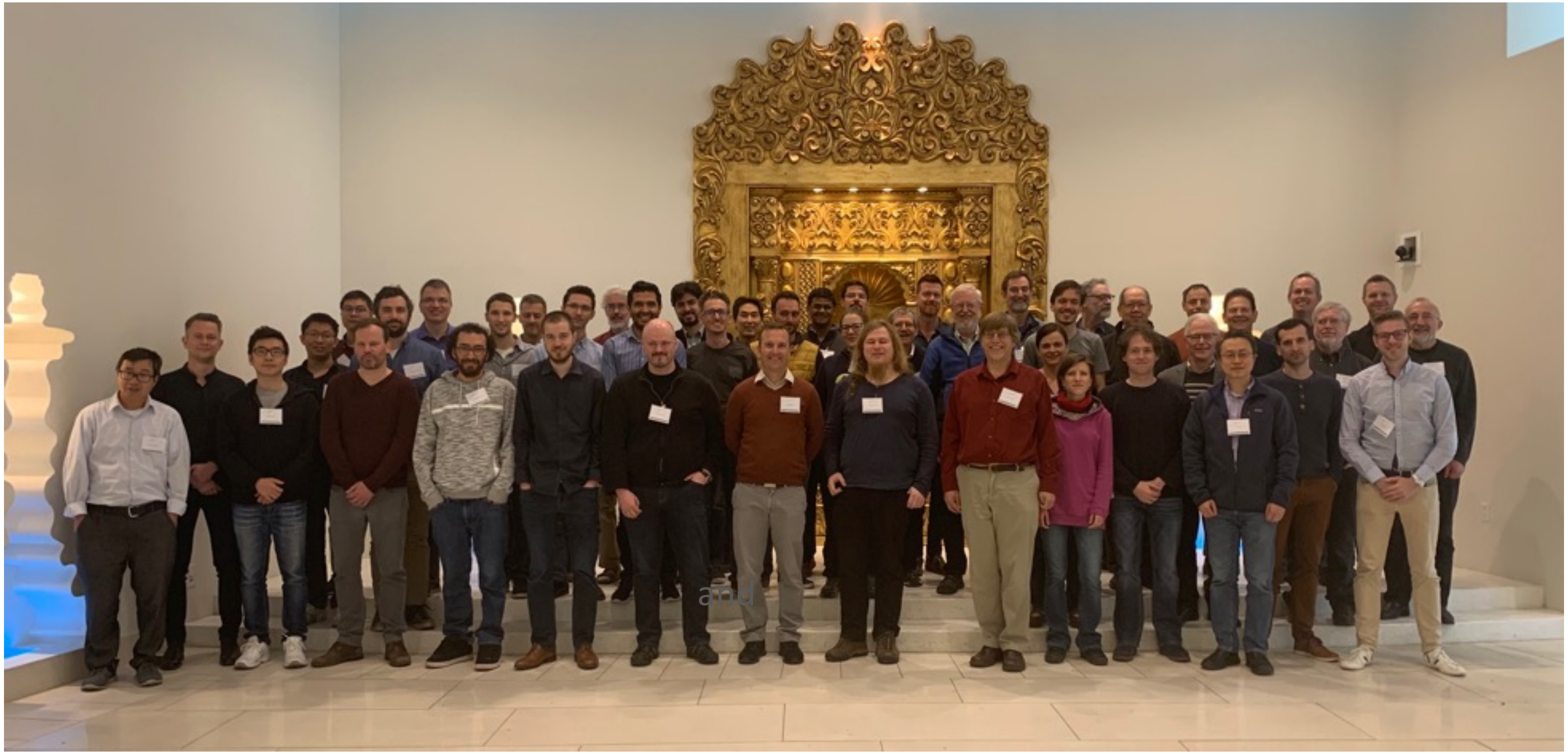
SciDAC-4 collaboration NUCLEI



Thomas Papenbrock, University of Tennessee / ORNL

SciDAC PI Meeting

July 17, 2019

Research funded by the US Department of Energy

SciDAC
Scientific Discovery through Advanced Computing

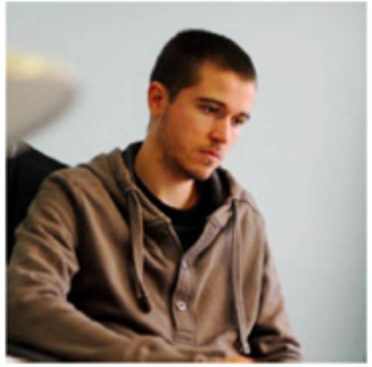
NUCLEI
Nuclear Computational Low-Energy Initiative

Good news! NUCLEI researcher successes

Metin Aktulga: NSF Career Award

Pieter Maris: leads NESAP award team

Stefan Wild: SIAG/CSE program director



Kevin Fossez FRIB Fellow ANL/MSU

Sarah Wesolowski faculty Salisbury U.

