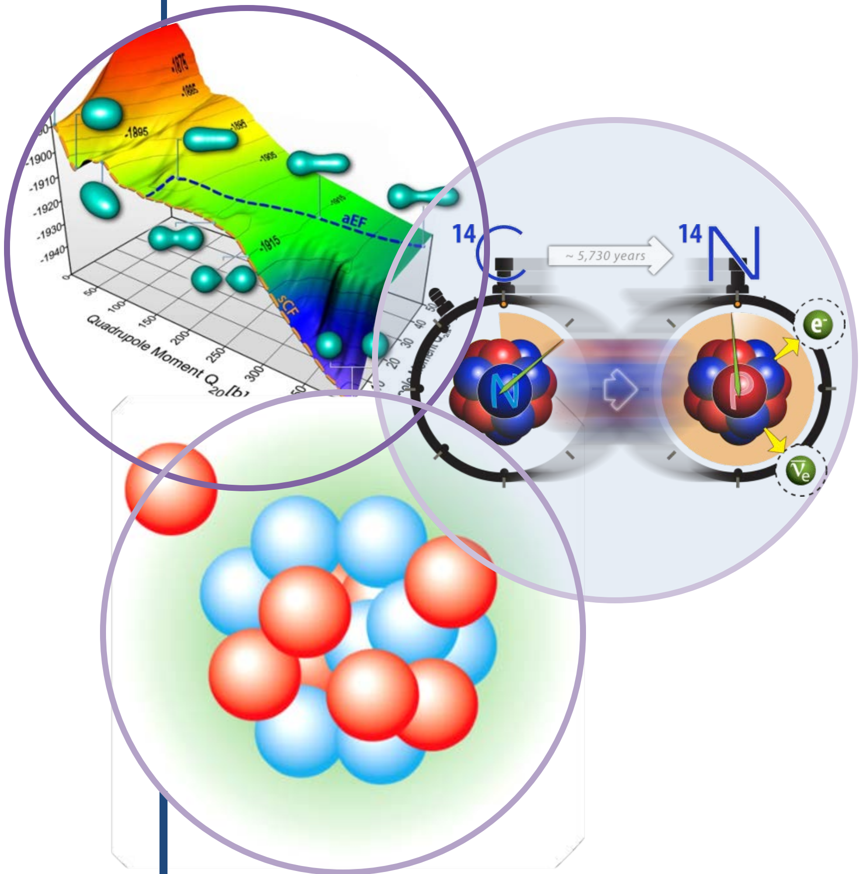
NUCLEI – Highlights from coupled-cluster computations of medium mass and neutron rich nuclei

Gaute Hagen (ORNL)



SciDAC-3 PI meeting,
Washington DC, July 30, 2014

U.S. DEPARTMENT OF ENERGY
NUCLEI Nuclear Computational Low-Energy Initiative
BSF United States – Israel Binational Science Foundation
OAK RIDGE NATIONAL LABORATORY
MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY

NUclear Computational Low-Energy Initiative

(2012-2017)

TJNAF

NIF

LENP facilities

FRIB

Validated Nuclear Interactions

Chiral EFT
Ab-initio

Optimization
Model validation
Uncertainty Quantification

Structure and Reactions: Light and Medium Nuclei

Neutron drops

EOS
Correlations

Structure and Reactions: Heavy Nuclei

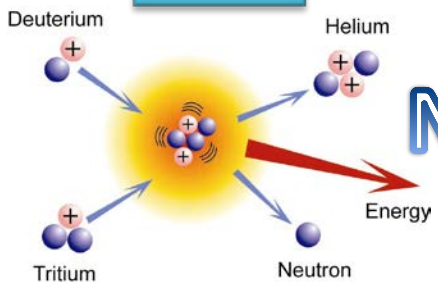
Ab-initio
RGM
CI

Load balancing
Eigensolvers
Nonlinear solvers
Model validation
Uncertainty Quantification

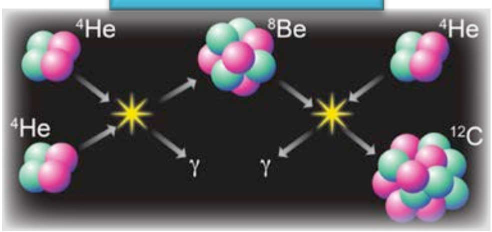
DFT
TDDFT

Load balancing
Optimization
Model validation
Uncertainty Quantification
Eigensolvers
Nonlinear solvers
Multiresolution analysis

