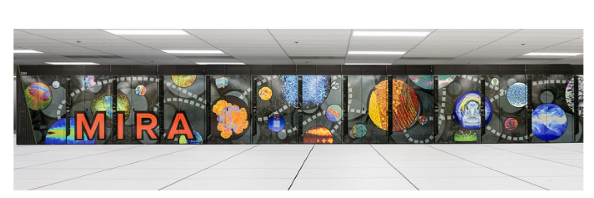
NUCLEI project members are advancing low-energy nuclear physics using DOE's Leadership Computing Facilities through the INCITE program. These computing resources are crucial to developing a microscopic description of nuclear structure and nuclear reactions that retains predictive power and carries quantified uncertainties, which is vital for the future development of nuclear energy and nuclear security and in industrial and medical applications that use stable or radioactive isotopes.

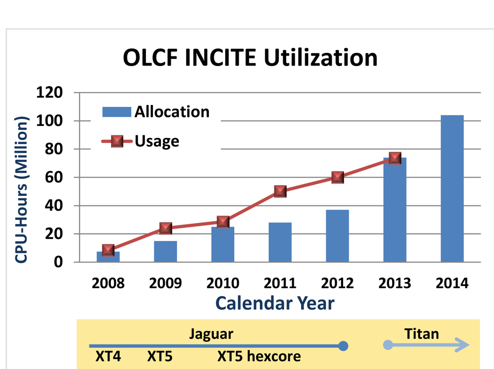
NUCLEI at Leadership-Class

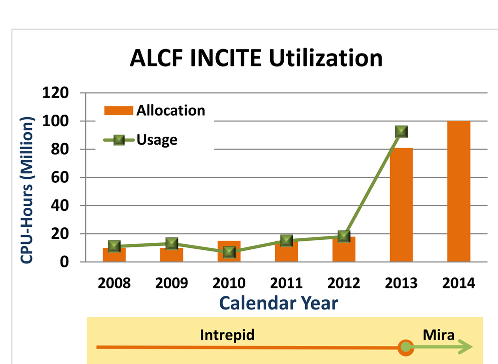
The NUCLEI (NUclear Computational Low-Energy Initiative) SciDAC project

- 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.



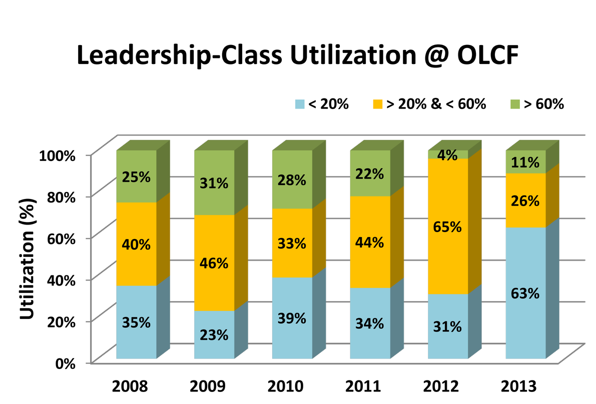




Allocation and utilization at the OLCF the ALCF during CY 2008 – 2013 and allocation for 2014.

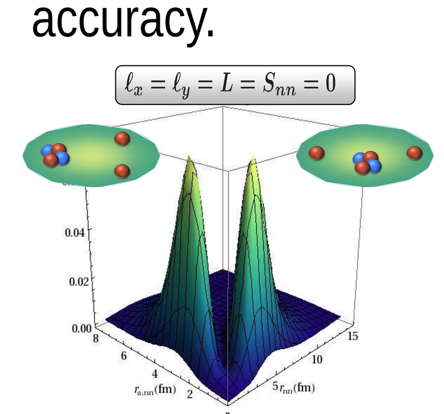
NUCLEI applications running at the OLCF consistently use over 35% of the allocation on leadership-class jobs utilizing 20% of the machine or more.

