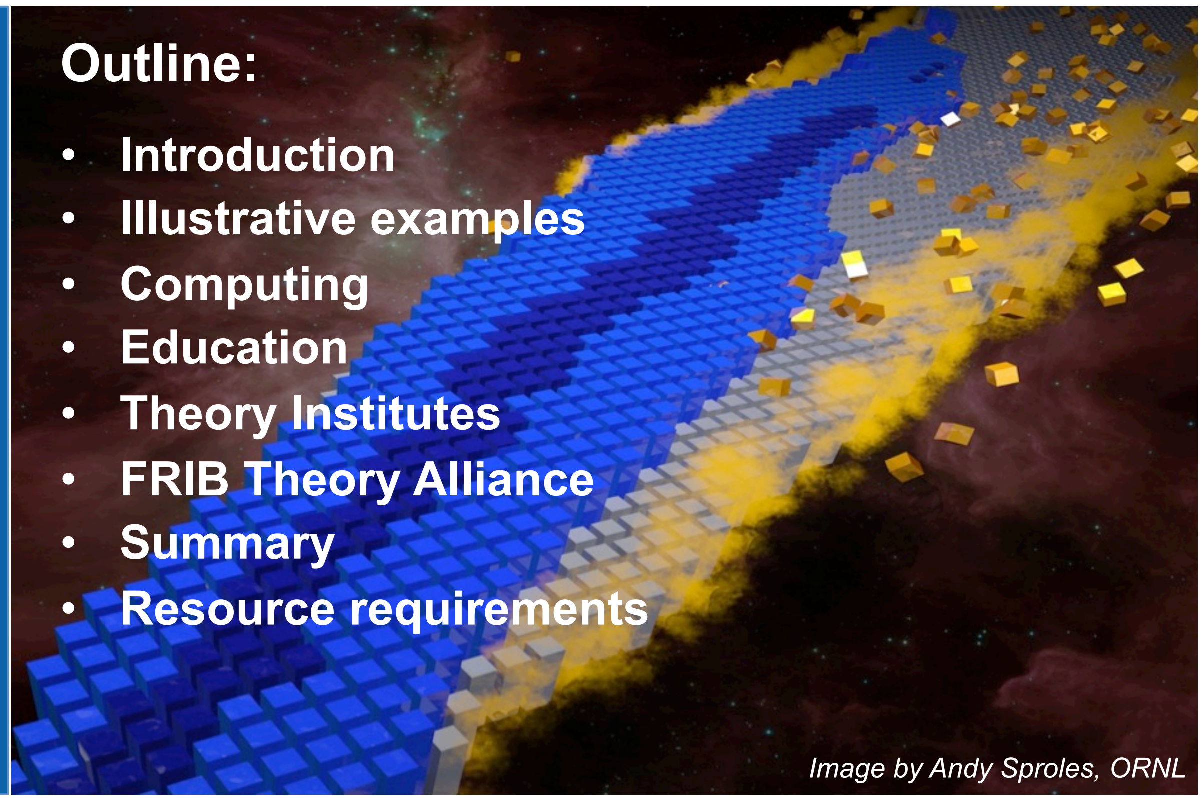
Frontiers of (Low-Energy) Nuclear Theory

2015 Low-Energy Community Meeting

Michigan State University, Aug 21-22, 2015

Sofia Quaglioni

Lawrence Livermore National Laboratory



Outline:

- **Introduction**
- **Illustrative examples**
- **Computing**
- **Education**
- **Theory Institutes**
- **FRIB Theory Alliance**
- **Summary**
- **Resource requirements**

Image by Andy Sproles, ORNL

LLNL-PRES-676478

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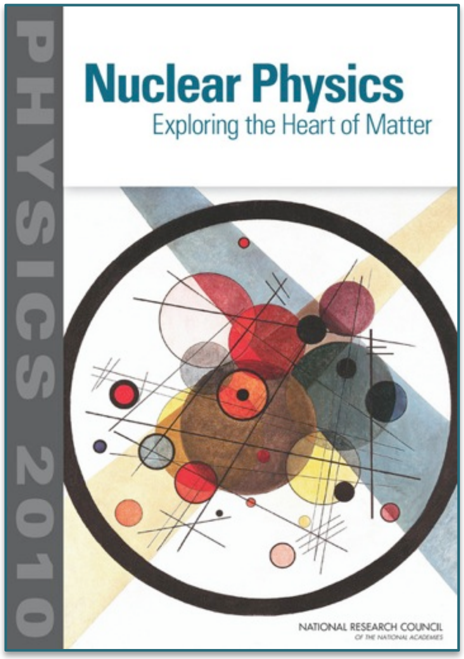
Low-energy nuclear science is fueled by exciting intellectual challenges, captured in NRC decadal survey