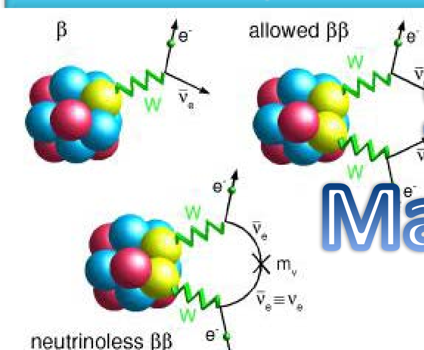
fusion



Stellar burning



Neutrinos and Fundamental Symmetries

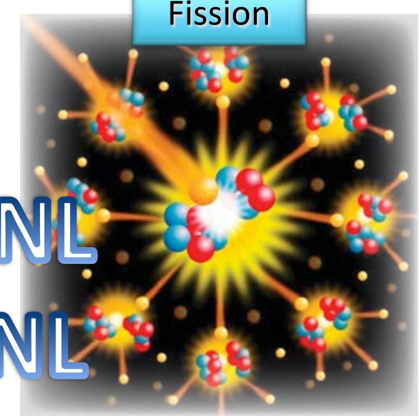


SNS

Majorana

Neutron Stars

Fission

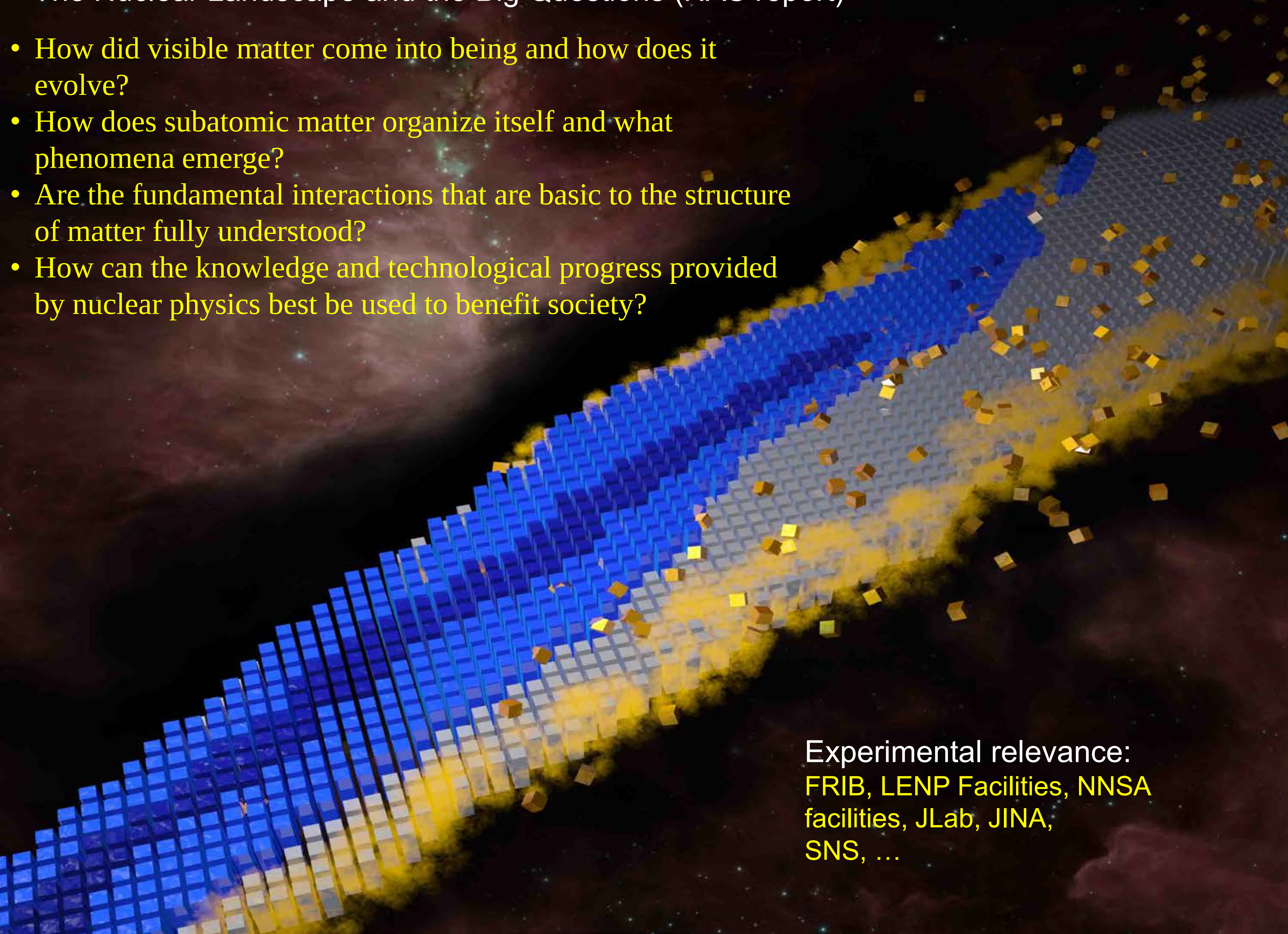


LANL

LLNL

The Nuclear Landscape and the Big Questions (NAS report)

- How did visible matter come into being and how does it evolve?
- How does subatomic matter organize itself and what phenomena emerge?
- Are the fundamental interactions that are basic to the structure of matter fully understood?
- How can the knowledge and technological progress provided by nuclear physics best be used to benefit society?



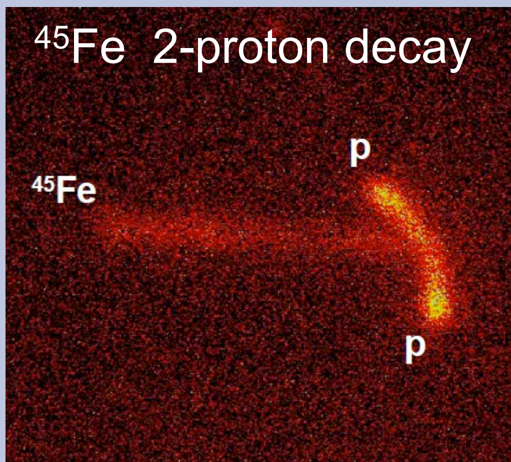
Experimental relevance:
FRIB, LENP Facilities, NNSA facilities, JLab, JINA, SNS, …

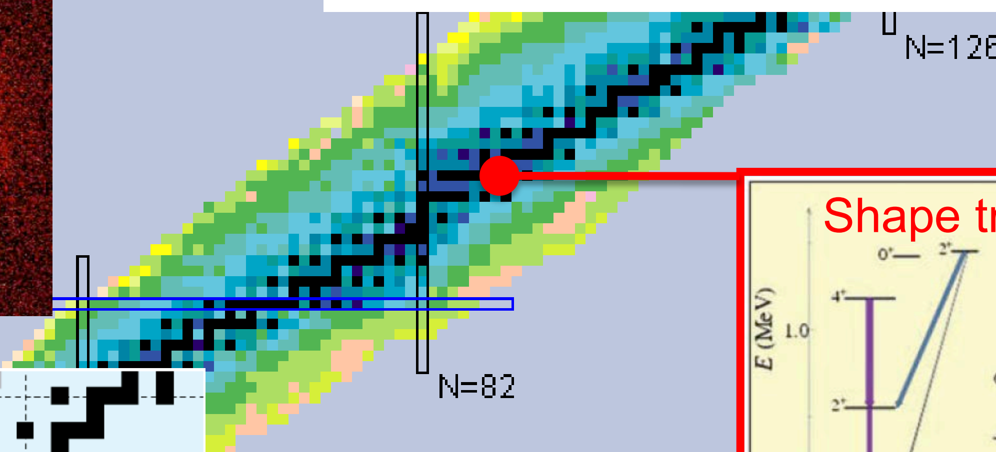
Nuclei across the chart

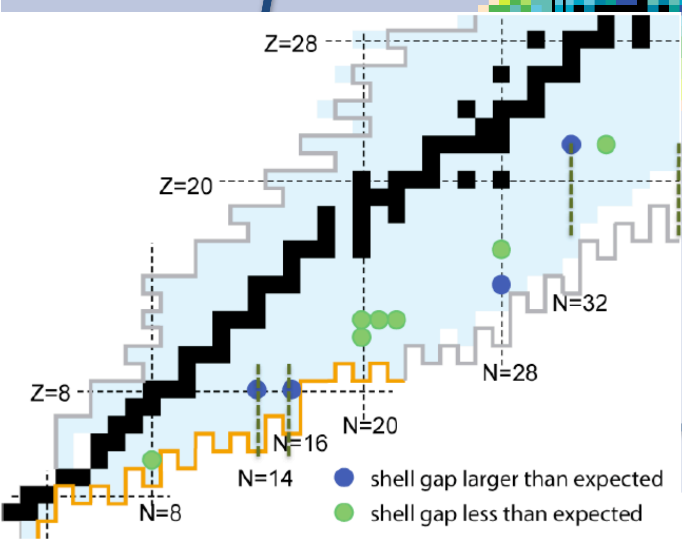
118 chemical elements (94 naturally found on Earth)
288 stable (primordial) isotopes

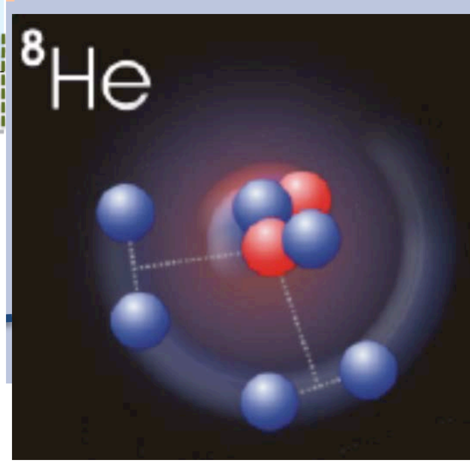
Thousands of short-lived isotopes – many with interesting properties

