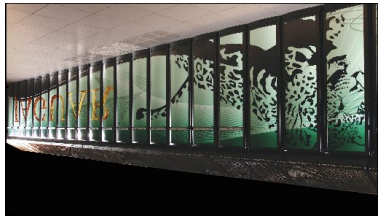
Theory of Nuclei and Their Reactions

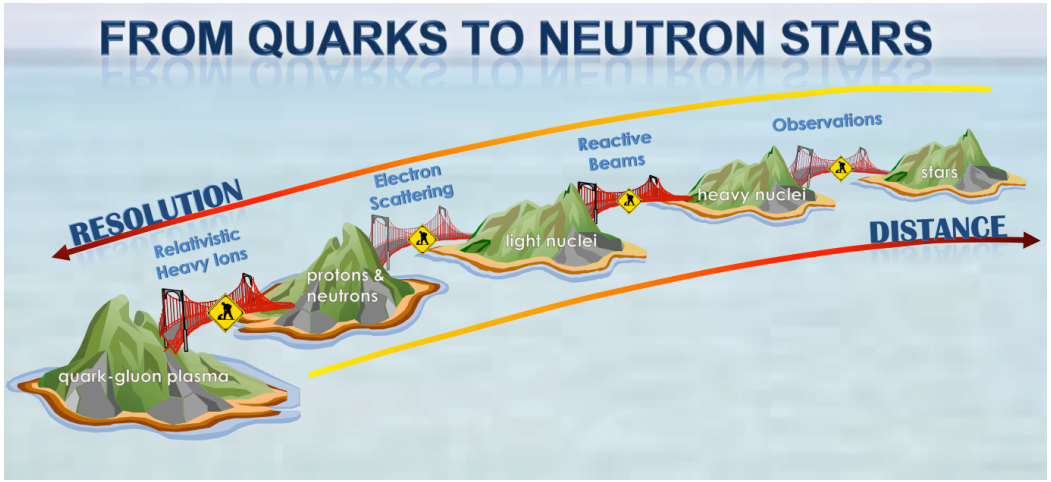
Witek Nazarewicz (MSU/ORNL)

Joint DNP Town Meetings on Nuclear Structure and Nuclear Astrophysics

Texas A&M, August 21-23, 2014

- Introduction
- General principles
- Examples: quantitative nuclear theory; predictive capability
- Initiatives
- Challenges
- Summary





Thanks for the input!

The Nuclear Landscape and the Big Questions (NAS report)

- How did visible matter come into being and how does it evolve? (origin of nuclei and atoms)
- How does subatomic matter organize itself and what phenomena emerge? (self-organization)
- 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?