Ingo Tews LANL staff scientist

NUCLEI – a national collaboration

Argonne NATIONAL LABORATORY

UNIVERSITY OF OREGON

THE UNIVERSITY of TENNESSEE UT KNOXVILLE

BERKELEY LAB
Lawrence Berkeley National Laboratory

THE UNIVERSITY of NORTH CAROLINA at CHAPEL HILL

NUCLEI
Nuclear Computational Low-Energy Initiative
A SciDAC-4 Project

THE OHIO STATE UNIVERSITY

INDIANA UNIVERSITY

OAK RIDGE National Laboratory

IOWA STATE UNIVERSITY

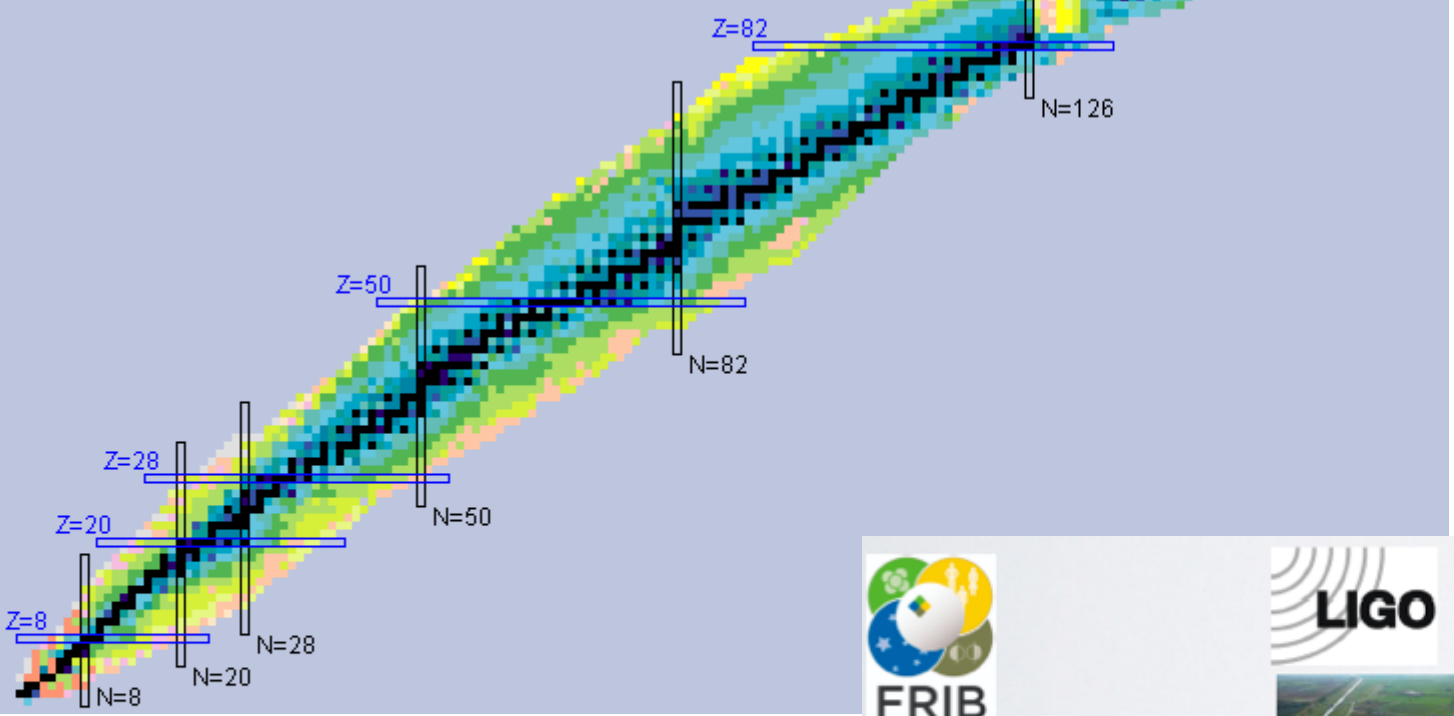
Lawrence Livermore National Laboratory

Los Alamos NATIONAL LABORATORY EST. 1943

MICHIGAN STATE UNIVERSITY

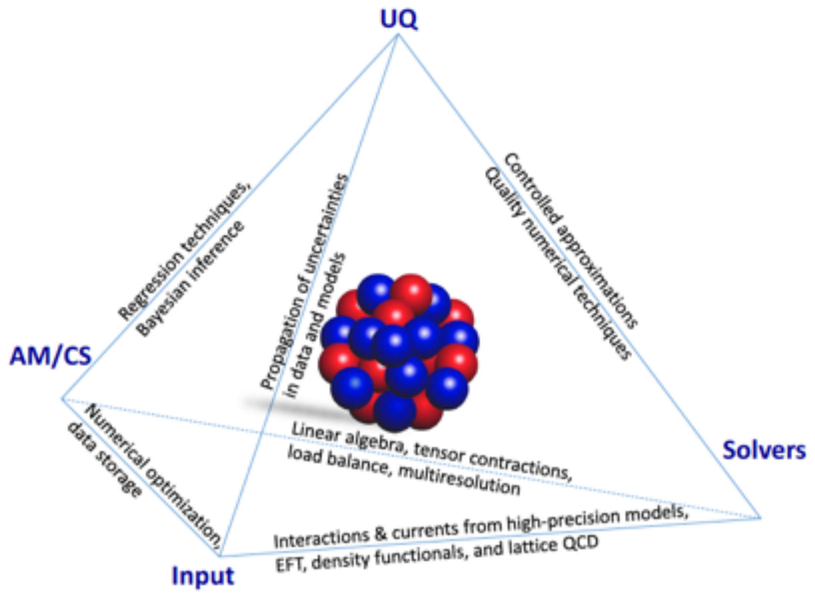
Physics of atomic nuclei

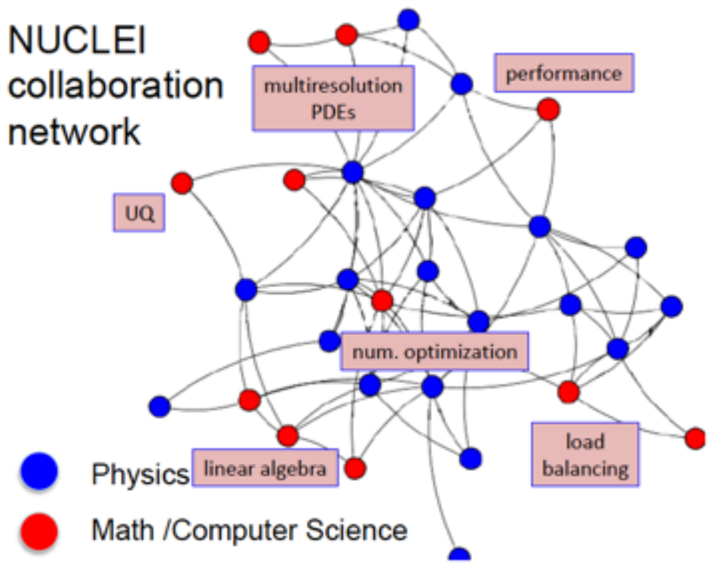
118 chemical elements (94 naturally found on Earth)
288 stable (primordial) isotopes
Thousands of short-lived isotopes