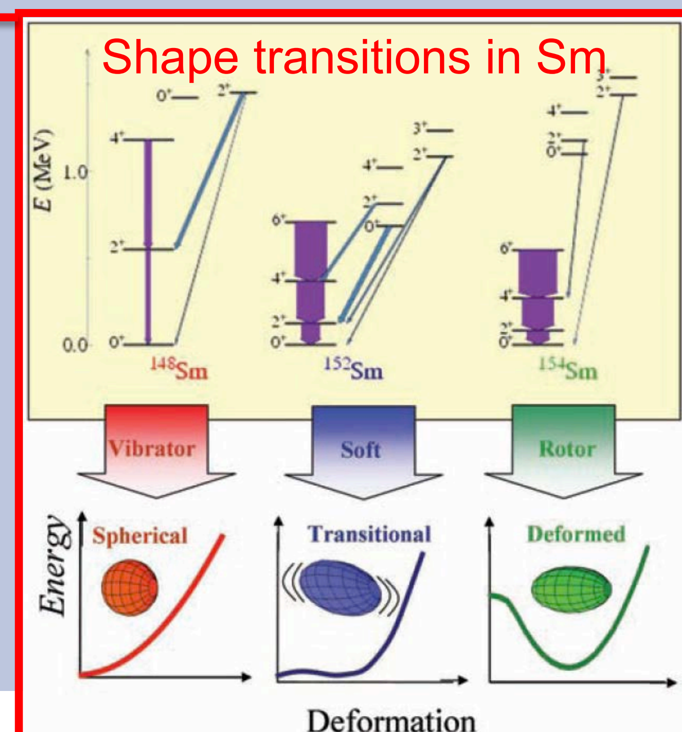
large isospin magnifies unknown physics
clustering behavior
novel evolution in structure









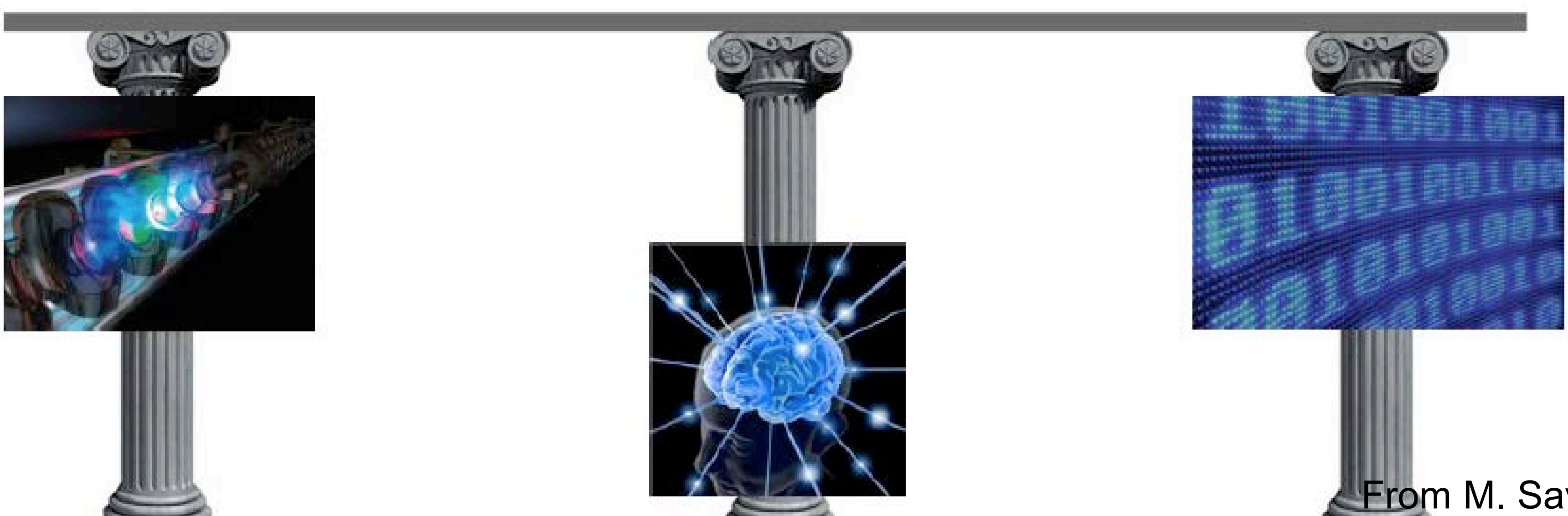


Computational Nuclear Physics

Computing is Essential

High Performance Computing provides answers to questions that neither experiment nor analytic theory can address; hence, it becomes the third leg supporting the field of nuclear physics

National Academy Report
(2012)

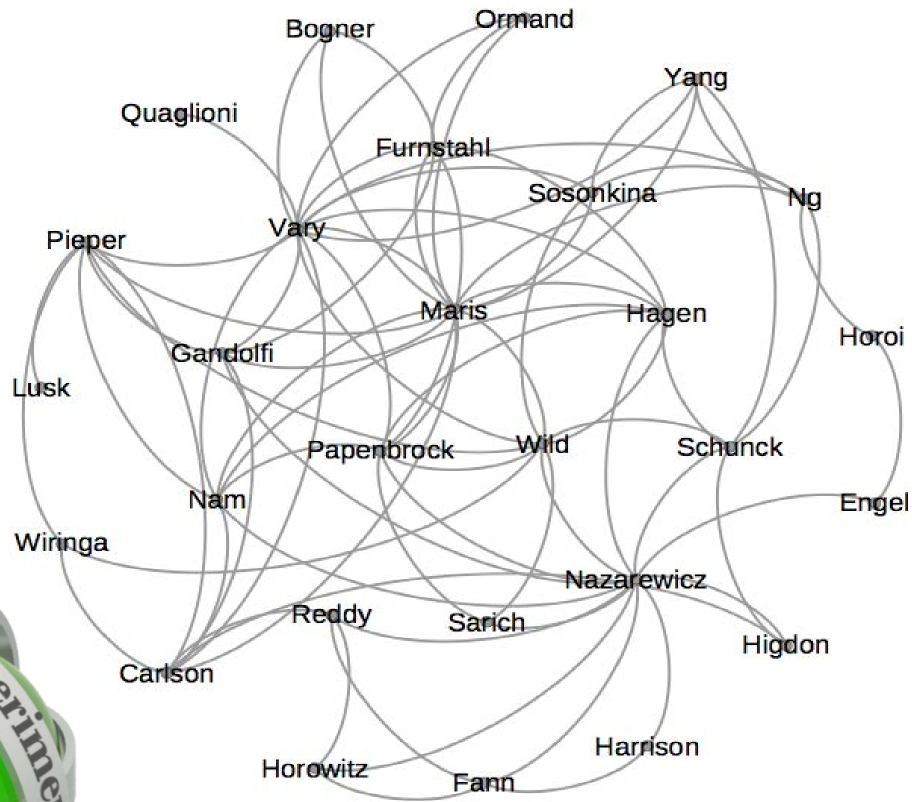


From M. Savage

Bridging Physics and Math/CS efforts

- Working with math/CS collaborators to enable science on new architectures (e.g. Titan, Cori)
- Bridge positions between physics and math/CS could help to establish computational physics as the third leg
- The SciDAC3 NUCLEI efforts have already initiated vast number of collaborations