TIMESCALE

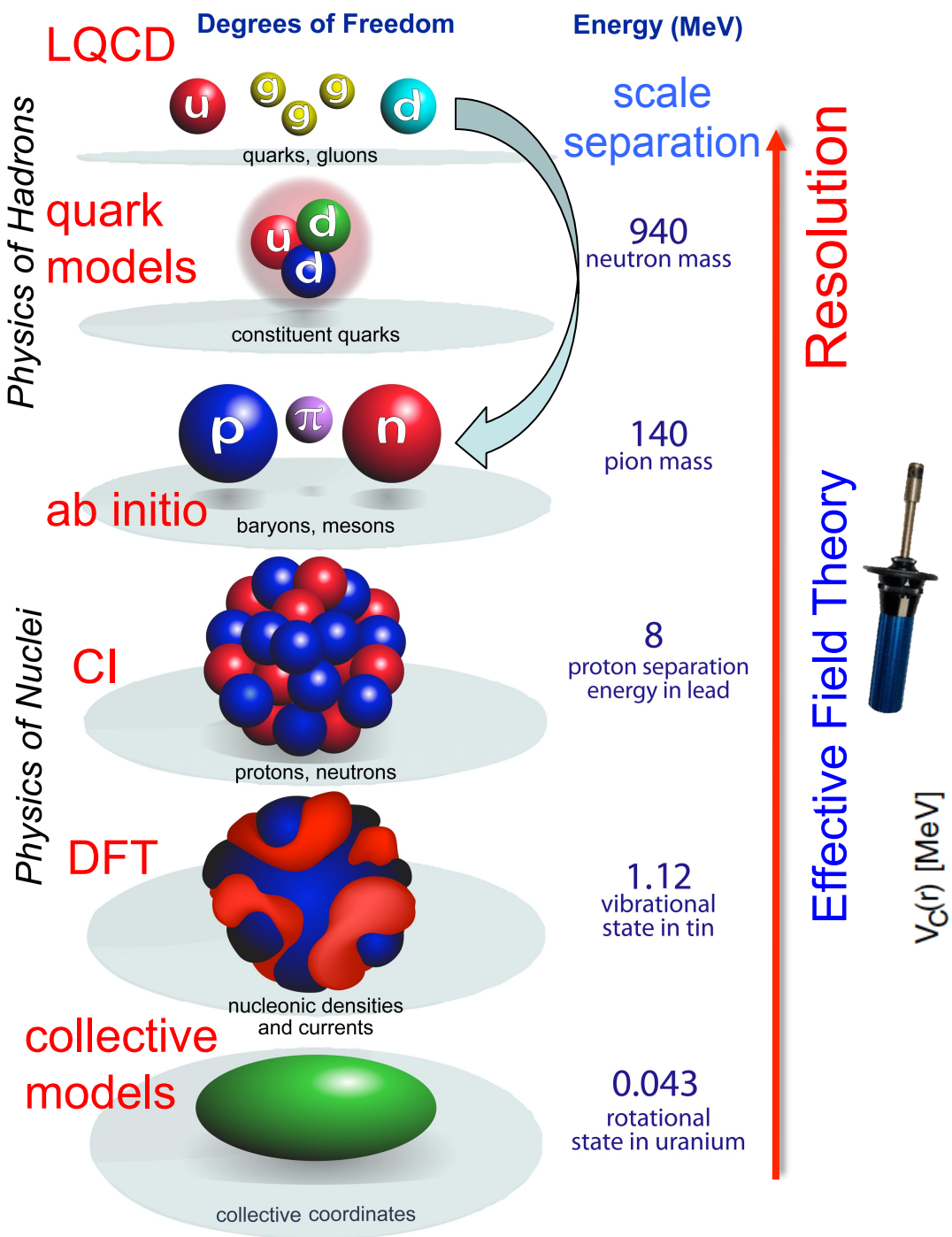
➡ from QCD transition (color singlets formed, 10 ms after Big Bang) till today (13.8 billion years later)