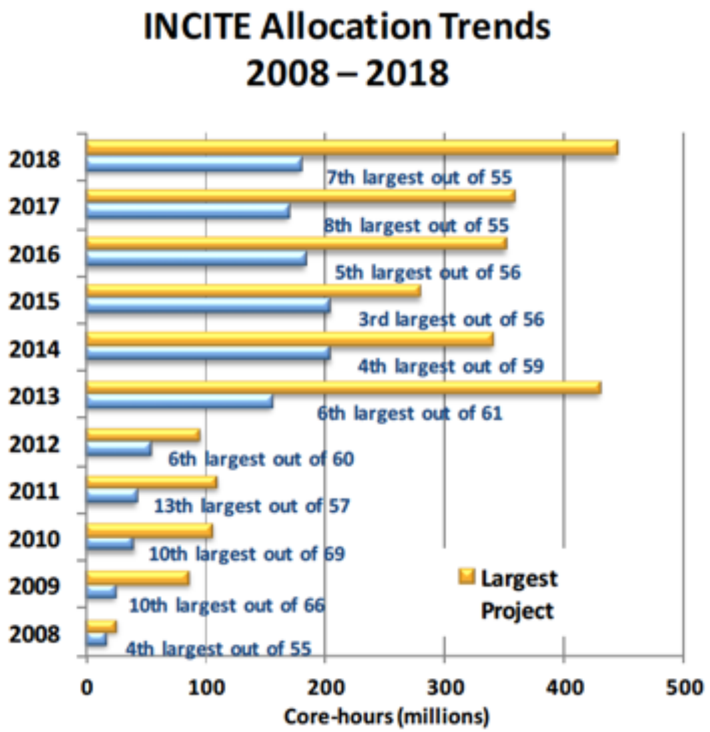


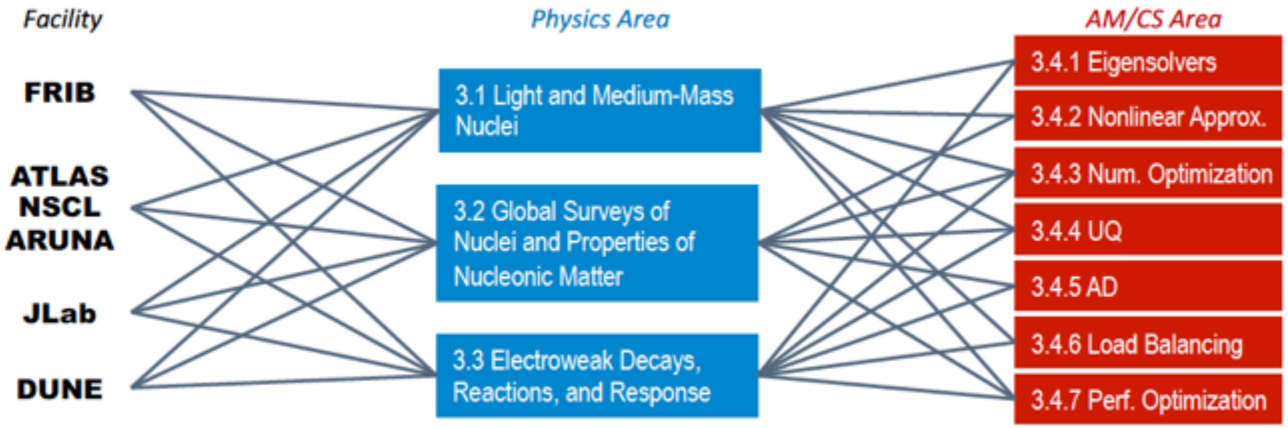
Aims:
Explore limits of nuclear binding
Link nuclei to neutron stars
Understand electroweak reactions

NUCLEI – connections between ASCR and NP

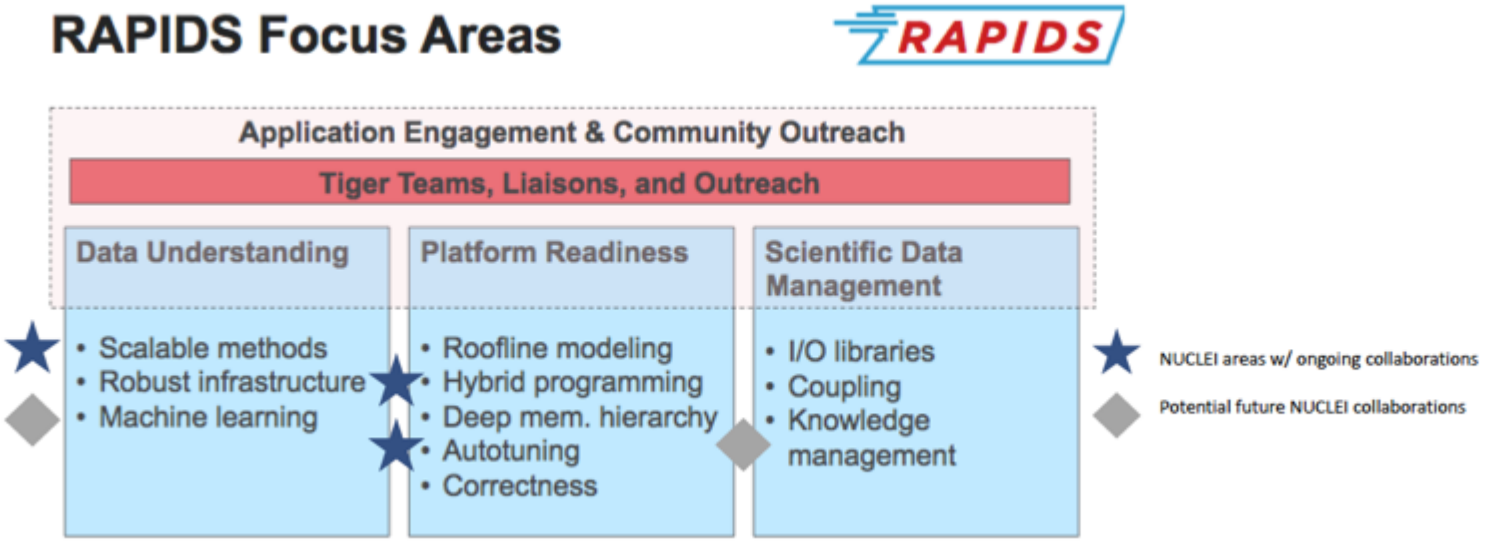


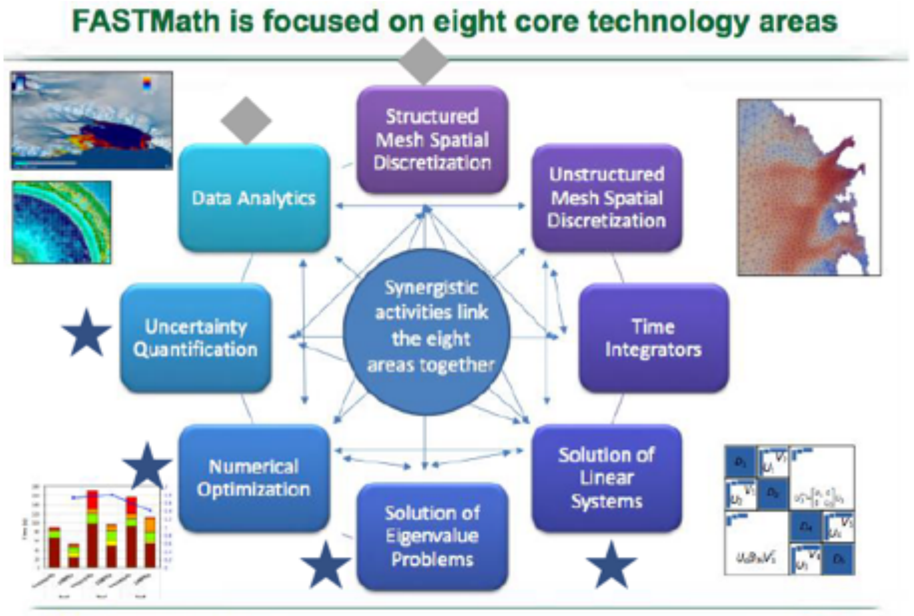






NUCLEI and SciDAC Institutes





Sustained impact of optimization for nuclear theory

Scientific Achievement

- **Parallel optimization code POUNDERS for optimizing low-energy functional**
- **Disrupted conventional manual and underoptimized approaches**

Math of complex systems: POUNDERS foundation

UNEDF SciDAC-2: UNEDF0

UNEDF SciDAC-2: UNEDF1

NUCLEI SciDAC-3: N2LOopt

NUCLEI SciDAC-4

Derivative-free optimization method developed under ASCR math program on complex systems and ASCR + NP SciDAC partnership

Nuclear energy density optimization. Kortelainen, Lesinski, Moré, Nazarewicz, Sarich, Schunck, Stoitsov, Wild. *Phys Rev C*, 2010.

Nuclear energy density optimization: Large deformations. Kortelainen, McDonnell, Nazarewicz, Reinhard, Sarich, Schunck, Stoitsov, Wild. *Phys Rev C* 2012.

An optimized chiral nucleon-nucleon interaction at next-to-next-to-leading order. Ekström, Baardsen, Forssén, Hagen, Hjorth-Jensen, Jansen, Machleidt, Nazarewicz, Papenbrock, Sarich, Wild. *Phys Rev Lett*, 2013.