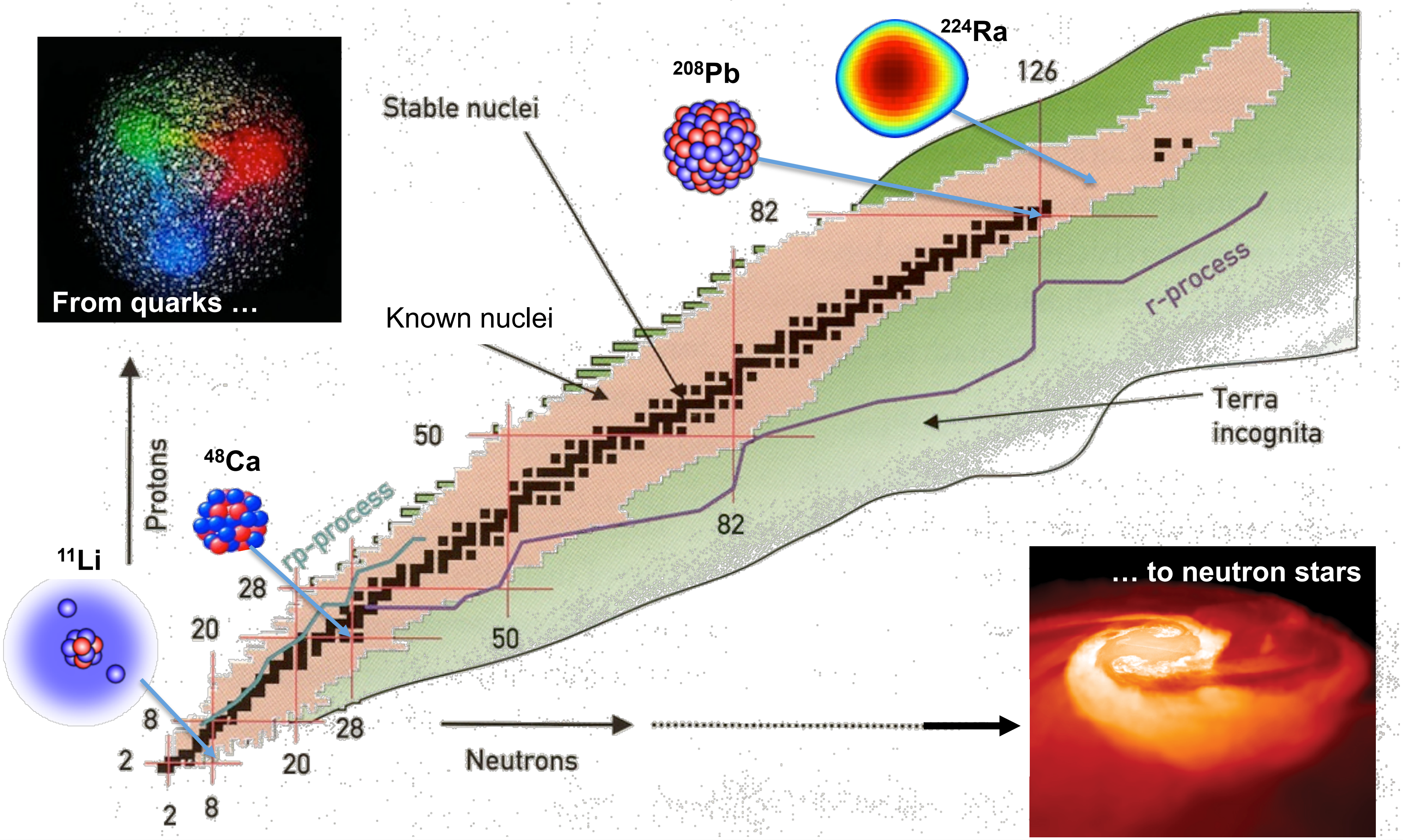
http://www.nap.edu/catalog/13438



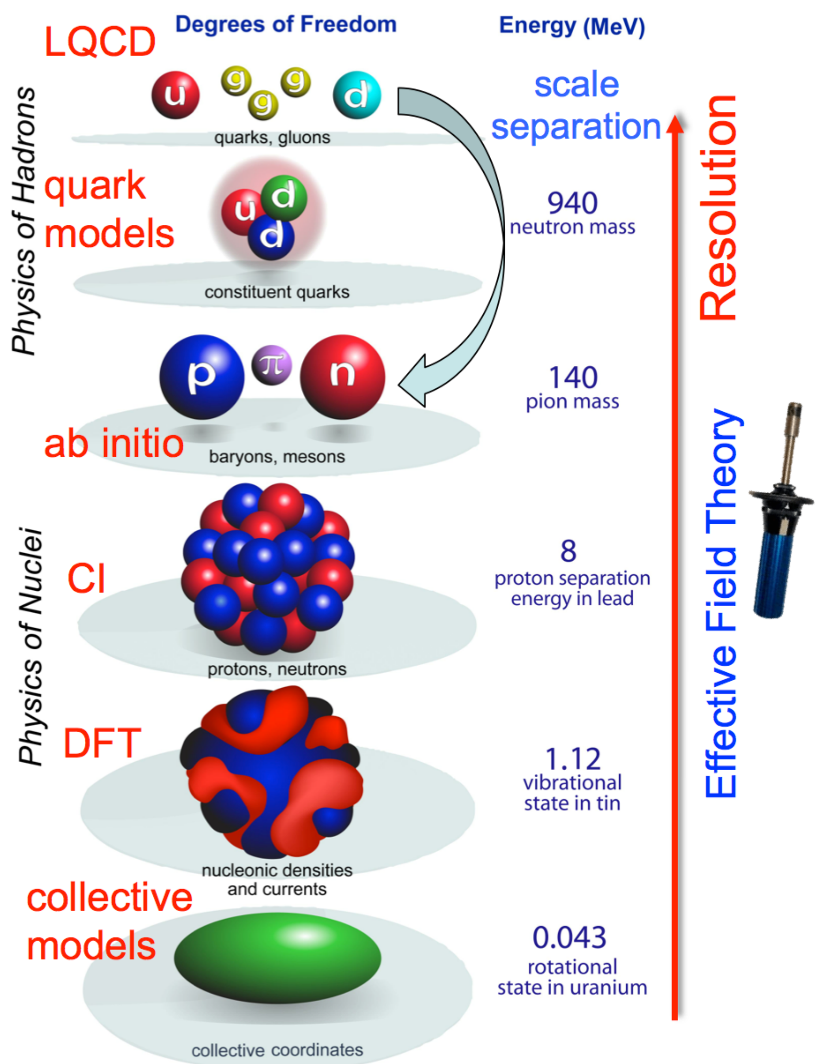
- How did visible matter come into being and how does it evolve?
- How does subatomic matter organize itself and what phenomena emerge?
- Are the fundamental interactions that are basic to the structure of matter fully understood?
- How can the knowledge and technological progress provided by nuclear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

"The ultimate goal is to develop <u>a predictive understanding</u> of nuclei and their interactions grounded in fundamental QCD and electroweak theory."
(*White Paper on Nuclear Astrophysics and Low-Energy Nuclear Physics, Jan 31, 2015***)**

We want to describe the entire landscape of nuclear properties in a controlled & unified way grounded in QCD

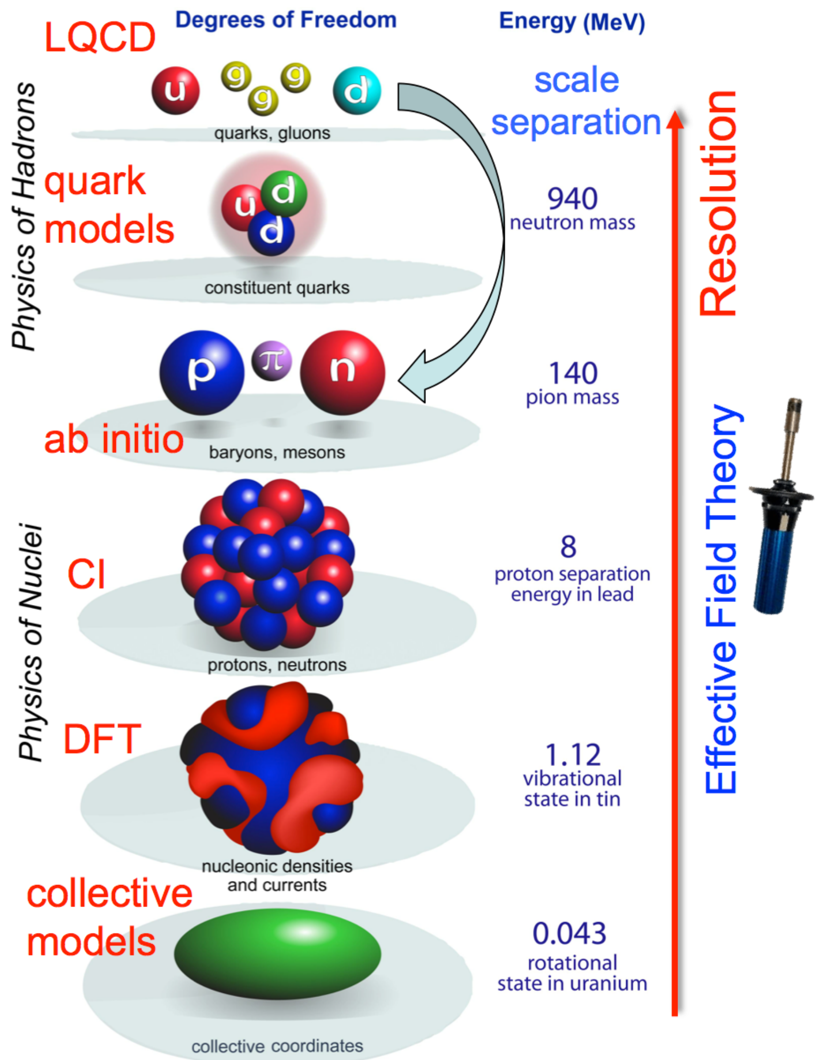


The physics of nuclei is complex, computationally difficult and interdisciplinary