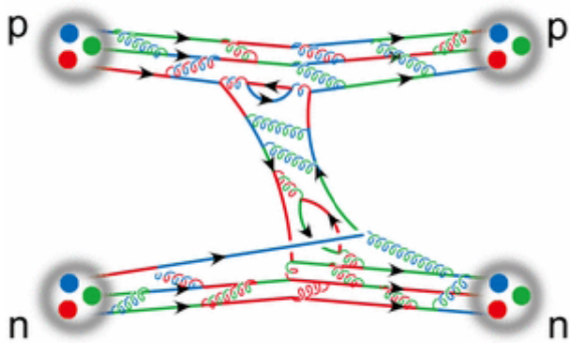
DISTANCE SCALE

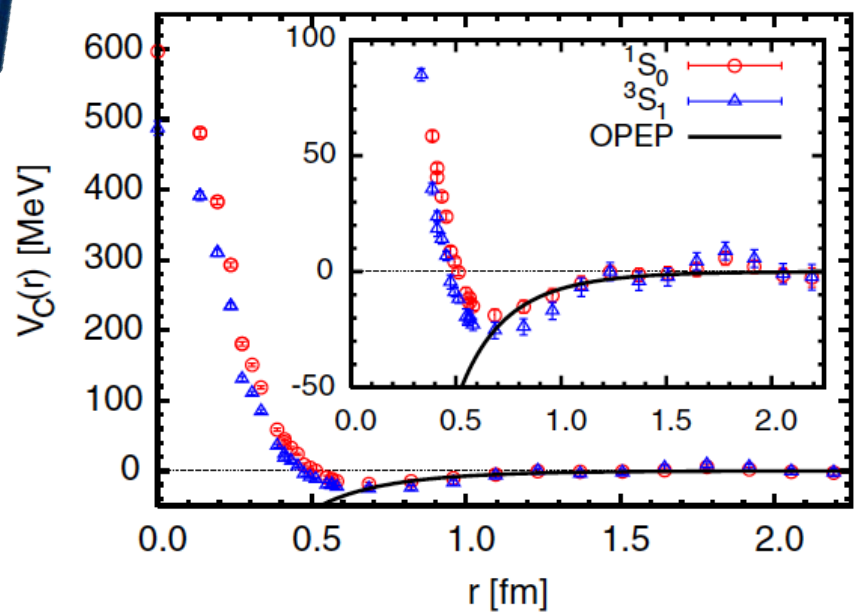
➡ from 10^{-15} m (proton's radius) to 12 km (neutron star radius)

SCIENCE AND SOCIETY RELY ON OUR UNDERSTANDING OF THE ATOMIC NUCLEUS AND THE GRAND NUCLEAR LANDSCAPE

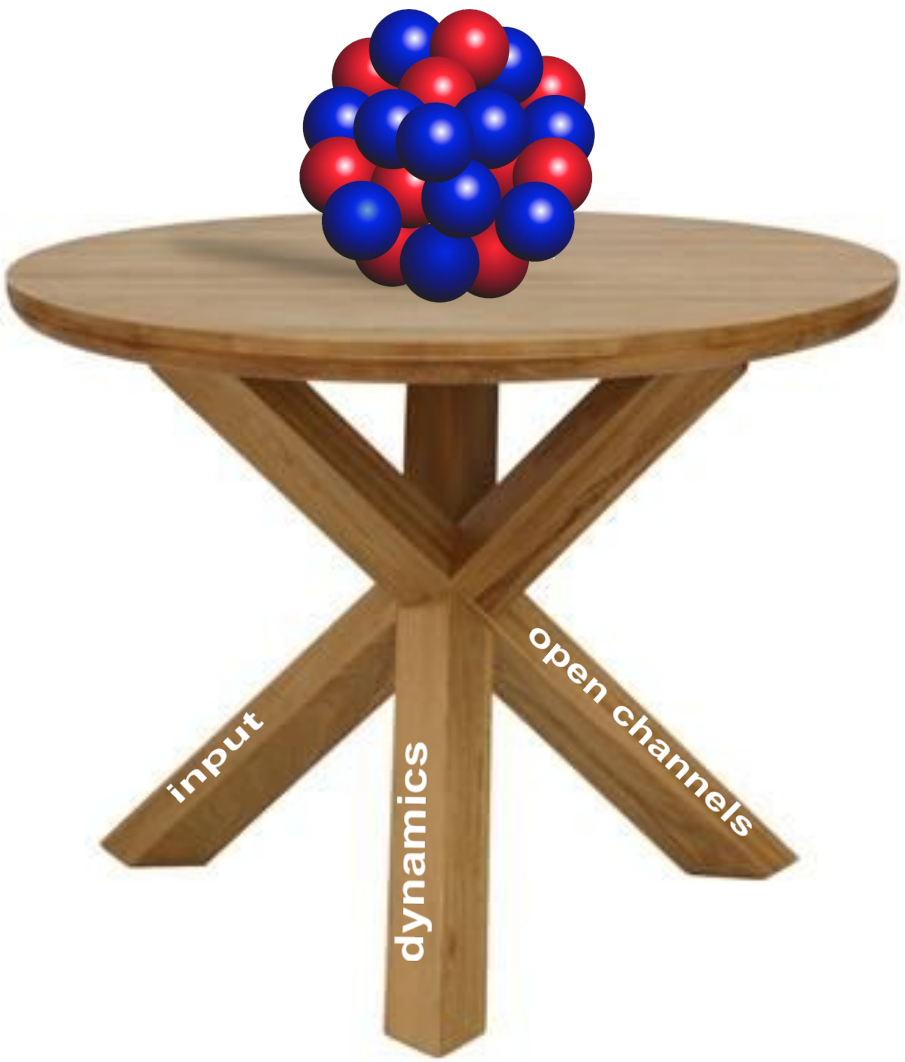
The challenge and the prospect: physics of nuclei directly from QCD