Existing collaborations within NUCLEI
From Rusty Lusk



Coupled-cluster theory

- Microscopic many-body theory that was introduced in nuclear physics in the late 50's
- Has become the state-of-the-art many-body method in computational quantum chemistry
- In the last decade, coupled-cluster theory was re-introduced in nuclear physics
- It is currently the only microscopic method that can compute properties of medium mass nuclei and take into account coupling to continuum and with inclusion of three-nucleon forces and two-body currents.
- A typical medium mass nucleus (ground state + spectrum) requires around 1,000,000 cpu hours

Computational challenges of CC

- Large sparse distributed matrices (several hundred GBytes)
  - IO takes significant walltime
  - The matrices are accessed differently for different terms in the coupled-cluster equations
  - No obvious distribution scheme
- Large set of non-linear equations (up to 10^9 unknowns)
  - Convergence issues
  - Need iterative solvers with Krylov sub-space methods (Broyden, DIIS)
- Large scale diagonalization of non-Hermitian complex matrices (dim ~ 10^9)
  - Arnoldi and non-symmetric Lanczos algorithms
  - Davidson method to access non-extremal eigenvalues

I/O Performance Improvements

Problem

- Time spent doing IO did not scale with the number of ranks
- Interaction-elements read one by one from a large binary file
- Packed disk-format does not correspond to distribution scheme
- Does not utilize parallel IO resources

Solution

- All interaction files in hdf5
- Read and write whole matrices at the time
- Optimized library on titan
- Can utilize parallel IO

Effect

- Time spent doing IO decreased by an order of magnitude
- Scales with the number of ranks
- Portable (Fortran, C/C++, Python, Java, etc.) and cleaner code
- Easier to maintain and share
- Decrease in directory clutter(multiple datasets in a single file)

The HDF Group

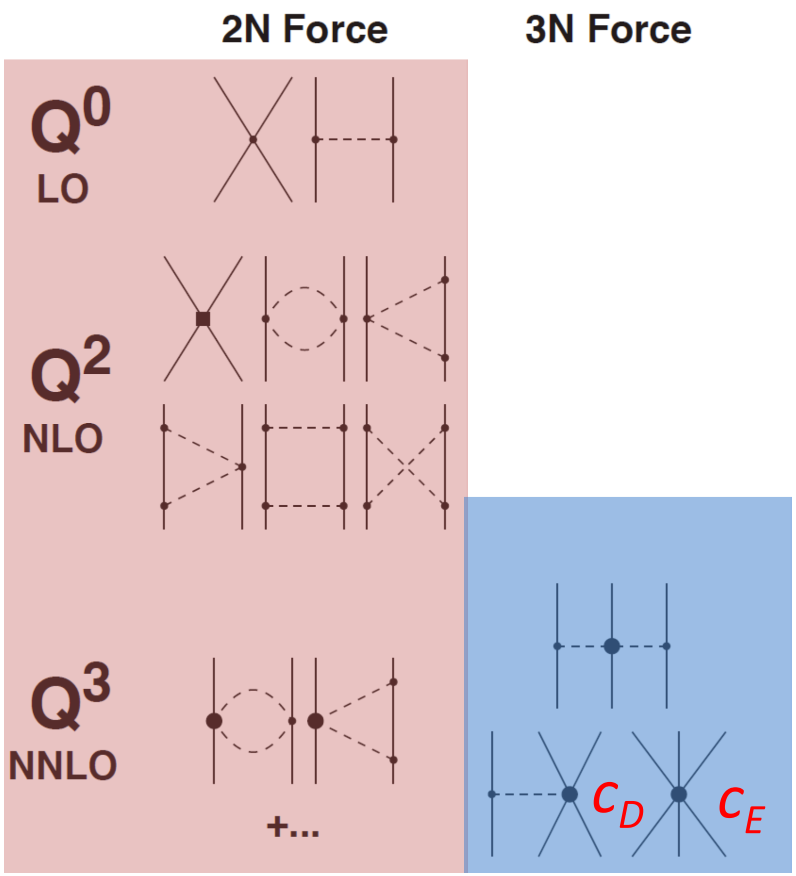
A data model, library, and file format for storing and managing data

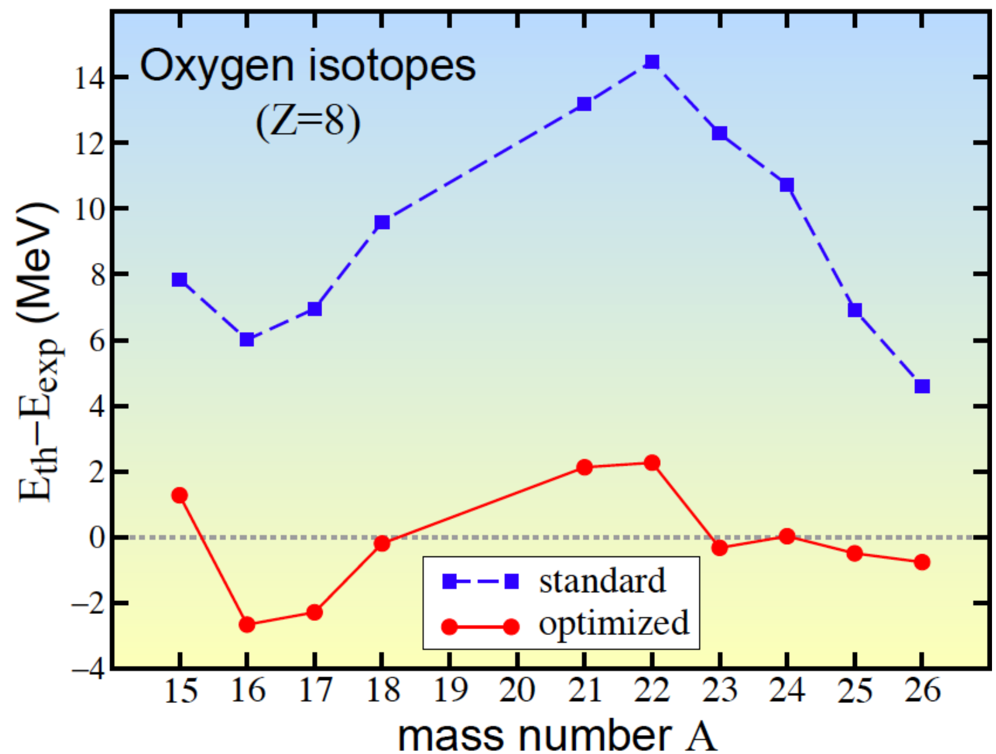
Optimizing the nuclear force

A. Ekström et al. Phys. Rev. Lett. 110, 192502 (2013)

DOE Office of Science highlight http://science.energy.gov/np/highlights/2014/np-2014-05-e/