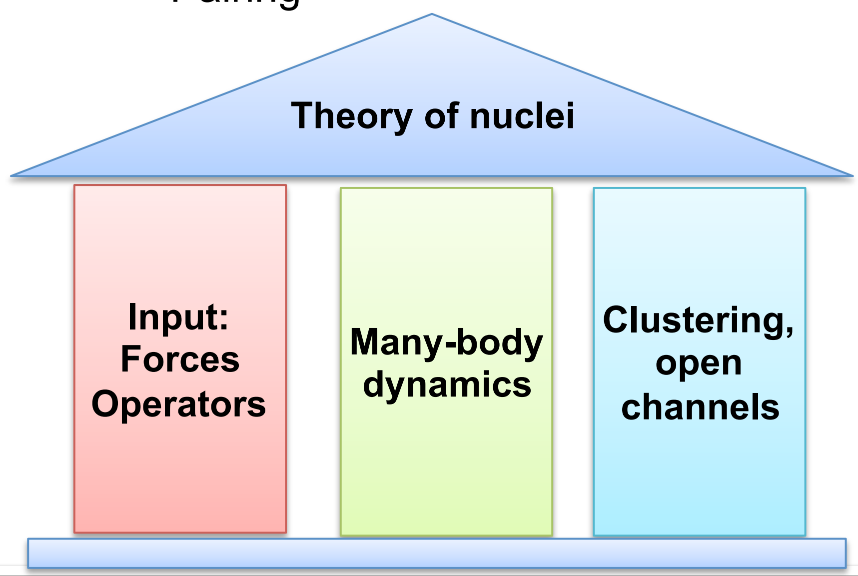


- Rich variety of phenomena, e.g.:
  - Nuclear structure at the extremes of isospin
  - Reactions at low (astrophysical) and high (accelerator) energies involving light and heavy nuclei
  - Fission of the heavy elements
  - Electroweak transitions and double-beta decay in nuclei
  - Equation of state and electroweak response in nucleonic matter
  - …

The physics of nuclei is complex, computationally difficult and interdisciplinary



- Nuclei are strongly correlated open quantum systems
  - Many-body correlations
  - Coupling to the continuum
  - Shell closures
  - Pairing



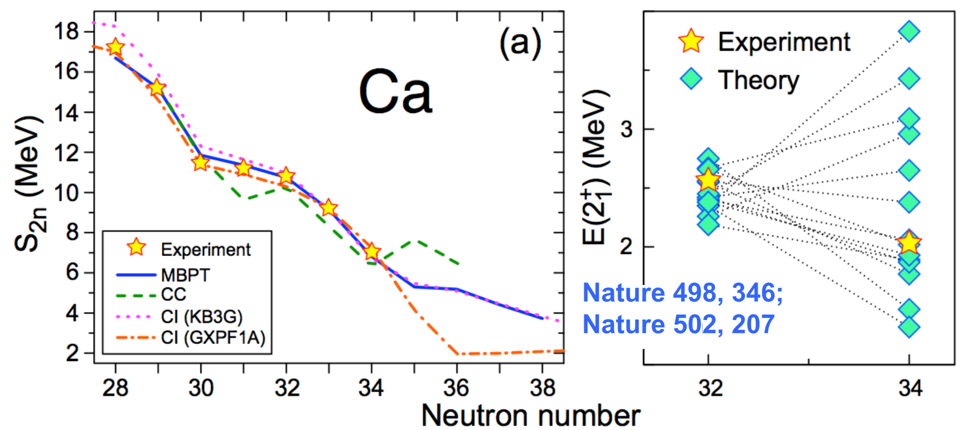
Summary of progress and opportunities in main areas of the theory of nuclei

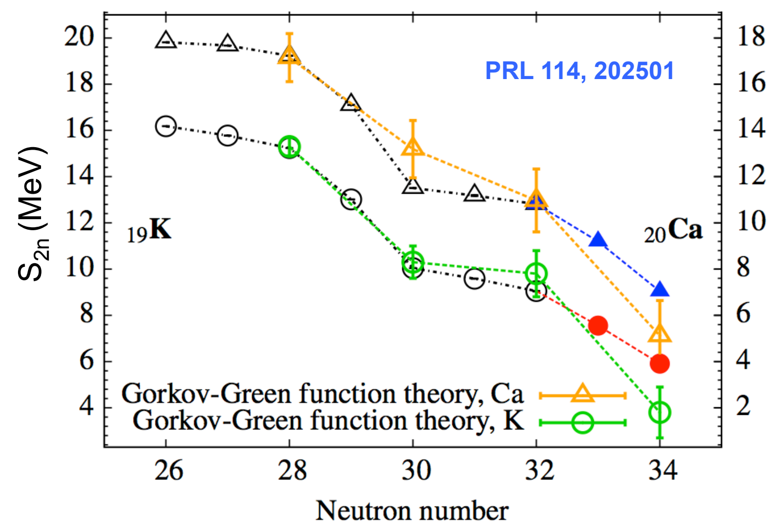
Illustrative examples

Nuclear structure renaissance driven by new ideas, data on exotic nuclei, high-performance computing

- Explosion of *ab initio* methods pushing to medium-mass nuclei
  - Coupled Cluster (CC)
  - In-Medium Similarity Renormalization Group (IM-SRG)
  - Gorkov-Green function theory
  - Many-Body Perturbation Theory
  - Ab initio valence-space shell model
- Complementary methods
  - allow unprecedented theory/ experiment confrontations
- Some of the challenges ahead
  - heavier, open-shell nuclei
  - coupling to the particle continuum

Frontier for probing nuclear forces and shell structure



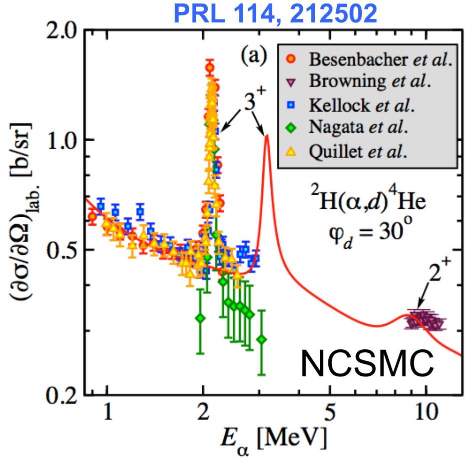


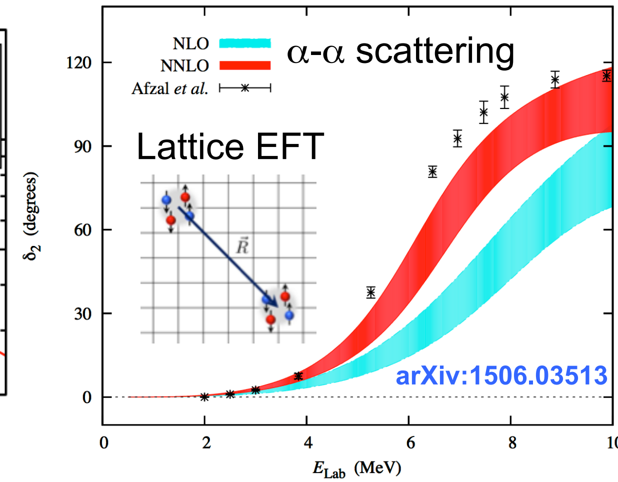
A parallel (though not as far along) development of unified ab initio approaches to structure and reactions

- Light-nucleus reactions with EFT NN+3N Hamiltonians
  - No-Core Shell Model with Continuum
  - Green' Function Monte Carlo
  - Lattice EFT with Adiabatic Projection Method
- Electroweak responses
  - Euclidean response with Green's Function Monte Carlo (GFMC)
  - Lorentz Integral Transform with Coupled Cluster
- Prospect/challenge:
  - Quantitative predictions of light-nucleus fusion reactions, e.g.: $^{12}C(\alpha,\gamma)^{16}O$