Open-source, scalable implementation available in PETSc

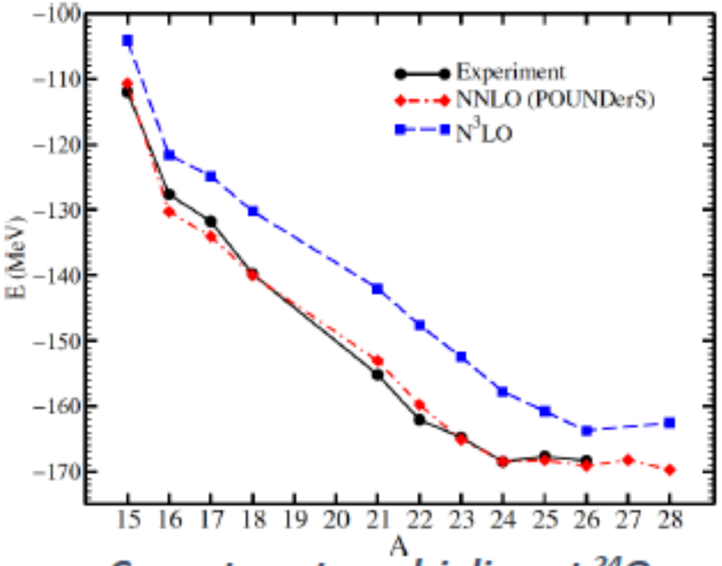
Latest developments account for correlations

mcs.anl.gov/petsc

Now Designated Essential Science Indicator Highly Cited Papers in Physics

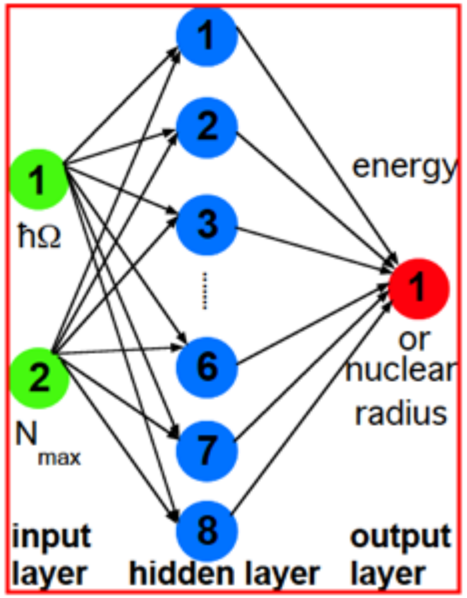
NP researchers

ASCR researchers

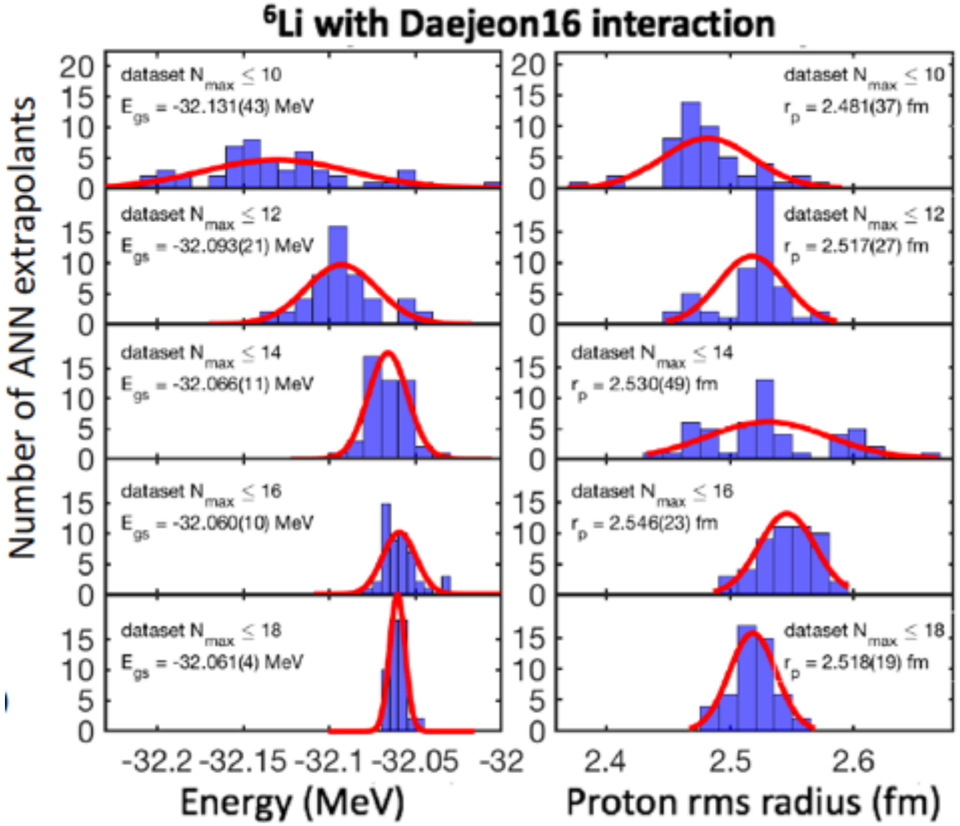


Correct neutron dripline at ^{24}O

Deep learning for nuclear binding energy and radius



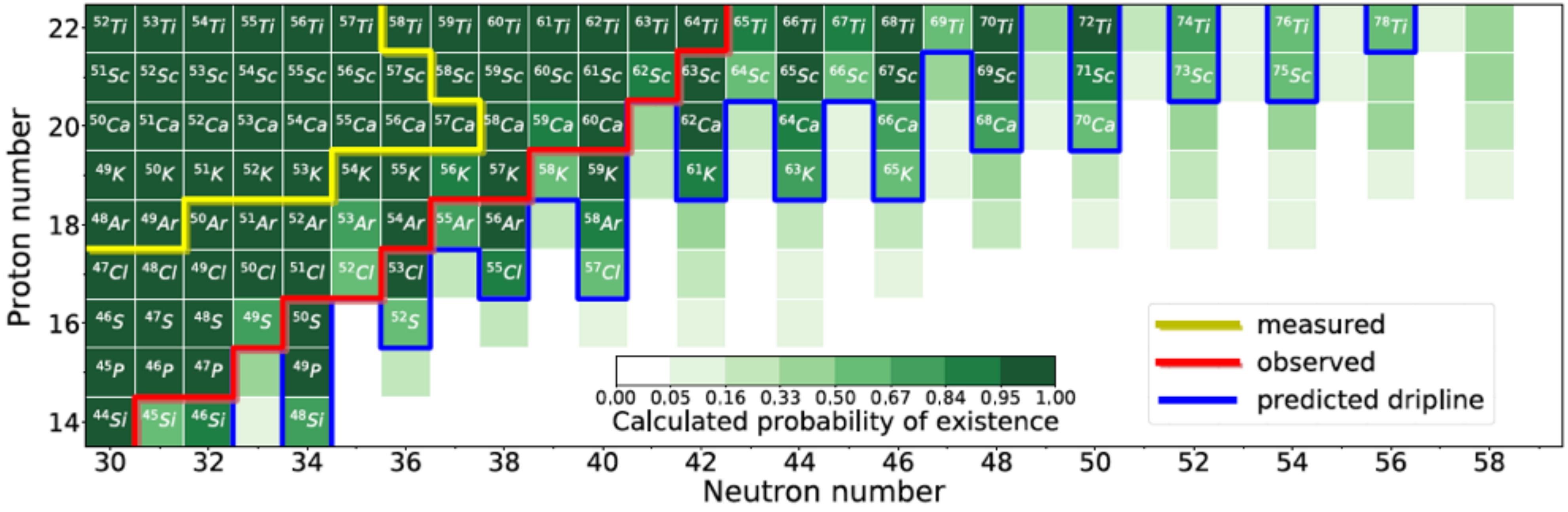
- Develop ANNs that extend the reach of high performance computing simulations of nuclei
- Predict properties of nuclei based on ab initio structure calculations in achievable basis spaces
- Produce accurate predictions of nuclear properties with quantified uncertainties using fundamental inter-nucleon interactions