- The derivative-free, nonlinear least squares solver POUNDERS in TAO was used to systematically optimize potentials based solely on two-nucleon forces
- The optimization of the low-energy constants of the new interaction $NNLO_{opt}$ yields a χ^2/datum ≈ 1 for laboratory scattering energies below 125 MeV. The new interaction yields very good agreement with binding energies and radii for A=3,4 nuclei and oxygen isotopes

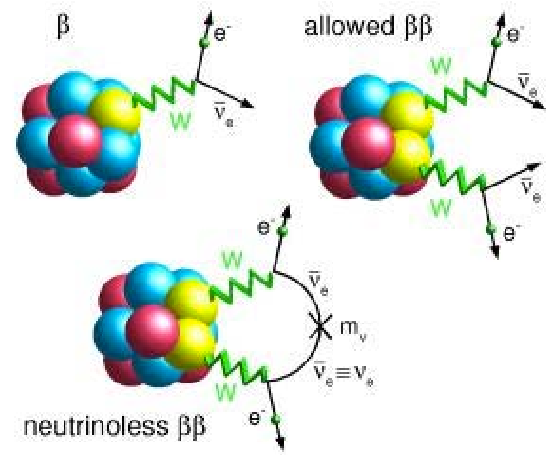




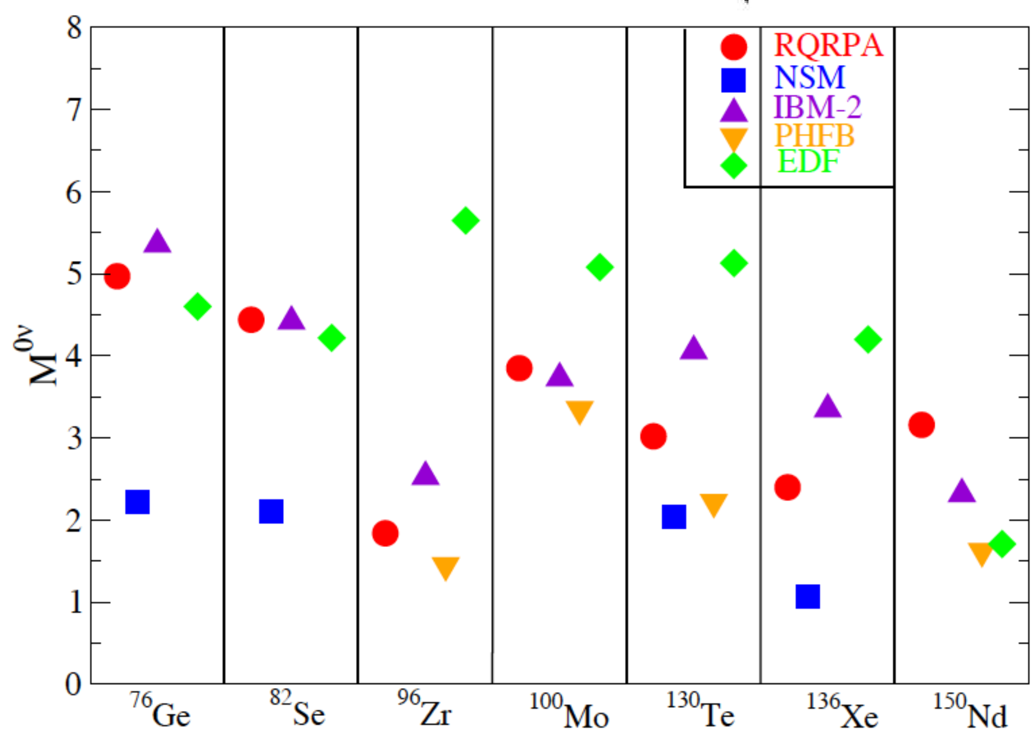
Neutrinoless double beta decay

Thanks to ASCR and DOE/NP for extra funding for neutrinoless double beta decay

- Fundamental questions:
  - Are neutrinos their own antiparticles?
  - Is the mass hierarchy inverted or normal?
  - What is the neutrino mass scale?



- Significance
  - If neutrinoless double beta decay happens neutrinos are their own anti-particles
  - If the decay happens fast enough to be observed by coming multimillion dollar experiments the mass hierachy is inverted
  - **But to extract the mass scale, we need to know the nuclear matrix element**

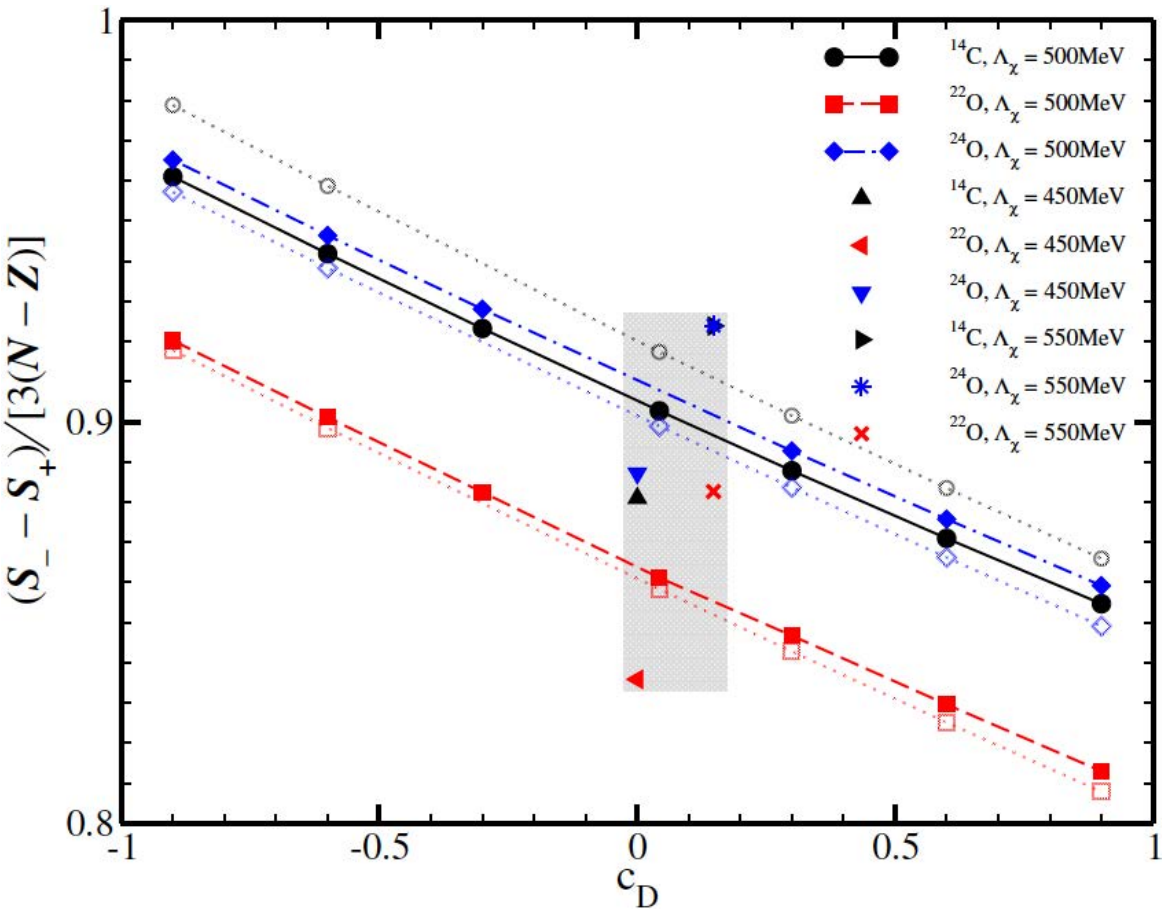


Taken from P. Vogel arXiv:1208.1992 (2012)