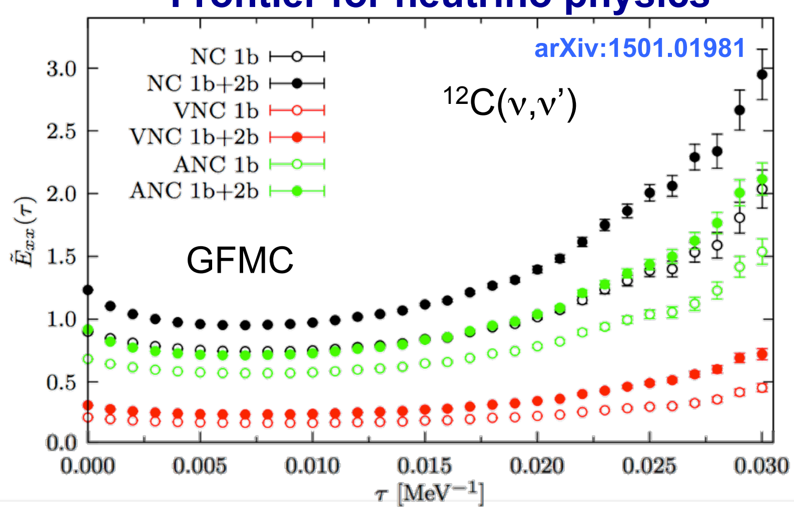
Quantitative predictions/Open nuclear systems frontier

PRL 114, 212502





Frontier for neutrino physics

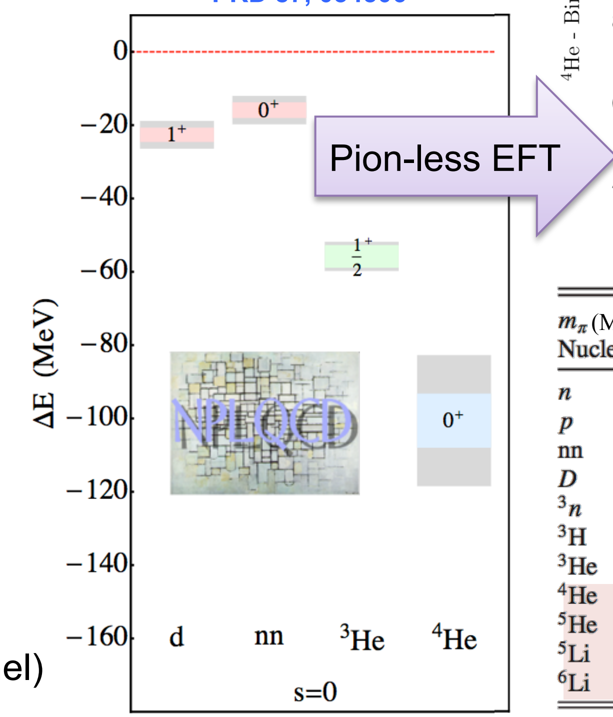


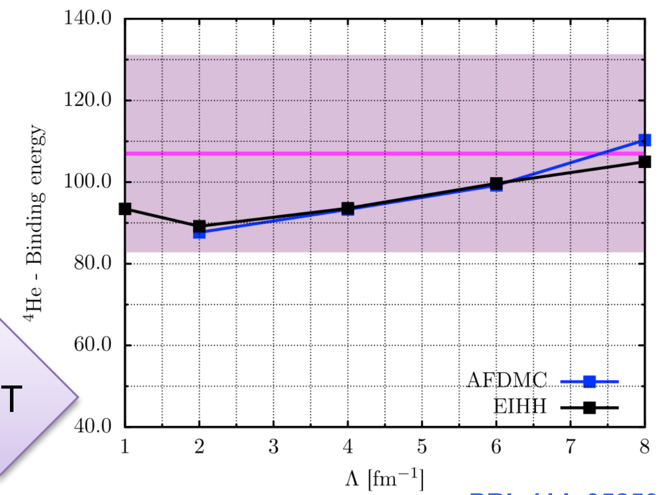
These efforts revealed deficiencies, and spurred multiple new formulations of EFT Hamiltonians

- New regularizations (Epelbaum, Krebs, Meissner)
- New optimizations (Ekstrom et al., Carlsson et al.)
- EFT Hamiltonian constrained on Lattice QCD for nuclei
- Prospects/challenges:
  - Robust uncertainty quantification
  - Lattice QCD to provide additional measurements to constrain EFT forces (e.g., T=3/2 A=3 channel)

Frontier for nuclear structure theory

PRD 87, 034506





PRL 114, 052501

m_π (MeV) Nucleus	140 (Nature)	510 (Ref. [5])	805 (Ref. [6])	805 (This work)
n	939.6	1320.0	1634.0	1634.0
p	938.3	1320.0	1634.0	1634.0
nn	...	7.4 ± 1.4	15.9 ± 3.8	15.9 ± 3.8*
D	2.224	11.5 ± 1.3	19.5 ± 4.8	19.5 ± 4.8*
^3n	...			...
^{3}H	8.482	20.3 ± 4.5	53.9 ± 10.7	53.9 ± 10.7*
^{3}He	7.718	20.3 ± 4.5	53.9 ± 10.7	53.9 ± 10.7
^{4}He	28.30	43.0 ± 14.4	107.0 ± 24.2	89 ± 36
^{5}He	27.50			98 ± 39
^{5}Li	26.61			98 ± 39
^{6}Li	32.00			122 ± 50

B.E. in MeV

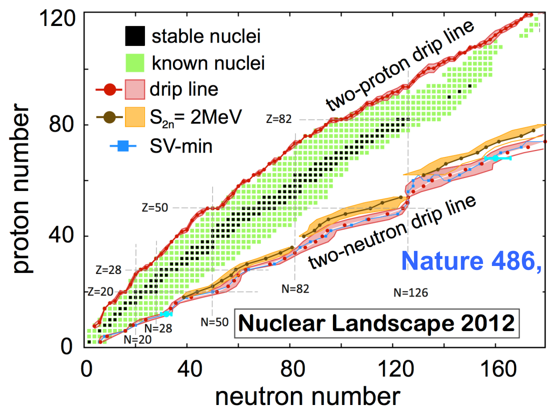
Large-scale surveys with Density Functional Theory (DFT) drive the quest for universal energy density functional

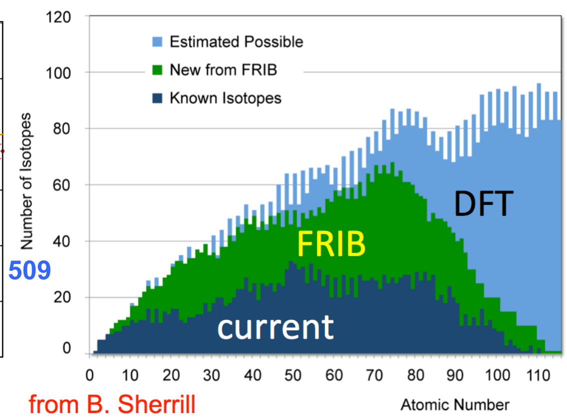
- Unprecedented large-scale applications of DFT
  - Driplines, superheavies, spectroscopy
  - Fission, fundamental symmetries
  - Nuclear astrophysics

- Challenge: Predictive and quantified energy functional routed in first-principles theory

- Prospects:
  - Predictive theory of structure and decay of heavy nuclei
  - Accurate inputs for applications for science and society