Application	Production Run Size	Dense Linear Alg.	Sparse Linear Alg.
MFDn: Many Fermion Dynamics - nuclear	260K cores @ 4 hrs 500K cores @ 1.33 hrs		X
NUCCOR: Nuclear Coupled-Cluster Oak Ridge, m-scheme & spherical	100K cores @ 5 hrs (1 nucleus, multiple parameters)		X
DFT Code Suite: Density Functional Theory, mean-field methods	100K cores @ 10 hrs (entire mass table, fission barriers)	X	
NCSM_RGM: Resonating Group Method for scattering	98,304 cores @ 8 hrs	X	X



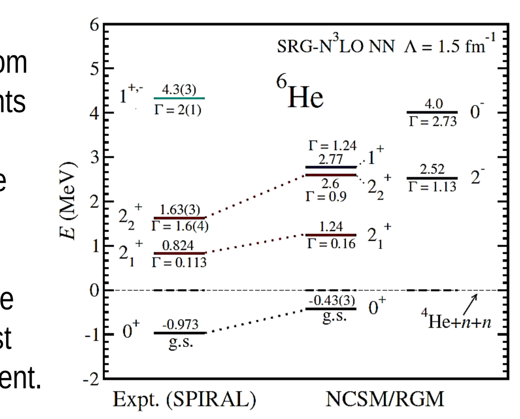
Structure of the Exotic Halo Nucleus ^{6}He

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 ^{6}He as a ^{4}He+n+n system starting from a nucleon-nucleon (NN) interaction that describes two-nucleon properties with high accuracy.



Information about the three-cluster structure of the ^{6}He ground state can be obtained by studying the probability distribution arising from the main component of the ^{4}He+n+n relative motion wave function. One peak shows the "dineutron" configuration in which the neutrons are close together and the ^{4}He core is separated from their center of mass at a distance of about 3 fm, whereas the second peak, corresponds to a "cigar" configuration with an almost-linear structure where the two neutrons are far apart.

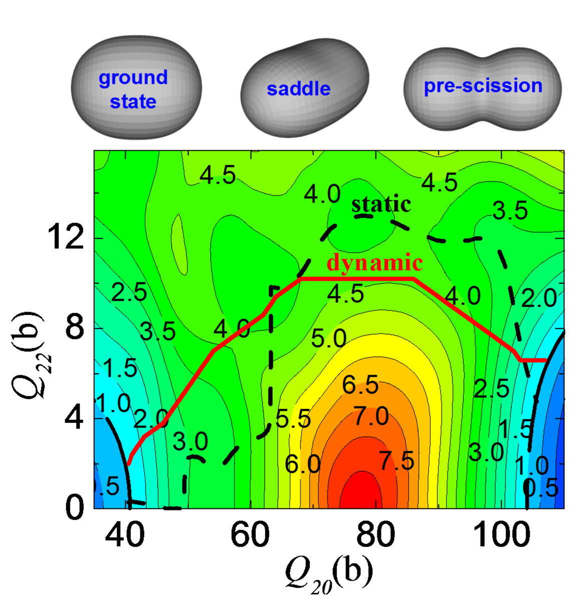
Comparison of the energy spectrum from recent measurements at GANIL show consistency with the presence of the second low-lying narrow 2^+ resonance observed for the first time in this experiment. Additional resonant states emerge in these calculations in the 2^- and 1^+ channels near the second 2^+ resonance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



^{4}He+n+n continuum within an ab initio framework, C. Romero-Redondo, S. Quaglioni, P. Navratil, G. Hupin, Phy. Rev. Lett. 113, 032503 (2014); *Three-cluster dynamics within an ab initio framework*, S. Quaglioni, C. Romero-Redondo, P. Navratil, Phys. Rev. C 88, 034320 (2013)

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 tin-132 nuclei.