Quenching of Gamow-Teller strength in nuclei

A. Ekström, G. Jansen, K. Wendt et al, arXiv:1406.4696 (2014)

- **Longstanding problem:** Experimental beta-decay strengths quenched compared to theoretical results.
- **Our approach:** perform the most sophisticated calculation of beta decay to date: include three-nucleon forces and consistent two-body currents

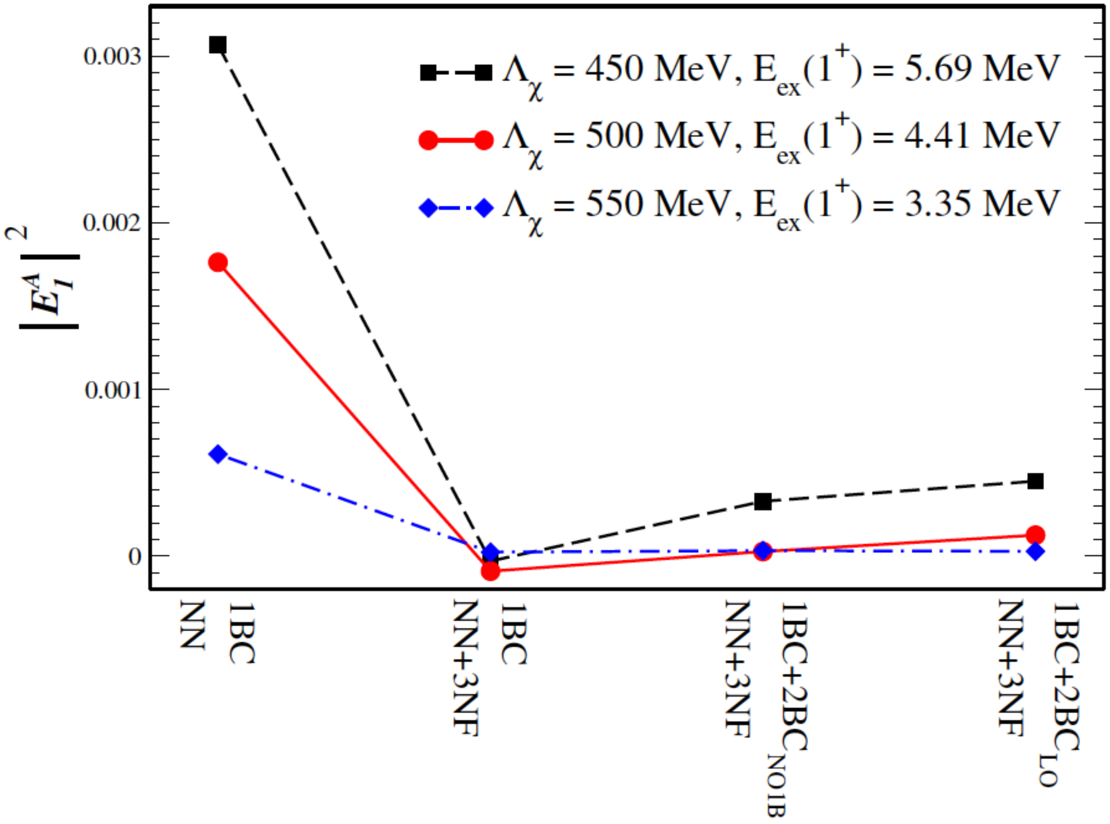


- We find a quenching of the Ikeda sum rule in ^{14}C and ^{22,24}O
- Grey area reproduce triton half-life
- The quenching of g_A is about 4-8%, and smaller than estimates from shell model

The anomalous life-time of ^{14}C

A. Ekström, G. Jansen, K. Wendt et al, arXiv:14.06:4696

The half life of ^{14}C is anomalous long and is used to determine the age of organic material such as Neanderthal bones. What are the mechanisms in the nucleus that gives us this powerful archeological tool?

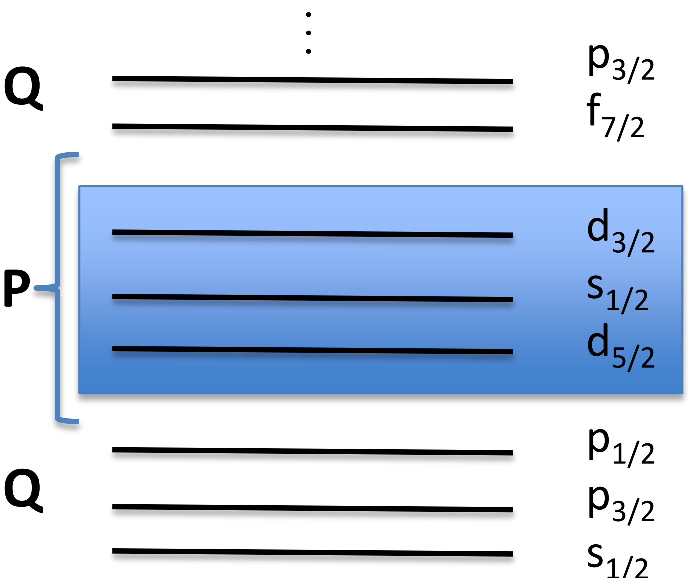


- 3NFs decrease the transition matrix element significantly
- 2BC counter the effect of 3NFs to some degree.
- The matrix element depends on the first excited 1^+ state in ^{14}N.