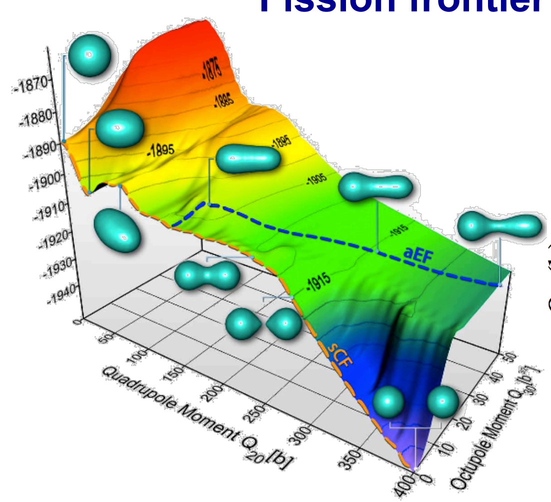
Frontier for the limits of stability



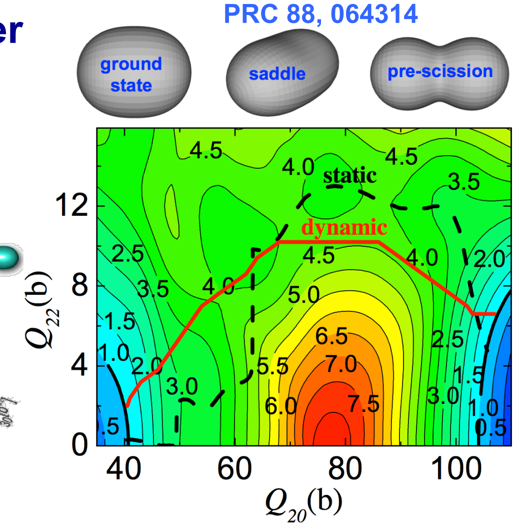


from B. Sherrill

Fission frontier

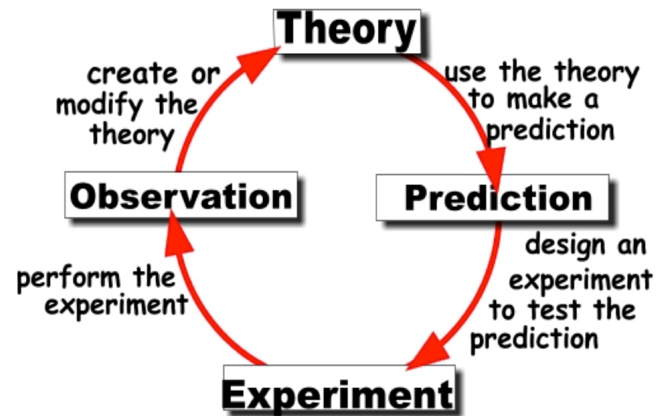


PRC 88, 064314



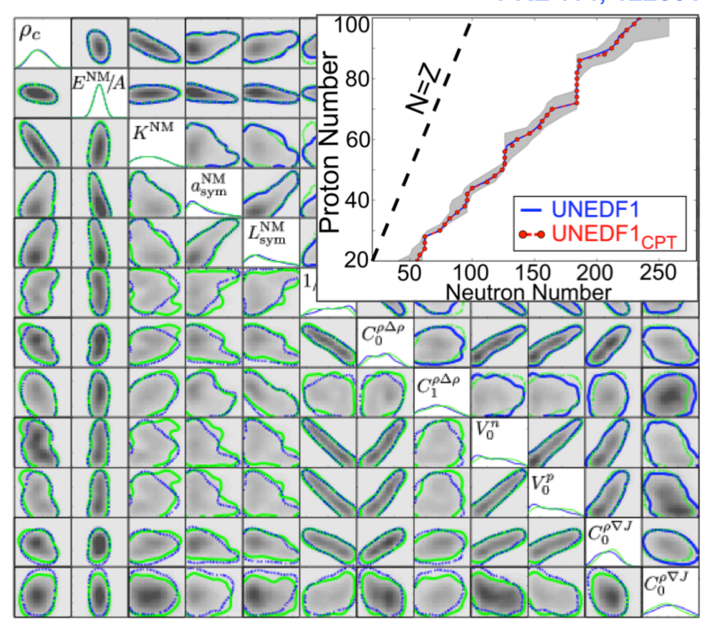
New tools to efficiently optimize nuclear interactions and quantify propagated uncertainties were/are instrumental

- Uncertainty Quantification (UQ) needed to enhance feedback in scientific method's cycle …
- … and to assess predictive power in regions not accessible to experiment
- Density Functional Theory provided the template for applying UQ methodology to nuclear structure and reactions
- Enabled by algorithmic developments and high-performance computing
- Prospect: paradigm shift that will enhance coupling between theory and experiment throughout low-energy nuclear theory



UQ frontier

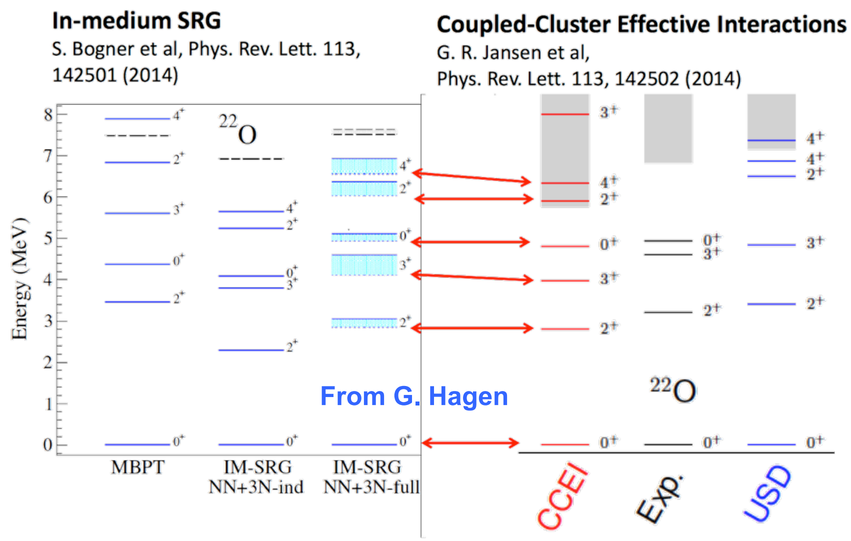
PRL 114, 122501

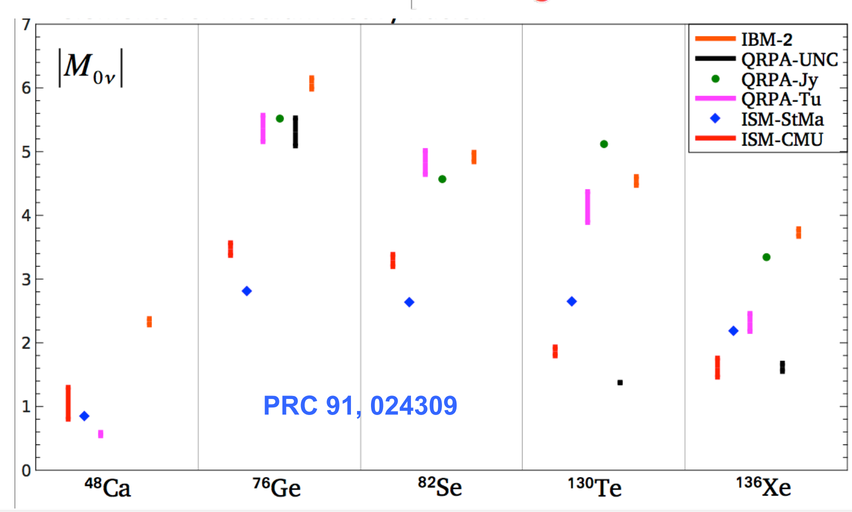


Nuclear structure and effective field theory ready to produce significantly more accurate $0\nu\beta\beta$ matrix elements

- Ab initio theory starting to deliver improved effective interactions for shell model calculations
- Shell Model codes becoming more efficient, allowing unprecedented large-scale calculations
- Emphasis on improving predictions by Density Functional Theory, Interacting Boson Model
- Effective Field Theory constructing and assessing many-body week currents, exotic $0\nu\beta\beta$ operators
- Sustained effort in & coordination between different areas are key!