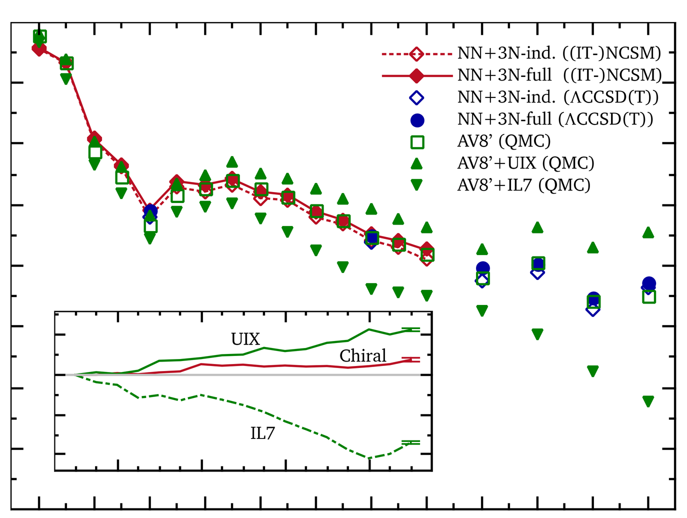


Dynamic and static paths for spontaneous fission of 264Fm in the 2D plane of elongation (Q_{20}) and triaxiality (Q_{22}) obtained by minimizing the collective action integral. It is seen that the fission pathway connects the slightly deformed ground-state of ^{264}Fm with the ^{132}Sn+^{132}Sn pre-scission configuration through the family of elongated triaxial shapes, thus bypassing the axial saddle (inner fission barrier).

Spontaneous fission lifetimes from the minimization of self-consistent collective action, J. Sadhukhan, K. Mazurek, A. Baran, J. Dobaczewski, W. Nazarewicz, J. A. Sheikh, Phys. Rev. C 88, 064314 (2013)

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.



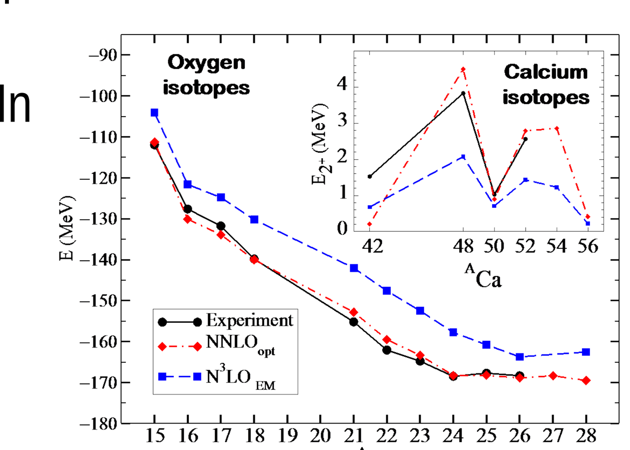
Comparison of ground state energies of systems with N neutrons trapped in a harmonic oscillator with strength 10 MeV. Solid red diamonds and blue dots signify new results with two-nucleon (NN) plus three-nucleon (3N) interactions derived from chiral effective field theory related to QCD. Inset displays the ratio of NN+3N to NN alone for the different interactions. Note that with increasing N, the chiral predictions lie between results from different high-precision phenomenological interactions, i.e. between AV8'+UIX and AV8'+IL7.

Properties of trapped neutrons interactive with realistic nuclear Hamiltonians, P. Maris, J. P. Vary, S. Gandolfi, J. Carlson, S. Pieper, Phys. Rev. C 87, 054318 (2013); Ab initio study of neutron drops with chiral Hamiltonians, H.D. Potter et al., arxiv1406.1160 (submitted)

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 and NUCCOR 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 POUNDERS in TAO was used to systematically optimize potentials from chiral effective field theory at next-to-next-to leading order in the phase-shift analysis based solely on two-nucleon forces.
- The optimization of the low-energy constants of the new interaction $NNLO_{opt}$ yields a chi^2/datum of about one for laboratory scattering energies below 125 MeV. The new interaction yields very good agreement with experiment for binding energies and radii for A=3,4 nuclei.
- Massively parallel sensitivity analysis performed to guide nuclear structure modeling.



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

An optimized chiral nucleon-nucleon interaction at next-to-next-to-leading order, A. Ekström, G. Baardsen, C. Forssén, G. Hagen, M. Hjorth-Jensen, G. R. Jansen, R. Machleidt, W. Nazarewicz, T. Papenbrock, J. Sarich, S. M. Wild, Phys. Rev. Lett. 110, 192502 (2013).

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