Road to ββ-decay of ^{76}Ge: Coupled-cluster effective interactions

G. R. Jansen, J. Engel, G. Hagen, P. Navratil, A. Signoracci, arXiv:1402.2563 (2014).

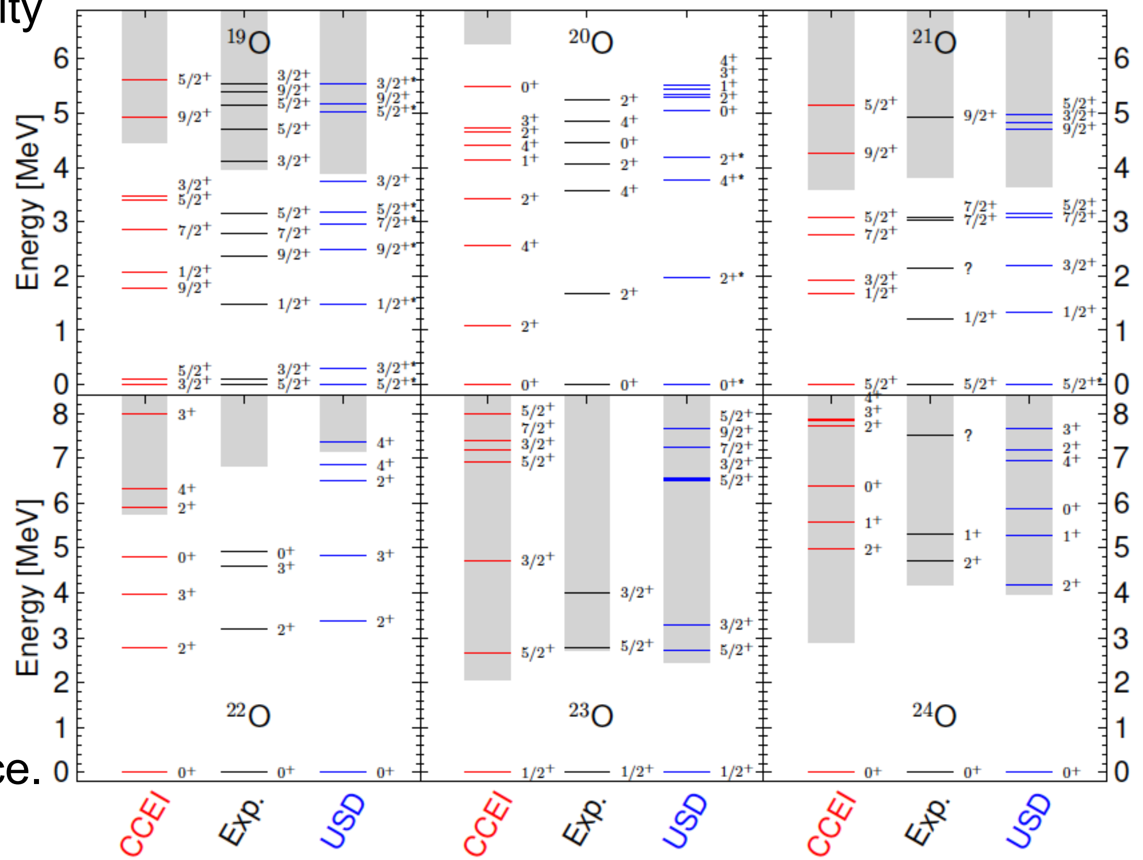
- Start from chiral NN(N3LO$_{EM}$) + 3NF(N2LO) interactions
- Solve for A+1 and A+2 using CC. Project A+1 and A+2 CC wave functions onto the *s-d* model space using Lee-Suzuki similarity transformation.



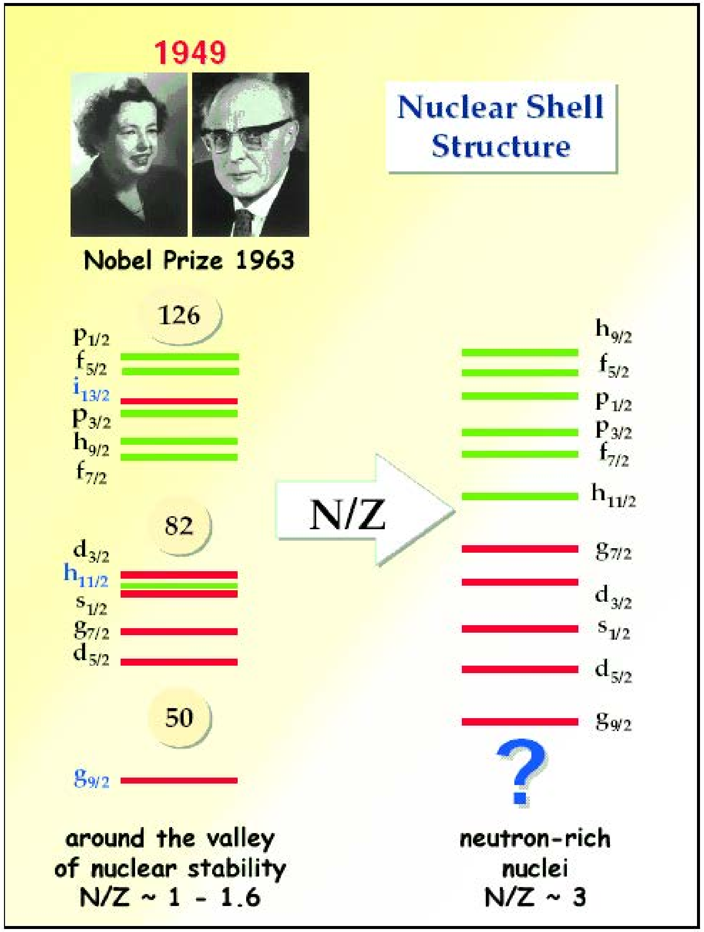
- Diagonalize the effective hamiltonian in the valence space.

Next step: Compute effective operators for use in neutrinoless double beta decay studies.

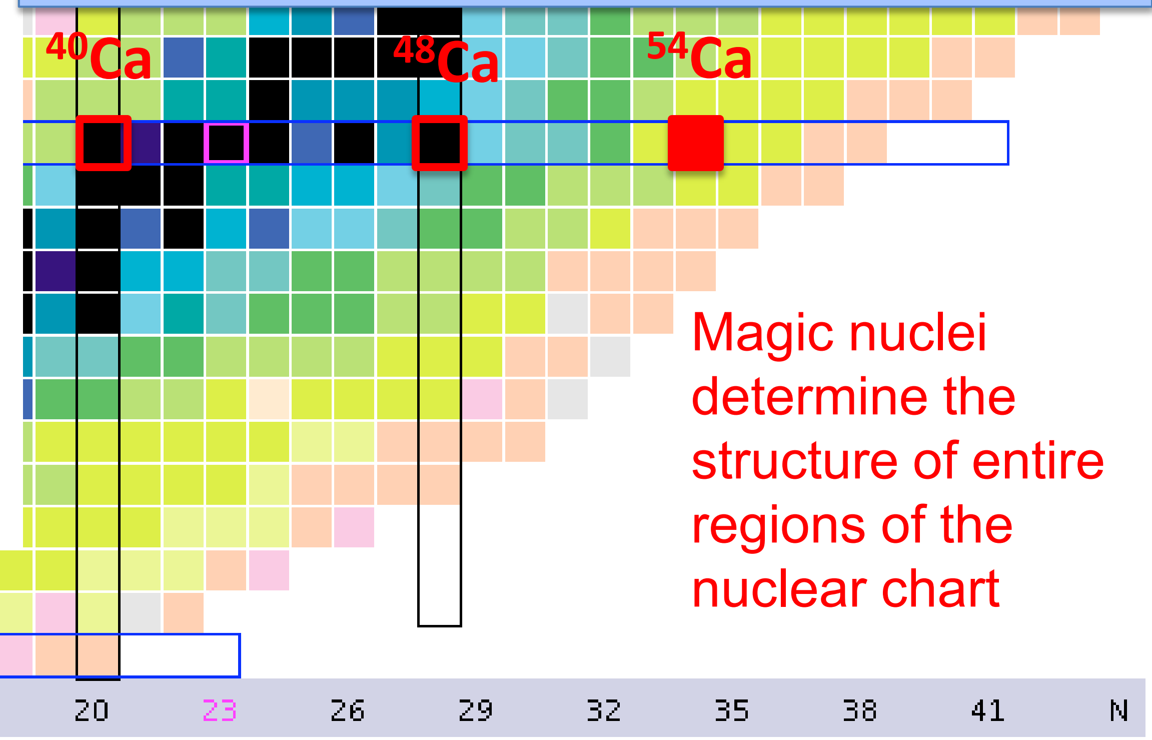
Spectra of oxygen isotopes computed with coupled-cluster effective interaction (CCEI)