Benchmarking different methods: Spectra in ^{22}O

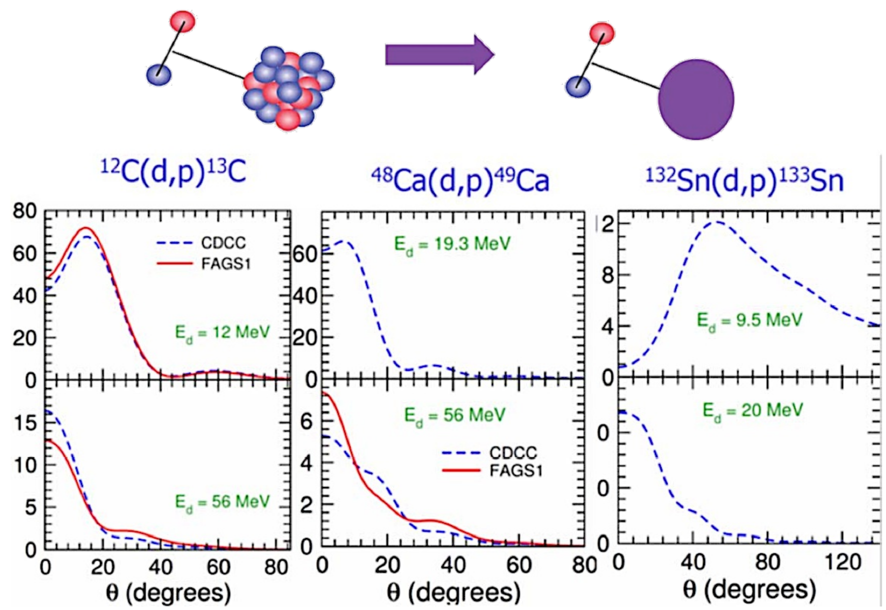




A complete description of nuclei cannot be achieved without understanding the reactions used to study them

- Emphasis on (d,p) reactions and connection to (n,γ) reactions
- Revealed shortcomings of Faddeev approach for heavy nuclei …
- … and spurred new Faddeev treatment of (d,p) reactions in momentum space
  - Mukhamedzhanov, Eremenko, Sattarov (theoretical formulation); Elster, Eremenko, Nunes (implementation)
- New treatments of transfer to the continuum using surface operator
- Neutron capture via giant-dipole excitations, isobaric analog states, target deformation
- Challenge: comprehensive description of direct, semi-direct, pre-equilibrium, and compound processes

(d,p) reactions as three-body problem

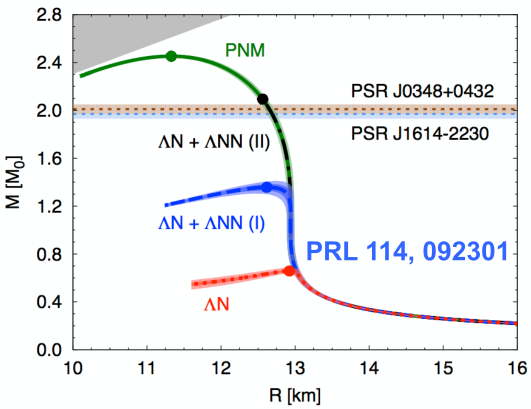


ReactionTheory.org

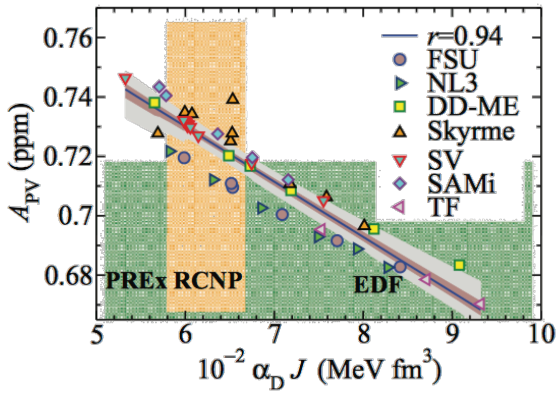
A Topical Collaboration for Nuclear Theory.
June 1, 2010 to May 31, 2015

Theory of atomic nuclei intimately tied to other parts of nuclear science and problems beyond nuclear science

Neutron Stars: Quantum Monte Carlo method for hyper-nuclear systems connected neutron star observations to many-body hyperon-nucleon forces in neutron matter in presence of Λ hyperons.

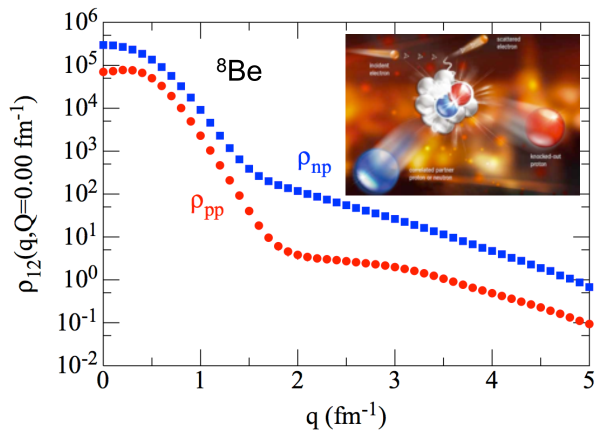


PRL 114, 092301

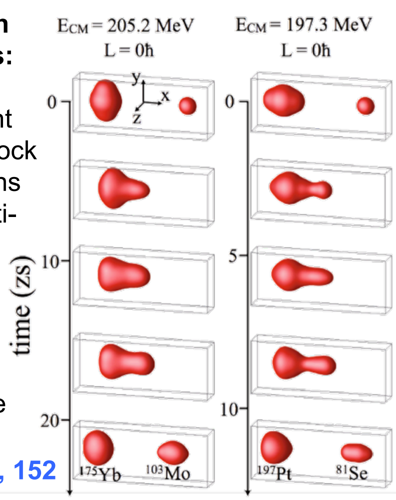


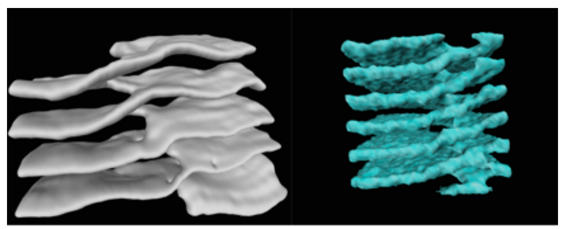
Neutron distribution: Parity-violating electron scattering together with measurements of electric dipole polarizabilities can provide a stringent test to our understanding of neutron-rich matter. PRC 88, 024316

Momentum distributions: Quantum Monte Carlo calculations explain JLAB enhanced np versus pp back-to-back ^{12}C(e,e'pN) cross sections. PRC 89, 024305



Heavy-ion collisions: Time-Dependent Hartree-Fock calculations show multi-nucleon transfer from the heavy fragment toward the light one. EPJ. A 48, 152



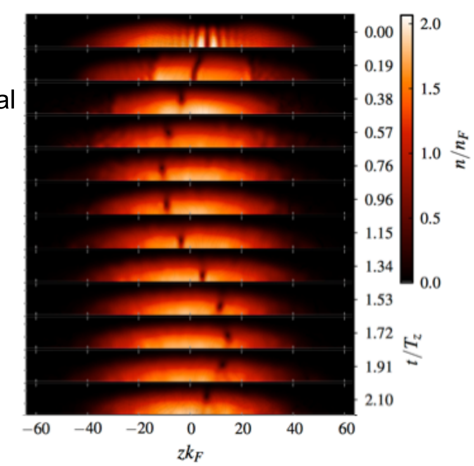


"Parking garage" Structures in Biophysics and Astrophysics: Large scale molecular dynamics simulations discovered helical defects in nuclear pasta that impact radio and X-ray obs. of neutron stars and provide model of an important biological structure.