- Developed artificial neural networks (ANNs) for extending the application range of the ab initio computations
- Demonstrated predictive power of ANNs for converged solutions of weakly converging simulations of the nuclear radius
- Provided a new paradigm for matching deep learning with results from high performance computing simulations

G. A. Negoita, et al., Phys. Rev. C 99, 054308 (2019)

Neutron drip line in the calcium region from Bayesian model averaging

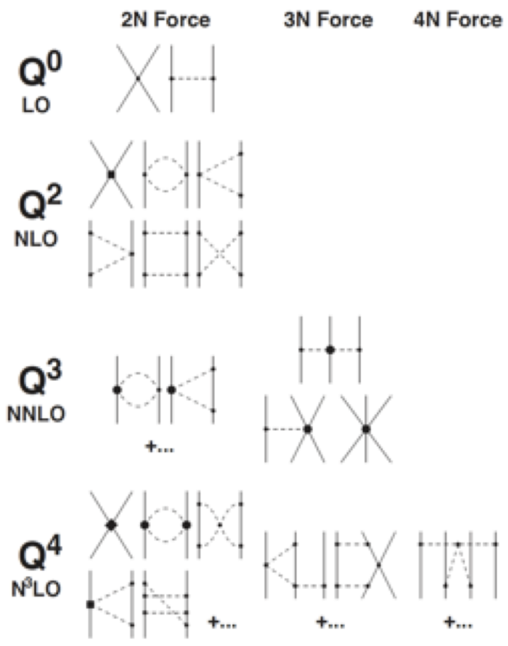


- Exploit recent discovery of eight new isotopes of the elements phosphorus, sulfur, chlorine, argon, potassium, scandium, and calcium
- Estimate the boundaries of nuclear existence in the calcium region with a full quantification of uncertainties, assessing the impact of the experimental discovery on nuclear structure research.

L. Neufcourt, Y. Cao, W. Nazarewicz, E. Olsen, and F. Viens, Phys. Rev. Lett. 122, 062502 (2019)

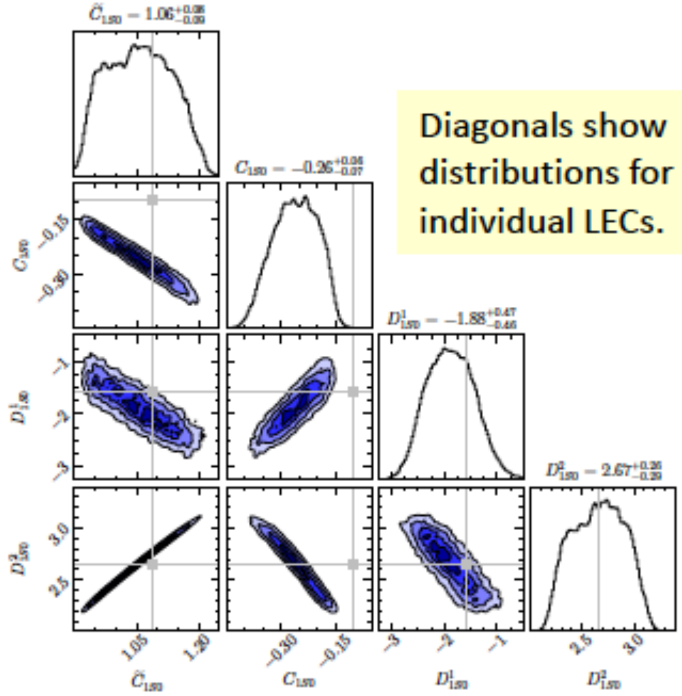
Scientific discovery through statistics

Objective: Develop statistical tools to provide theoretical error bars and to assist in scientific discovery



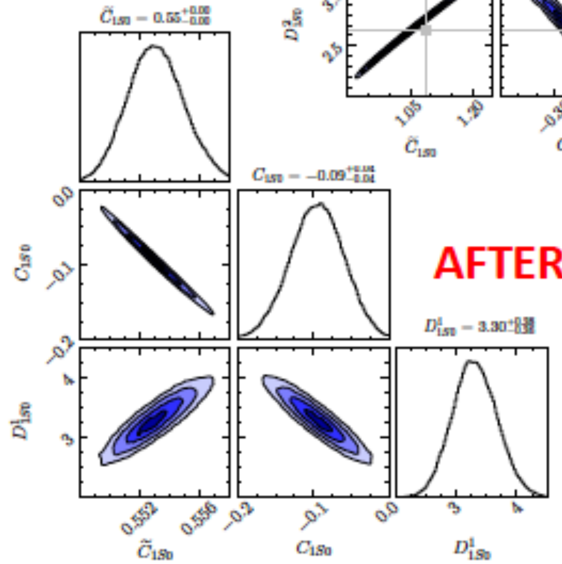
- Adapted Bayesian methods were to parameter estimation for chiral effective field theories.
- Identified a model redundancy caused by too many parameters and overfitting. This was unnoticed for over ten years.
- Resulted in new improved fits to experimental data with fewer parameters

BEFORE

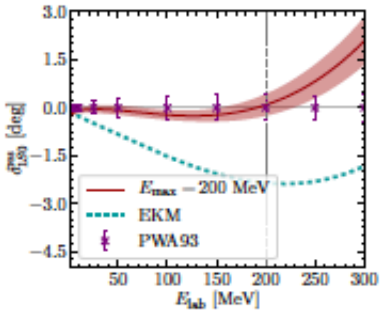


Diagonals show distributions for individual LECs.

Off-diagonals show *correlations* for pairs of LECs.