Shell structure in neutron rich calcium



- How do shell closures and magic numbers evolve towards the dripline?
- Is the naïve shell model picture valid at the neutron dripline?
- What are the mechanisms for new shell structure?

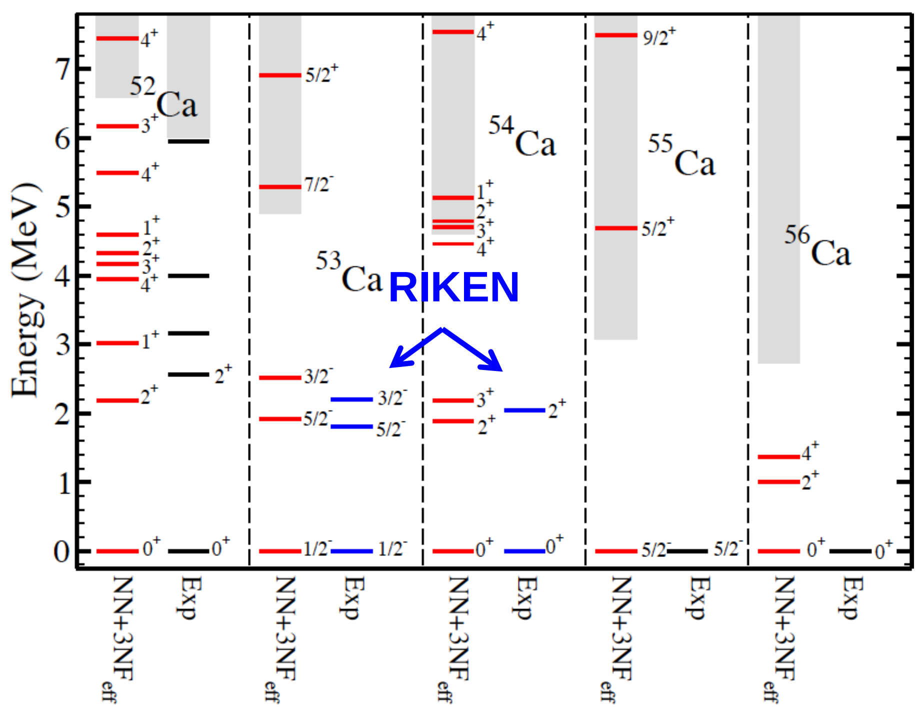


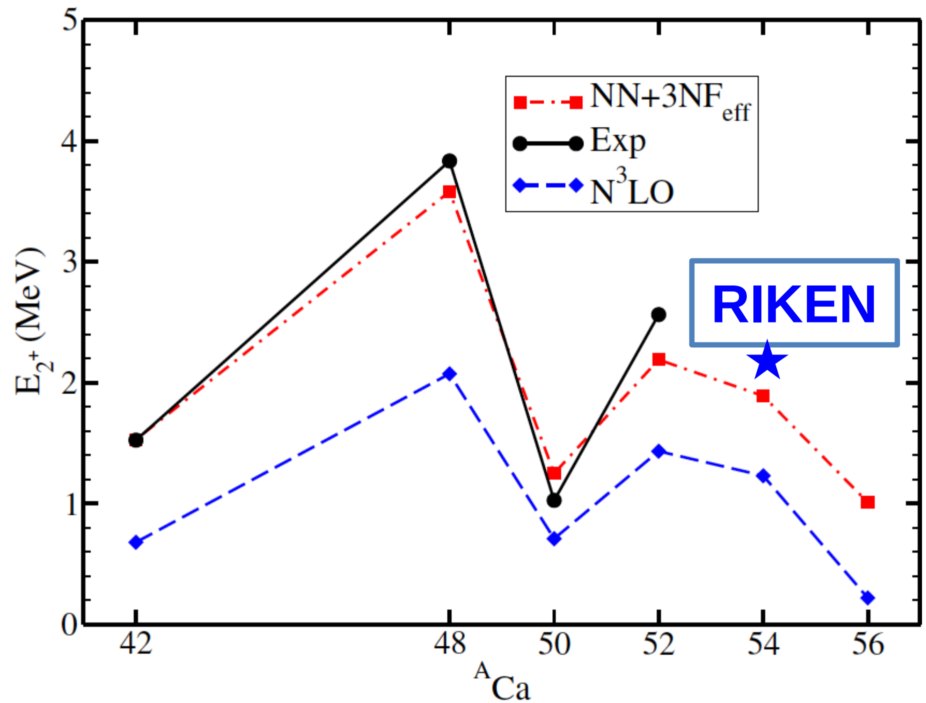
Magic nuclei determine the structure of entire regions of the nuclear chart

First-principles description of neutron-rich calcium

- Good agreement between theory and experiment for excited states
- Effects of three-nucleon forces and continuum is essential to describe shell structure
- We predict inversion of the *gds* orbitals
- Our prediction for excited states in ^{53}Ca and weak sub-shell closure in ^{54}Ca was recently verified by experiment at RIKEN (Nature 2013, D. Steppenbeck et al)

G. Hagen, M. Hjorth-Jensen, G. Jansen, R. Machleidt, T. Papenbrock, Phys. Rev. Lett. 109, 032502 (2012)





Predictions that defy textbook paradigms

Current and future Work

- Focus on porting the CC code suite (NUCCOR) to GPUs
  - Tool to analyze the memory access patterns of key CC diagrams (they have similar structures)
  - Repackage data, help guide algorithmic changes necessary to localize data
  - Port singels and doubles calculations to GPUs etc.
- Double Beta Decay
  - Solvers for large generalized eigenvalue problems for coupled-cluster & GPU porting for computational efficiency
  - GPU porting for configuration interaction codes to address efficiency and scalability

Summary

- Computing is an essential part of NUCLEI
- Bridging Physics and Math/CS efforts is vital to our work
- Science highlights:
  - Origin of quenched Gamow-Teller strengths traced to two-body currents
  - Revisited the anomalous life time of ^{14}C: depends on 3NFs, 2BC and 1+ state in ^{14}N
  - Coupled-cluster effective interactions for the shell model
  - Prediction of sub-shell closure in ^{54}Ca and excited states in ^{53}Ca verified at RIKEN.