Scientific Discovery in NUCLEI through Collaboration

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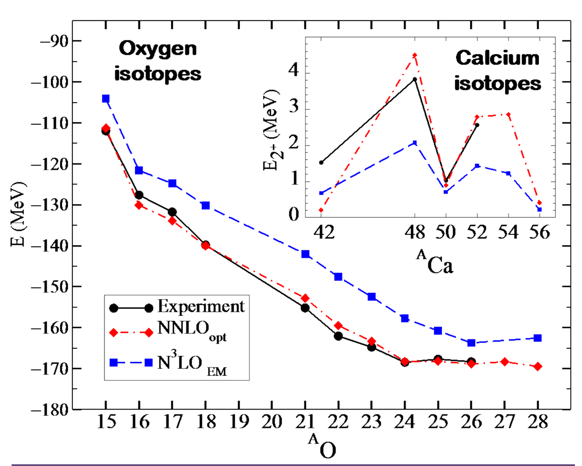
A microscopic description of nuclear structure and nuclear reactions that retains predictive power and carries quantified uncertainties is vital for the future development of nuclear energy and nuclear security and in industrial and medical applications that use stable or radioactive isotopes. This work highlights NUCLEI's close collaborations between domain scientists, applied mathematicians, and computer scientists to enable these complex calculations on leadership-class computing systems.

Streamlining the nuclear force with SUPER

The strong force can be systematically derived as a series of pion-exchanges. In the past decade very precise models of the strong force resulted from this procedure. In these models, the computationally expensive three-nucleon forces are believed to play a smaller but pivotal role in the description of nuclei and nuclear matter.



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.

Collaborators in NUCLEI and SUPER revisited these models and used state-of-the-art optimization methods to construct a high-precision potential. They showed that key aspects of atomic nuclei, such as the enhanced binding of "magic" nuclei, might be understood with two-nucleon forces alone. The new model requires less computational resources than the previous models.

- 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.

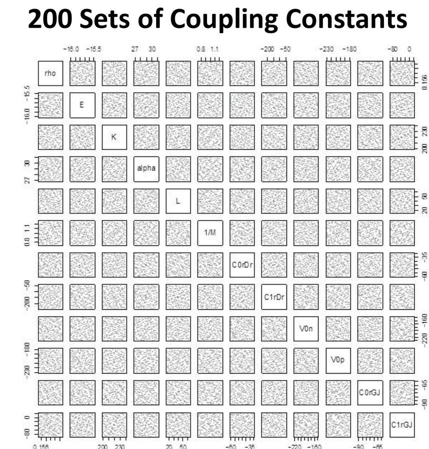
An optimized chiral nucleon-nucleon interaction at next-to-next-to-leading order, A. Ekström, G. Baardsen, C. Forssén, G. Hagen, M. Hjorth-Jensen, G. R. Jansen, R. Machleidt, W. Nazarewicz, T. Papenbrock, J. Sarich, S. M. Wild, Phys. Rev. Lett. 110, 192502 (2013).

Uncertainty quantification with QUEST

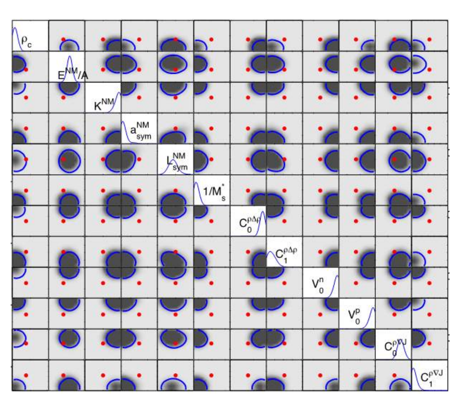
Density functional theory (DFT) has proven useful for describing the ground state properties of nuclei across the nuclear chart. To explore unknown nuclei, such as neutron-rich and super-heavy nuclei, we must quantify the reliability of our predictions.

We couple Bayesian model calibration with large-scale computing to understand the propagation of error in our models. **Bayesian Model Calibration** uses an ensemble of model runs and a Gaussian Process model to emulate the DFT model's output at untried input parameter settings. With this "emulator," the resulting posterior distribution for the DFT parameters is estimated with Markov Chain Monte Carlo.