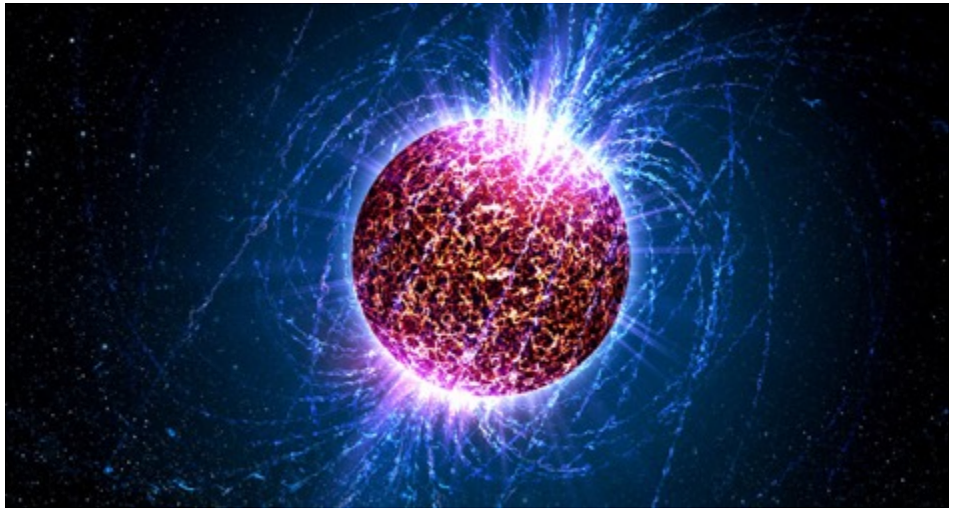


AFTER



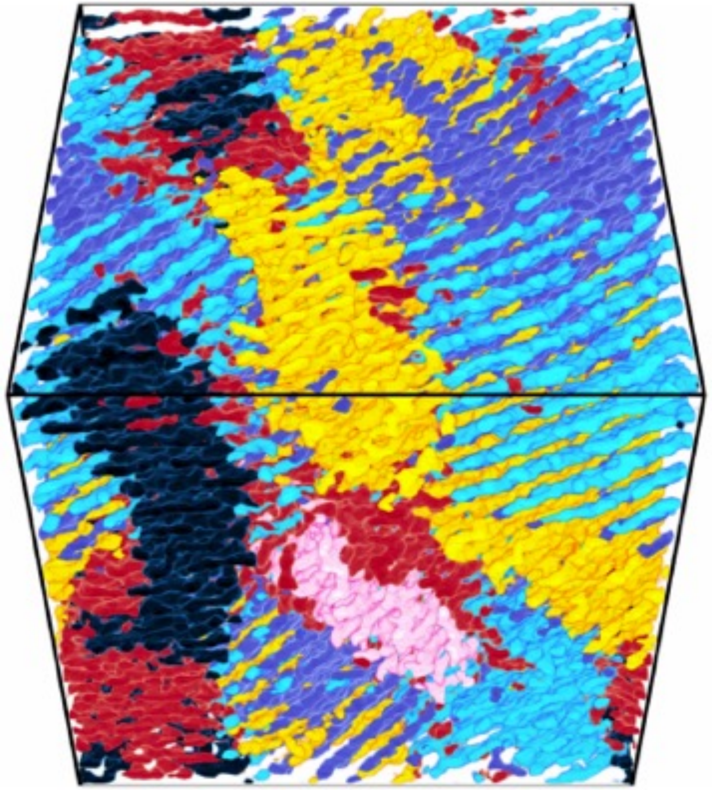
S. Wesolowski, R.J. Furnstahl, J. Melendez, and Daniel Phillips, J. Phys. G 46, 045102 (2019).

Nuclear pasta: strongest material in the universe



Casey Reed / Penn State University, Wikimedia Commons

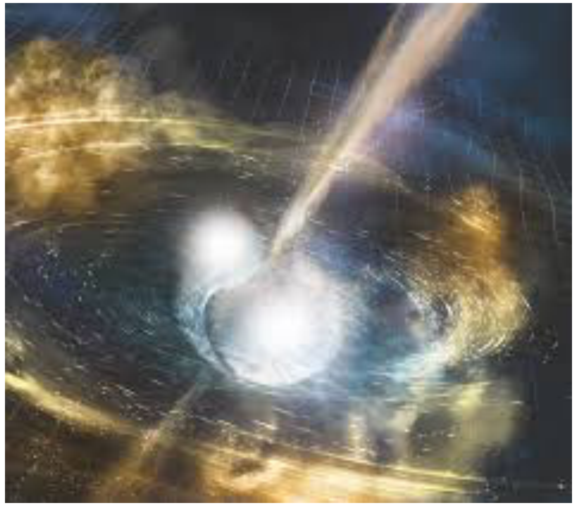
- Used large scale GPU computing to perform detailed molecular dynamics simulations of neutron star crust, including complex nuclear pasta phases
- Determined its elastic properties such as sheer modulus and breaking strain
- Found that the very strong breaking strain can support large crust mountains, which on rotating neutron stars can efficiently radiate gravitational waves. These could be observed in near future LIGO searches



Largest ever simulation of nuclear pasta, containing over three million protons and neutrons. The colors show "domains" where nuclear pasta is locally ordered.

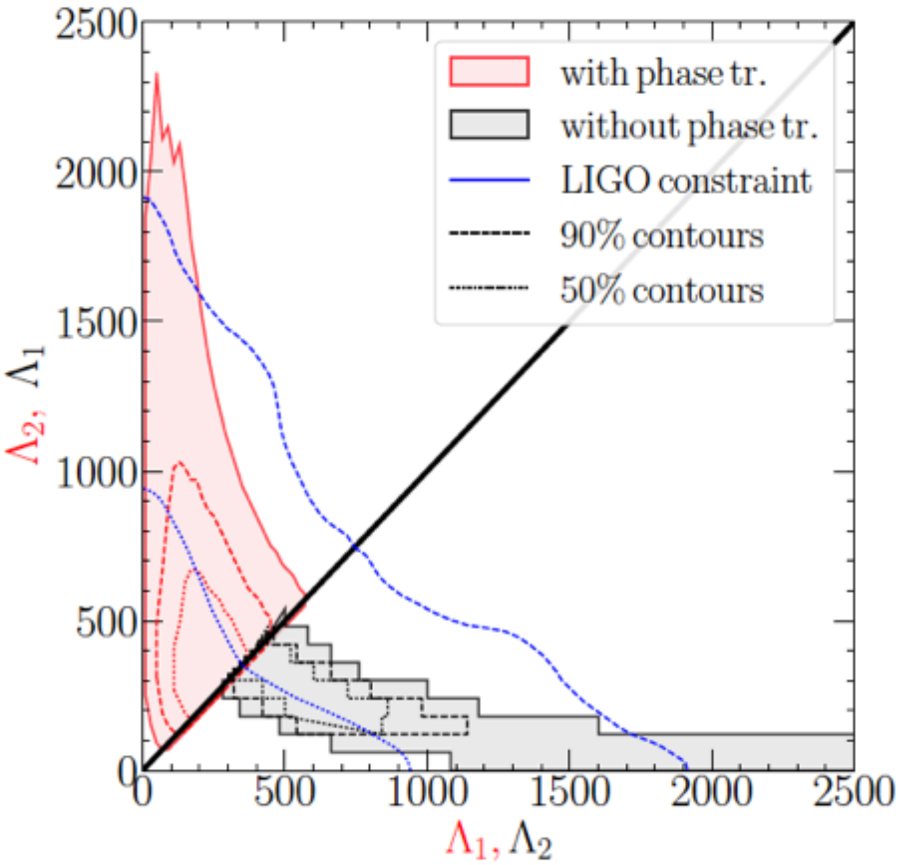
M. E. Caplan, A. S. Schneider, and C. J. Horowitz, Phys. Rev. Lett. **121**, 132701 (2018)