Theory of nuclei is demanding



Great recent progress

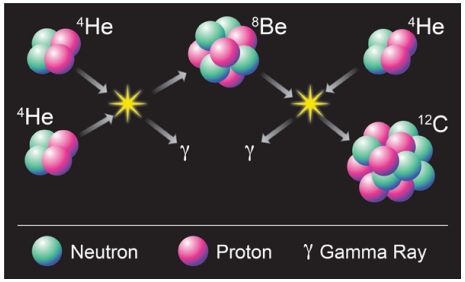
- New ideas
- Data on exotic nuclei crucial
  - long isotopic chains
  - low-energy reaction thresholds
  - large neutron-to-proton asymmetries
- High performance computing
  - algorithmic developments
  - benchmarking and validation
  - uncertainty quantification
  - large-scale computations

Illustrative physics examples

More excellent examples in the experimental overview

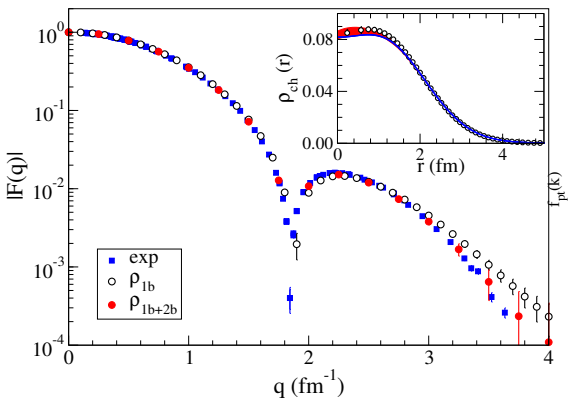
Janssens

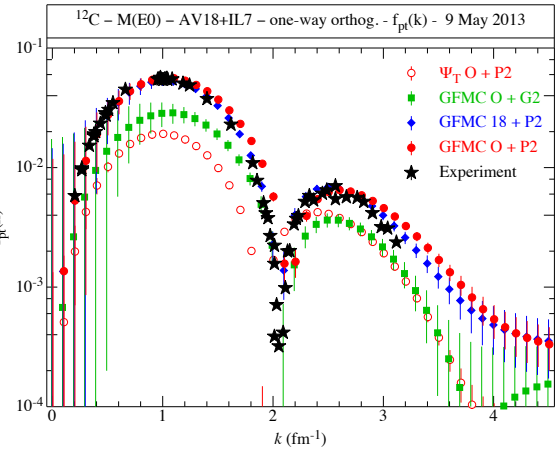
Ab-initio frontier: quantitative predictions