PRL 114, 031102

Cold atoms: Time Dependent Density Functional Theory explains recent MIT experiments which forms a vortex from an imprinted domain wall via a decaying vortex ring.

PRL 112, 025301



None of this would have been possible without high-performance computing

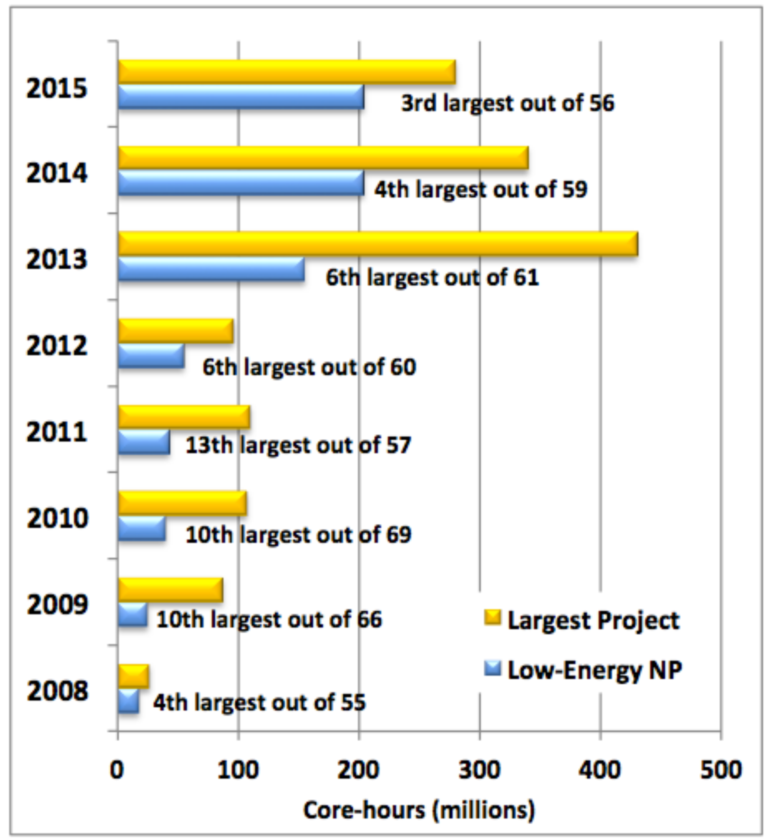
"High performance computing provides answers to questions that neither experiment nor analytic theory can address; hence, it becomes a third leg supporting the field of nuclear physics."
(NRC report, Nuclear Physics: Exploring The Heart of Matter)

- SciDAC collaborations between applied mathematicians, computer scientists, and nuclear physicists are key
- NUCLEI holds one of the largest INCITE allocations
- Other allocations: Astrophysics SciDAC, Lattice QCD SciDAC
- Other resources through ASCR, NNSA, …

UNEDF SciDAC Collaboration
Universal Nuclear Energy Density Functional

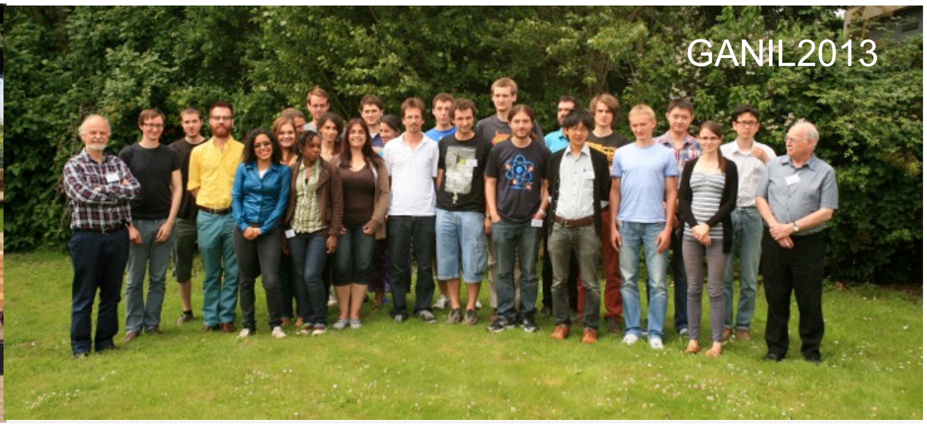
NUCLEI
Nuclear Computational Low-Energy Initiative

INCITE Allocation Trends 2008 – 2015



Training in nuclear theory is key to ensure a pipeline of new talents, future skilled workforce

- Problem: Small numbers and distributed expertise preclude University groups from adequately educating young scientists in state-of-the-art nuclear theory
- Excellent progress with TALENT (Training in Advanced Low-Energy Nuclear Theory, nucleartalent.org)
- Nine courses planned for 3-4 year cycle, ranging from nuclear forces to few- and many-body methods, to theory for experiments, astrophysics, and exotic nuclei, to high-performance computing. Now at second cycle.



International Theory Institutes for Physics with Exotic Nuclei: 2015 activities

- "New Directions fro Nuclear Structure and Reaction Theories", GANIL, 3/16-20/2015
- "Fission-fragments in low-energy fission: a gauge for macroscopic and microscopic influences", GANIL, 10/21-22/2015

- Topical Workshop on Nuclear Symmetry Energy, Southern China U., 1/9-12/2015
- "First FRIB-China Workshop on Physics od Nuclei and Hadrons", NSCL, 5/28-30/2015
- "Advances in the computations of nuclear structure and NN force", PKU, 8/1-6/2015
- "Properties of exotic nuclei and asymmetric nuclear matter", IMP-CAS, 8/7-12/2015

Theory Institutes: Upcoming Programs, Workshops (I)

*INSTITUTE FOR **N**UCLEAR **T**HEORY* (Programs)

- **"Nuclear Physics from Lattice QCD"** (INT-16-1)
  March 21 - May 27, 2016
  N. Barnea, S. Beane, Z. Davoudi, U. van Kolck
- **"Bayesian Methods in Nuclear Physics"** (INT-16-2a)
  June 13 - July 8, 2016
  R.J. Furnstahl, D. Higdon, N. Schunck, A.W. Steiner

*ECT**

- **"Interfacing Structure and Reaction Dynamics …"**
  01 Sep 2015 to 04 Sep 2015
  Gurgen Adamian, Alexis Diaz-Torres
- **ECT*-APCTP Joint Workshop: From Rare Isotopes to Neutron Stars**
  14 Sep 2015 to 18 Sep 2015
  Francesca Gulminelli, Chang-Hwan Lee, Yongseok Oh, Jürgen Schaffner-Bielich

Theory Institutes: Upcoming Programs, Workshops (II)

KAVLI INSTITUTE FOR THEORETICAL PHYSICS

- **"Frontiers in Nuclear Physics"**

  Aug 22 – Nov 4, 2016

  Barry Holstein, Wick Haxton, Ulf-G. Meißner, and Martin Savage

- **"Universality in Few-Body Systems"**

  Nov 7 13 – Dec 16, 2016

  Doerte Blume, Robin Côté, Olivier Dulieu, Chris H. Greene, and Alejandro Saenz

FRIB theory center steering committee

Constituted in Spring 2013 by NSCL director with the mandate to "*determine the required ingredients, including ramp-up funding options and an appropriate organizational structure for a future FRIB theory center, and then proceed to work with the agencies and develop a path forward.*"