Confronting gravitational waves with modern nuclear physics constraints



LIGO Caltech

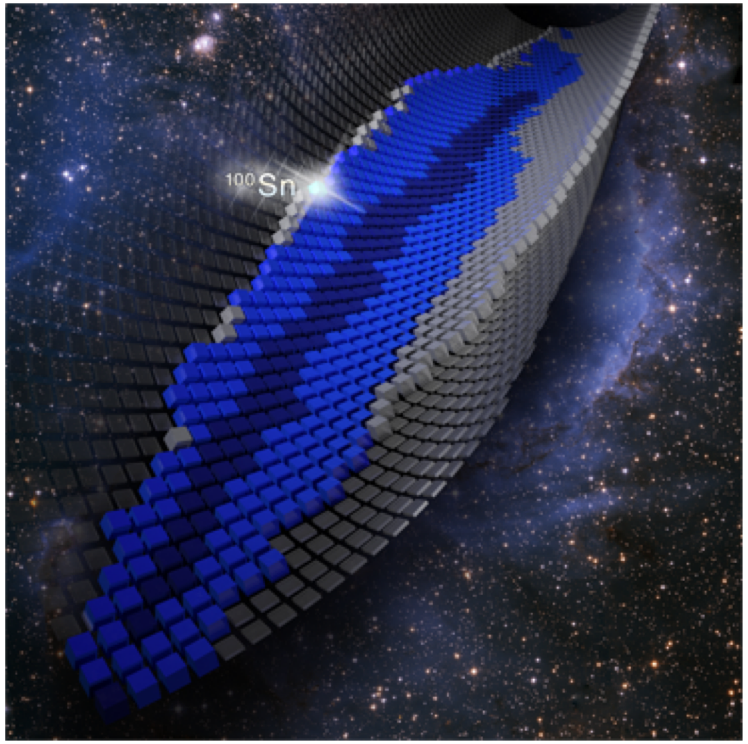
- Studied the impact of phase transitions on the gravitational-wave signal GW170817
- Constrained the radius of a 1.4 solar-mass neutron star to be between 8.7-12.6 km (10.9-12.0 km) when phase transitions are present (not present)
- Determined ranges for tidal polarizabilities that will allow to shed light on the existence of phase transitions to exotic forms of matter in the core of neutron stars when future neutron-star merger observations become available



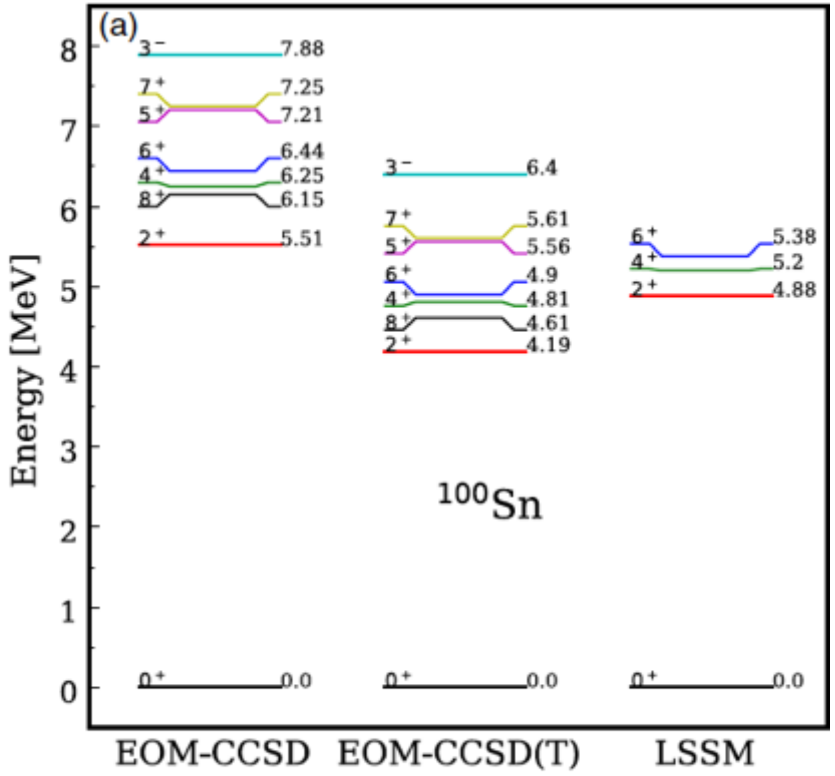
Tews, Carlson, Gandolfi, and Reddy, Astrophys. J. 860, 149 (2018); Tews, Margueron, and Reddy, Phys. Rev. C 98, 045804 (2018)

Structure of ^{100}Sn and its neighbors

- Determine the structure of the supposedly doubly magic nucleus ^{100}Sn consisting of 50 protons and 50 neutrons and its neighbors
- Tying the structure of this heavy nucleus to nuclear interactions that are constrained only in very light nuclei.



- Doubly magic nuclei such as ^{100}Sn have a simple structure and are the cornerstones for entire regions of the nuclear chart.
- Our results confirm that ^{100}Sn is doubly magic, and the predicted low-lying states of ^{100,101}Sn open the way for shell-model studies of many more rare isotopes.
- Separation energies enter models of nucleosynthesis.



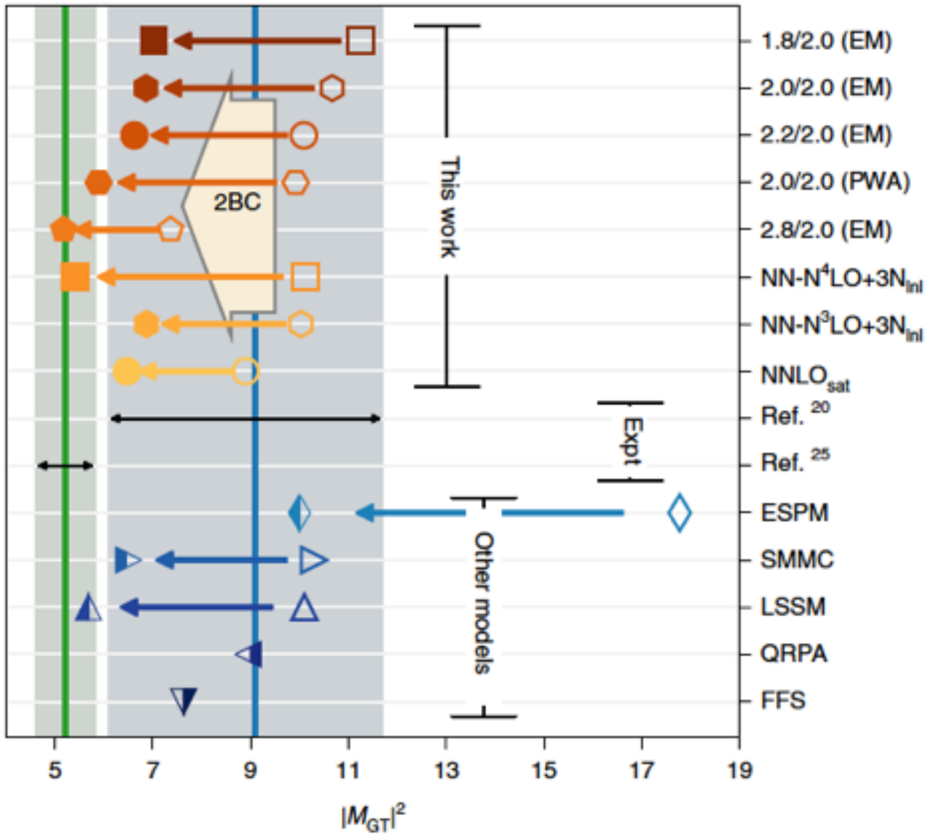
T. Morris, C. Simonis, R. Stroberg, C. Stumpf et al., Phys. Rev. Lett. **120,** 152503 (2018)