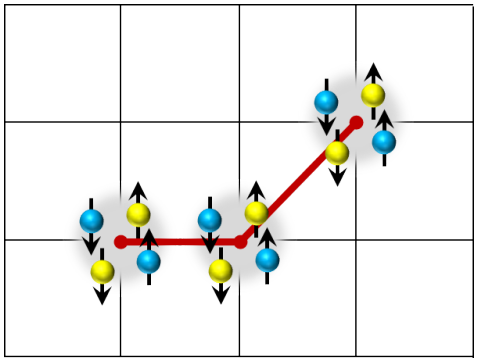
^{12}C ground state and Hoyle state

Green's Function Monte Carlo

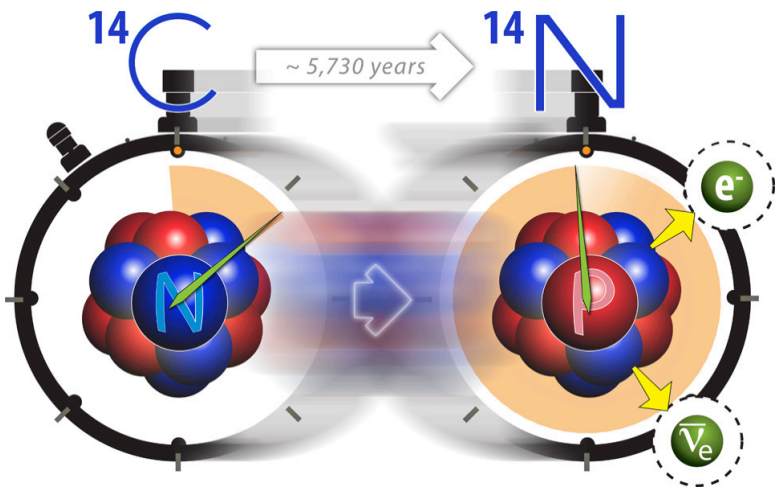


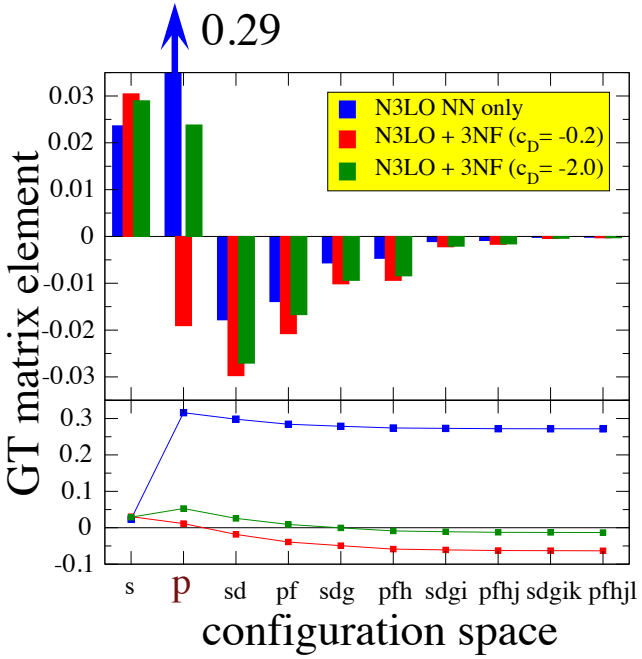


Lattice EFT