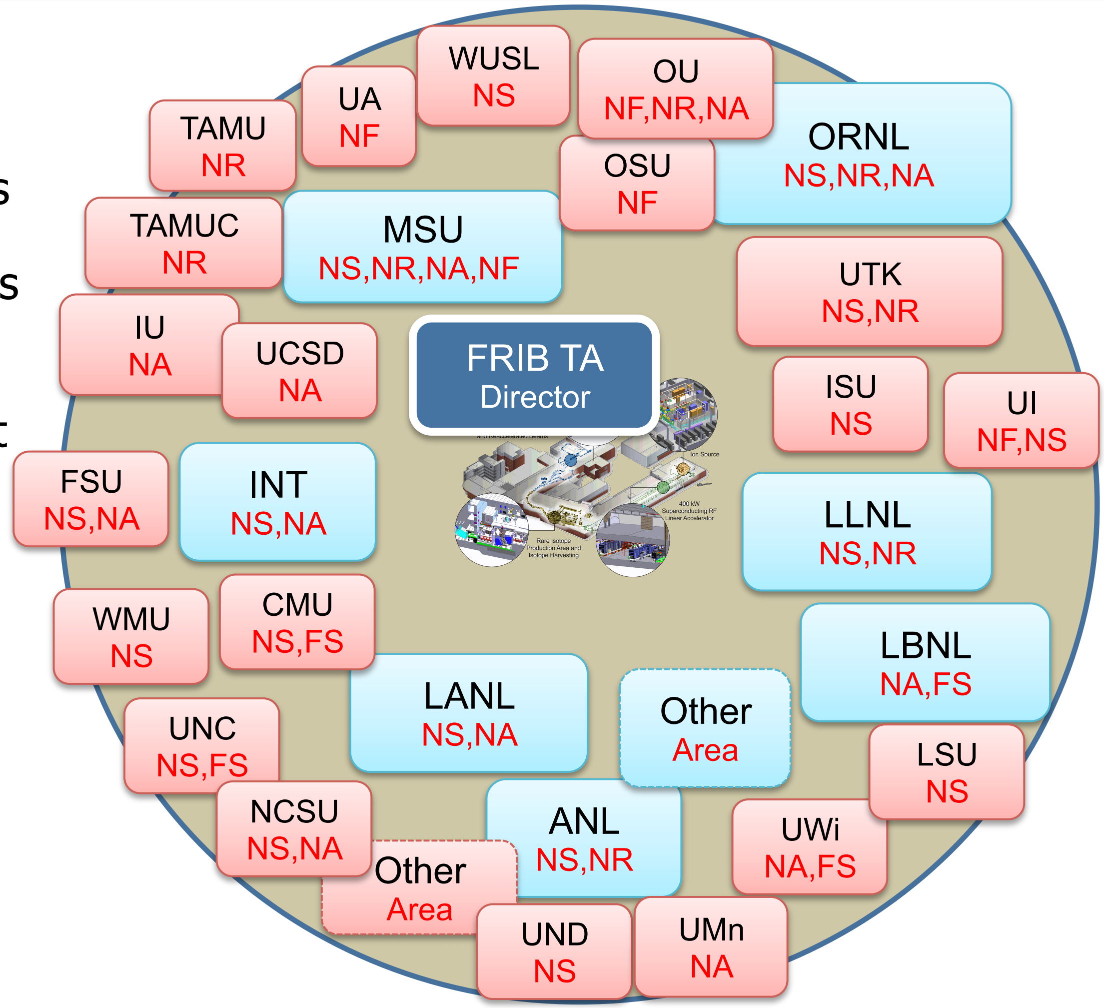
- Baha Balantekin (University of Wisconsin)
- Joseph Carlson (Los Alamos National Laboratory)
- David Dean (Oak Ridge National Laboratory)
- George Fuller (University of California San Diego)
- Richard Furnstahl (Ohio State University)
- Morten Hjorth-Jensen (NSCL, Michigan State University)
- Robert Janssens (Argonne National Laboratory)
- Bao-An Li (Texas A&M University - Commerce)
- Witek Nazarewicz (University of Tennessee)
- Filomena Nunes (**Chair**) (NSCL, Michigan State University)
- Erich Ormand (Lawrence Livermore National Laboratory)
- Sanjay Reddy (INT, University of Washington)
- Brad Sherrill (FRIB, Michigan State University)

FRIB theory alliance: Enhancing theory efforts nationally

FRIB theory alliance will:

- connect broadly across fields
- bring focus to those activities that are relevant
- identify and nurture the best talent
- take advantage of high performance computing
- be the natural home for training in advanced nuclear theory

Courtesy of F. Nunes



A possible snapshot for the FRIB theory alliance
(NF-nuclear forces; NS-nuclear structure; NR-nuclear reactions; NA-nuclear Astrophysics; FS-fundamental symmetries)

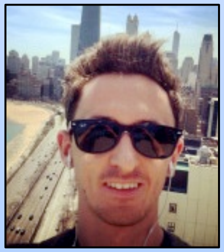
Key Elements of FRIB Theory Alliance

- A prestigious **national fellow program** (already started)
  - MSU FRIB Theory Fellow Program

Elena Litvinova
(Fellow: 2012-2013)
Faculty WMU

Heiko Hergert
(Fellow: 2014-2015)
Faculty MSU

  - Natl. FRIB Theory Fellow Program



Diego Lonardoni
(Fellow: 2015-present)
LANL

- **Bridge tenure-track positions** in nuclear theory

- Vibrant national/international visitors program (already started)
  - **Jul-Aug 2013:**
    "Symmetry energy in the context of new radioactive ion beam facilities and astrophysics":
    JPG 41, 093001
  - **May 2015**
    "Theory for open shell nuclei near the limits of stability"

Michigan State University
FRIB Theory Fellow (2015)

The FRIB Theory Alliance is seeking outstanding candidates for a FRIB Theory Fellowship. The successful candidate will conduct independent or collaborative research at Michigan State University on nuclear structure, astrophysics, and/or fundamental symmetries relevant to the Facility for Rare Isotope Beams (FRIB). The FRIB Theory Alliance is a consortium of universities and national laboratories actively engaged in theoretical research in FRIB science. FRIB will be a new national user facility for nuclear science, funded by the DOE Office of Science and operated by Michigan State University.

The FRIB Theory Fellowship is a 2-year position with the possibility of renewal for a maximum of 5 years. The initial stipend is $70K and this position has an annual travel budget of up to $5K. This FRIB Theory Fellow will be placed at Michigan State University. The successful candidate must demonstrate great promise for high scientific achievement in FRIB science and is expected to advance into open faculty or permanent staff positions in the field within 5 years of their initial appointment.

Benefits
MSU employees receive excellent benefits including health/dental plans, a generous retirement plan, and educational assistance.

For immediate consideration, send resume, research statement, publication list, and names and contacts of three references to **Dr. Erich Ormand**, Chair of the national FRIB Theory Fellow search committee (**theory-fellow2015@frib.msu.edu**). Deadline for applications: 1 October 2015.

Summary

- The theory of nuclei and their reactions plays an important role across the entire spectrum of U.S. nuclear science
- A major driver of progress is new data on very neutron-rich nuclei from FRIB
- Additional data is critical to obtaining a coherent picture of nuclear structure and dynamics
  - parity violating electron scattering at JLab
  - astrophysical observations
  - …
- Success of nuclear theory program enhanced by investments and initiatives
  - Institute for Nuclear Theory
  - Topical Collaborations
  - Inter-disciplinary connections
  - International programs
  - TALENT

Nuclear Theory Initiatives

The nuclear theory community is in the process of launching a suite of new initiatives to ensure that the experimental program reaches its full potential:

- Establishment of a national FRIB Theory Alliance, which will enhance the field through the national FRIB theory fellow program; establishing tenure-track bridge positions in nuclear theory; fostering interdisciplinary collaborations; and shepherding international initiatives.
- New investments in computational nuclear physics theory, including expansion of SciDAC programs and workforce development to fully exploit U.S. leadership in high-performance computing.
- Expansion of educational initiatives, including TALENT.