Solution of the puzzle of quenched β decays

Andy Sproles / ORNL

Addressed the long-standing puzzle of why computations of β-decay rates in atomic nuclei are about 25% faster than what's expected from the β-decay of the free neutron

Found that the coupling of the weak force to two nucleons and a proper treatment of strong correlations in the nucleus are necessary to correctly describe β-decay rates from light nuclei to the heavy nucleus ^{100}Sn

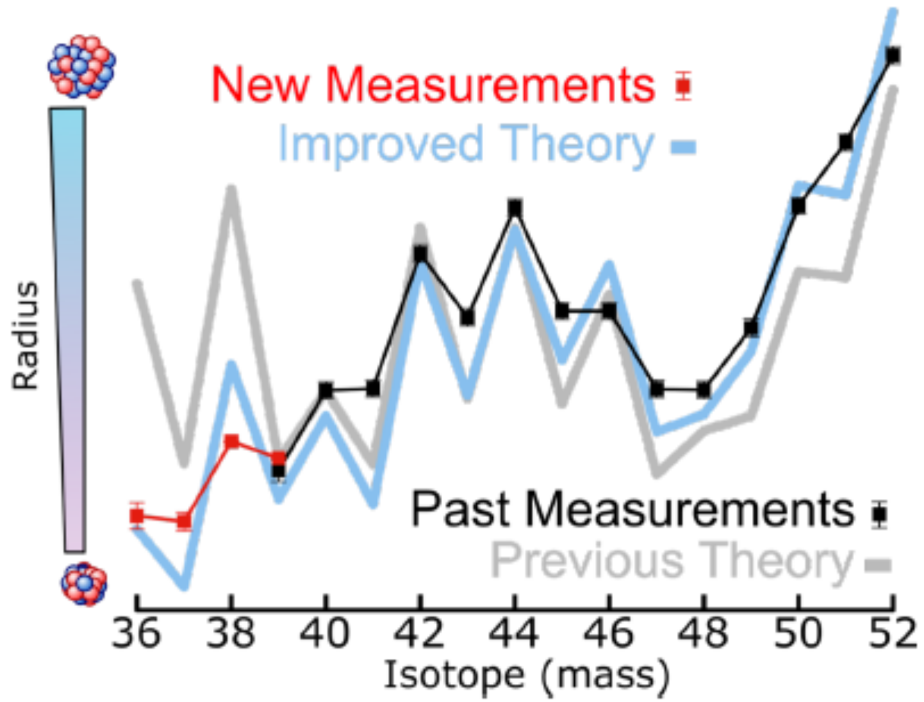


P. Gysbers et al., Nature Physics **15**, 428 (2019)

Puzzling sizes of extreme calcium isotopes

- The intricate behavior of charge radii along the chain of Ca isotopes, including the unexpectedly large charge radius of neutron-rich ^{52}Ca, poses a daunting challenge for nuclear theory.

- The charge radii of proton-rich isotopes $^{36,37,38}Ca$ are challenging as properties of these systems are impacted by the interplay between nuclear superfluidity and weak binding.

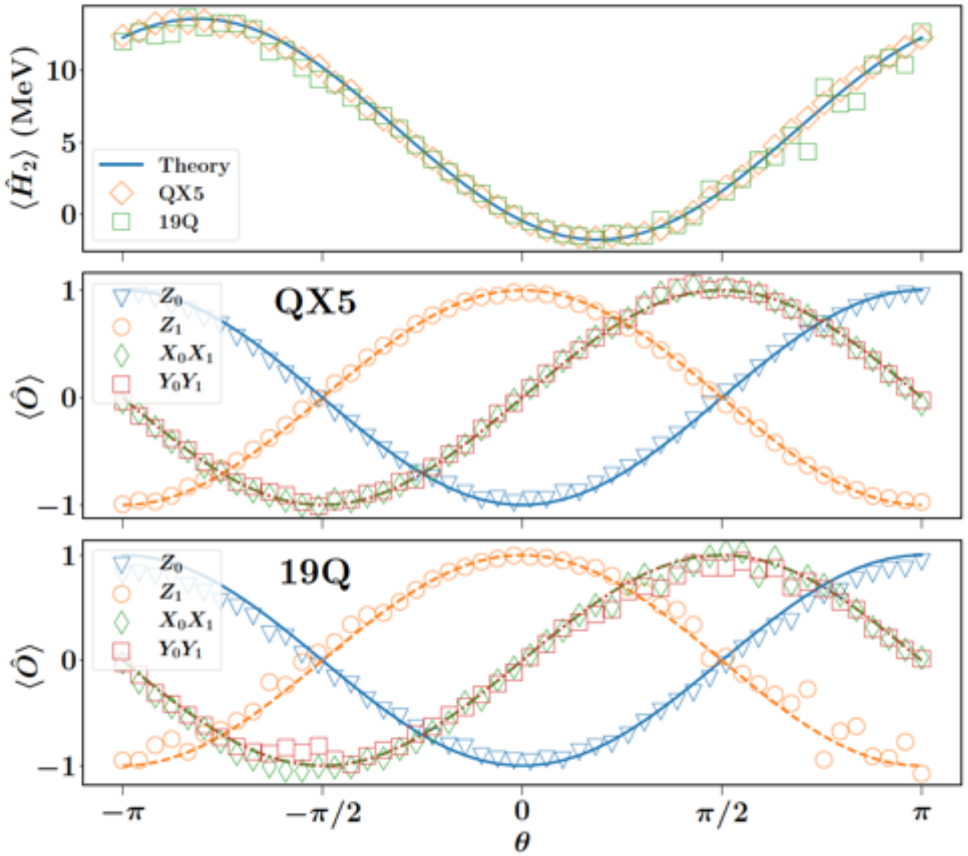


Charge radii of calcium isotopes. New data are shown in red squares and compared with theoretical values.

A.J. Miller et al., Nature Physics (2019)

Quantum computing of an atomic nucleus

Andy Sproles / ORNL



- Perform the first quantum computation of an atomic nucleus
- Learn how to map real-word physics problems onto existing quantum devices

Collaboration between nuclear physicists (NP) and quantum information scientists (ASCR):

Dumitrescu, McCaskey, Hagen, Jansen, Morris, TP, Pooser, Dean, Lougovski, Phys. Rev. Lett. **120**, 210501 (2018)

Summary

Year 3 of SciDAC-4 was successful for the NUCLEI collaboration

- Continued productive collaborations between AM/CS and NP
- Addressed exciting science problems