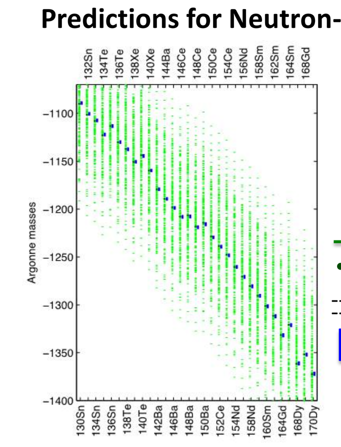
200 Sets of Coupling Constants



Posterior parameter uncertainties



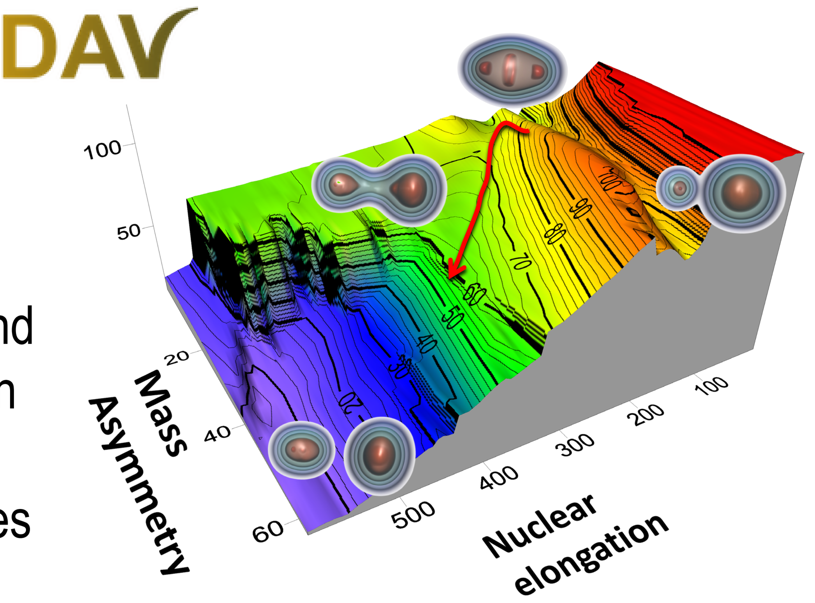
Predictions for Neutron-Rich Isotopes

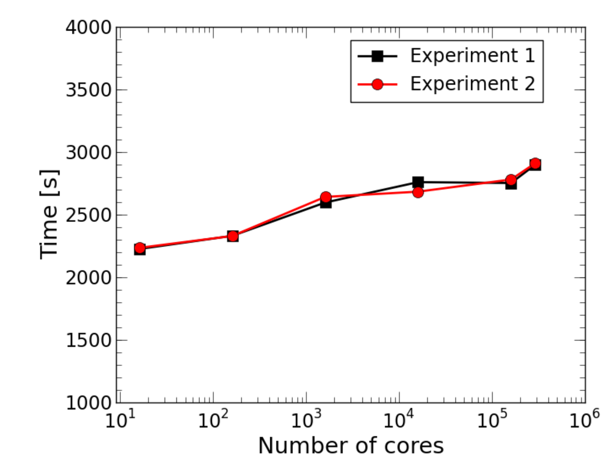


Resulting parameter uncertainty can be propagated to estimate the uncertainty for our predictions of masses across the table of isotopes, including new isotopes measured at Argonne National Laboratory or at the future FRIB. **Sensitivity analyses** can help determine the expected reduction in parameter uncertainty that would be produced by the information from new experiments. This provides an important guide for experimental campaigns to strategically target the measurements that will most refine our models and our understanding.

Scaling I/O with SDAV

DFT is the tool of choice to study complex decay modes of heavy elements such as nuclear fission. Simulation I/O, data management and workflow are significant challenges in the context of the large multi-dimensional potential energy surfaces needed to simulate fission.



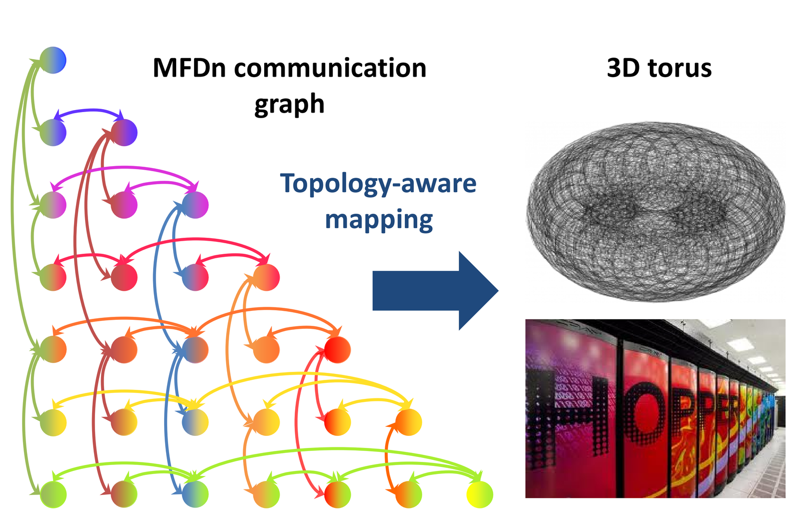


Working closely with SDAV members, we integrate the Adaptable IO System (ADIOS) framework from the SDAV toolkit into HFODD, a nuclear DFT application, to manage I/O from tens of thousands of files generated during a single simulation. ADIOS enables a flexible interface to manage data that may be written, read, or processed outside of the running simulation.

HFODD solves self-consistently a system of coupled nonlinear integro-differential equations to characterize nuclei with no assumption of symmetry. It should scale weakly as we increase the number of cores with the number of nuclear configurations under study. At large scale, the performance suffers due to I/O. ADIOS will address the performance degradation and is the first step toward workflow integration.

Scalable eigensolver for MFDn from FASTMATH

The Hamiltonian matrix evaluation and diagonalization code MFDn ("Many-Fermion Dynamics – nuclear"), has been the key tool used in over 75 publications to date, including 18 in *Physical Review Letters,* to solve the nuclear problem with the no-core shell model.



Topology-aware mapping of processes to the physical processors becomes more important as the gap between computational power and bandwidth widens. Communication groups are optimized through a column-major ordering of processes on the triangular grid.

The largest runs of MFDn use more than 250,000 cores and 4 hours of wall-clock time on Jaguar/Titan. MFDn was used on Jaguar to solve for a speculative nucleus, ^{14}F, which was later confirmed experimentally, and also resolved the puzzle of the anomalous long lifetime of the ^{14}C.

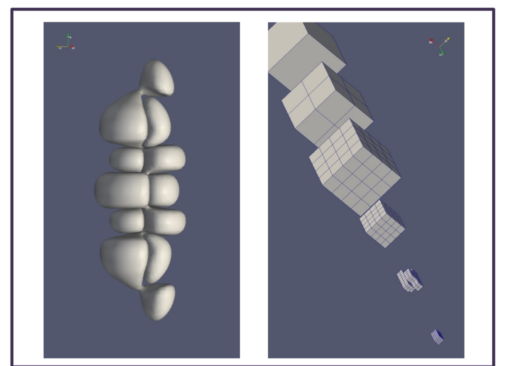
MFDn requires an efficient and scalable iterative solver for extreme scale eigenvalue problems arising in nuclear physics. Collaborations with members of FASTMATH have resulted in:

- Drastically reduced communication overheads through communication hiding and topology-aware mapping.
- Significant speed-ups over earlier version of MFDn (up to 6x on 18,000 cores)
- Almost perfect strong scaling up to 260,000 cores on Jaguar

Topology-Aware Mappings for Large-Scale Eigenvalue Problems, H.M. Aktulga, C. Yang, P. Maris, J.P. Vary, E.G. Ng, Euro-Par 2012 Conference.
Improving the Scalability of a Symmetric Iterative Eigensolver for Multi-core Platforms, H.M. Aktulga, C. Yang, E.G. Ng, P. Maris, J.P. Vary, CCP&E, accepted for publication.

Tackling complex topologies with MADNESS

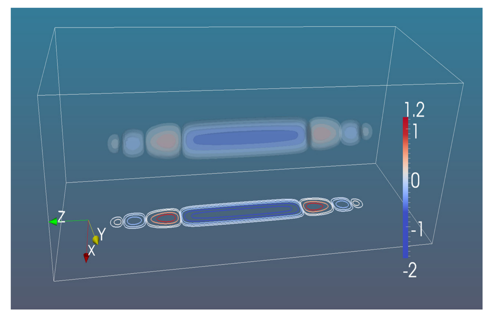
The description of superfluid Fermi systems with complex topologies and significant spatial extend is necessary to study systems such as fissioning nuclei, weakly-bound nuclei, nuclear matter in the neutron star crust, and ultracold Fermi atoms in elongated traps.



An isosurface of the 45th quasiparticle wavefunction for an ASLDA DFT simulation is shown, with six levels of multiresolution support structure. For a given precision, each wave functions is expanded in the multiwavelet basis with an oct-tree structure for the union of the supports of the multiwavelets. The multiresolution geometry adapts to include only the support with significant wavelet contributions during the course of computation. Cubes with trivial contributions to the computation are deleted.

MADNESS-HFB solves the self-consistent Hartree-Fock-Bogoliubov problem in large boxes accurately in coordinate space. It uses novel multi-resolution analysis based adaptive pseudo-spectral techniques to enable fully parallel 3D calculations of very large systems.

- MADNESS is a scalable and adaptive computational tool to describe many-body nuclear and atomic problems involving complex geometries within the superfluid density functional theory.
- MADNESS uses high-order adaptive spectral approximations with an Object-Oriented solver environment to reduce simulation uncertainties and numerical errors.
- MADNESS enables rigorous computational predictive modeling in complex physical systems in large and asymmetric domains.



The local 3-D pairing density for a HFB cold-fermion simulation computed by MADNESS-HFB is shown. The transversal oscillations of the pairing field are indicative of the Larkin-Ovchinnikov phase. The simulation used a box of width 320 fermis.

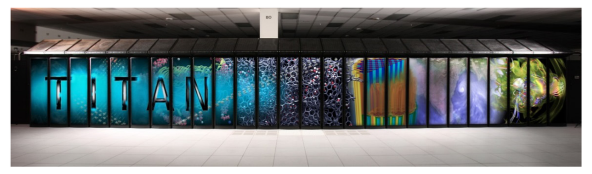
Coordinate-space Hartree-Fock-Bogoliubov Solvers for Superfluid Fermi systems in large boxes, J. Pei, G. Fann, R. J. Harrison, W. Nazarewicz, J. Hill, D. Galindo, J. Jia, J. Phys. Conf. Series **402** (2012) 012035.

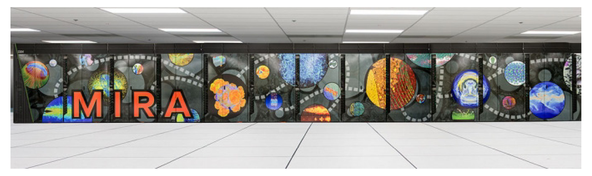
Computing at leadership-class with INCITE

To continue to push scientific frontiers in low-energy nuclear physics, NUCLEI application teams with diverse scientific backgrounds are addressing the challenges created by the considerable change in computing architectures. Close collaboration between nuclear physicists, applied mathematicians, and computer scientists enable NUCLEI researchers to effectively utilize high-performance computing resources.

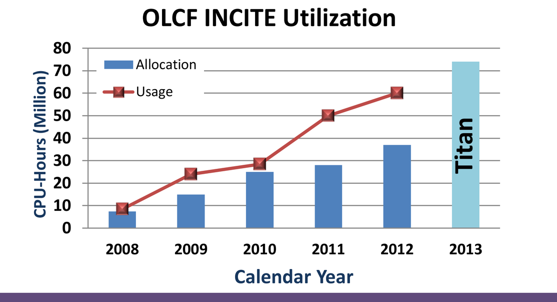
Leadership-class computing resources

NUCLEI project members have been awarded allocations at DOE's Leadership Computing Facilities through the INCITE program since 2008. These computing resources are crucial to scientific discovery in low-energy nuclear physics, both experiment and theory.

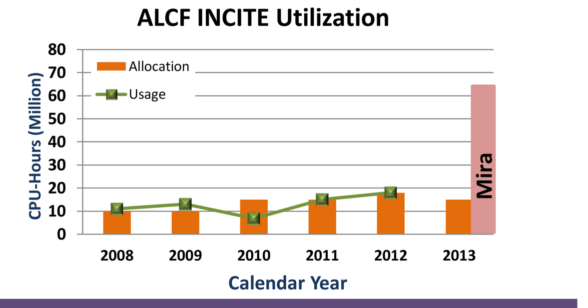




OLCF INCITE Utilization



ALCF INCITE Utilization



Allocation and utilization at the OLCF the ALCF during CY 2008 – 2012 and allocation for 2013.

NUCLEI
Nuclear Computational Low-Energy Initiative