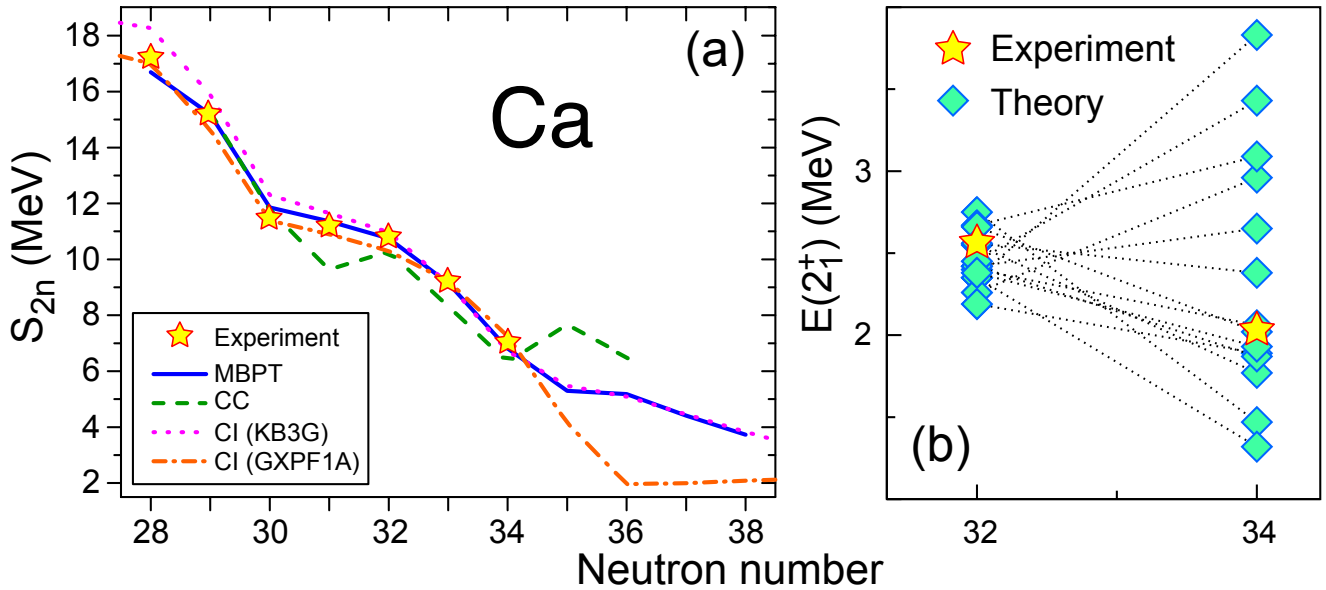


Anomalous Long Lifetime of ^{14}C

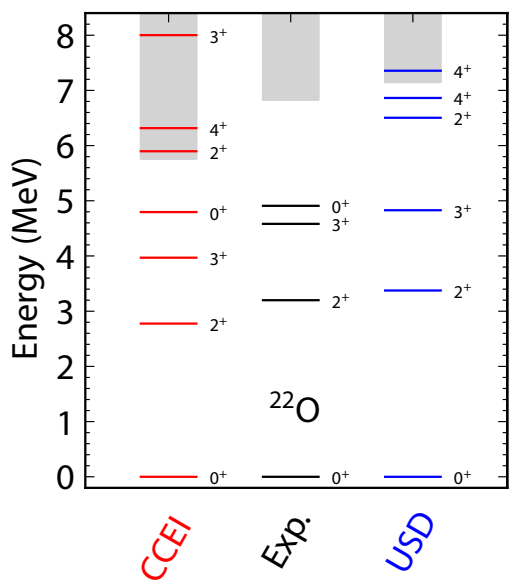




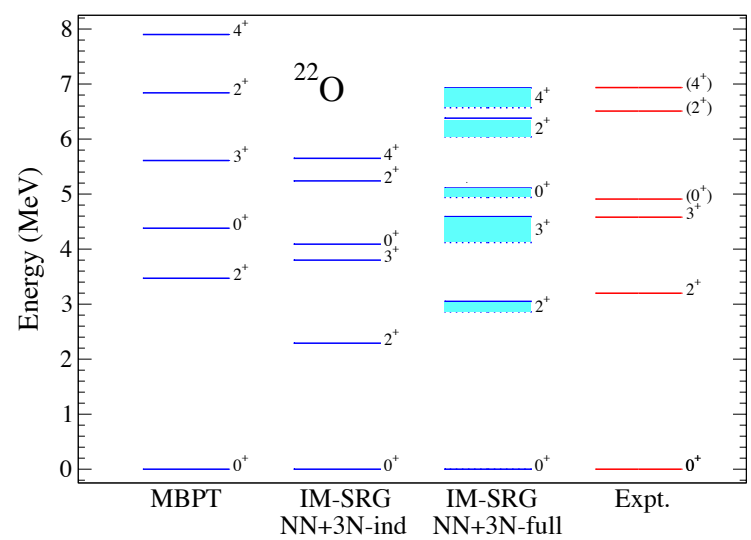
The frontier: medium-mass nuclei



Microscopic valence-space Shell Model

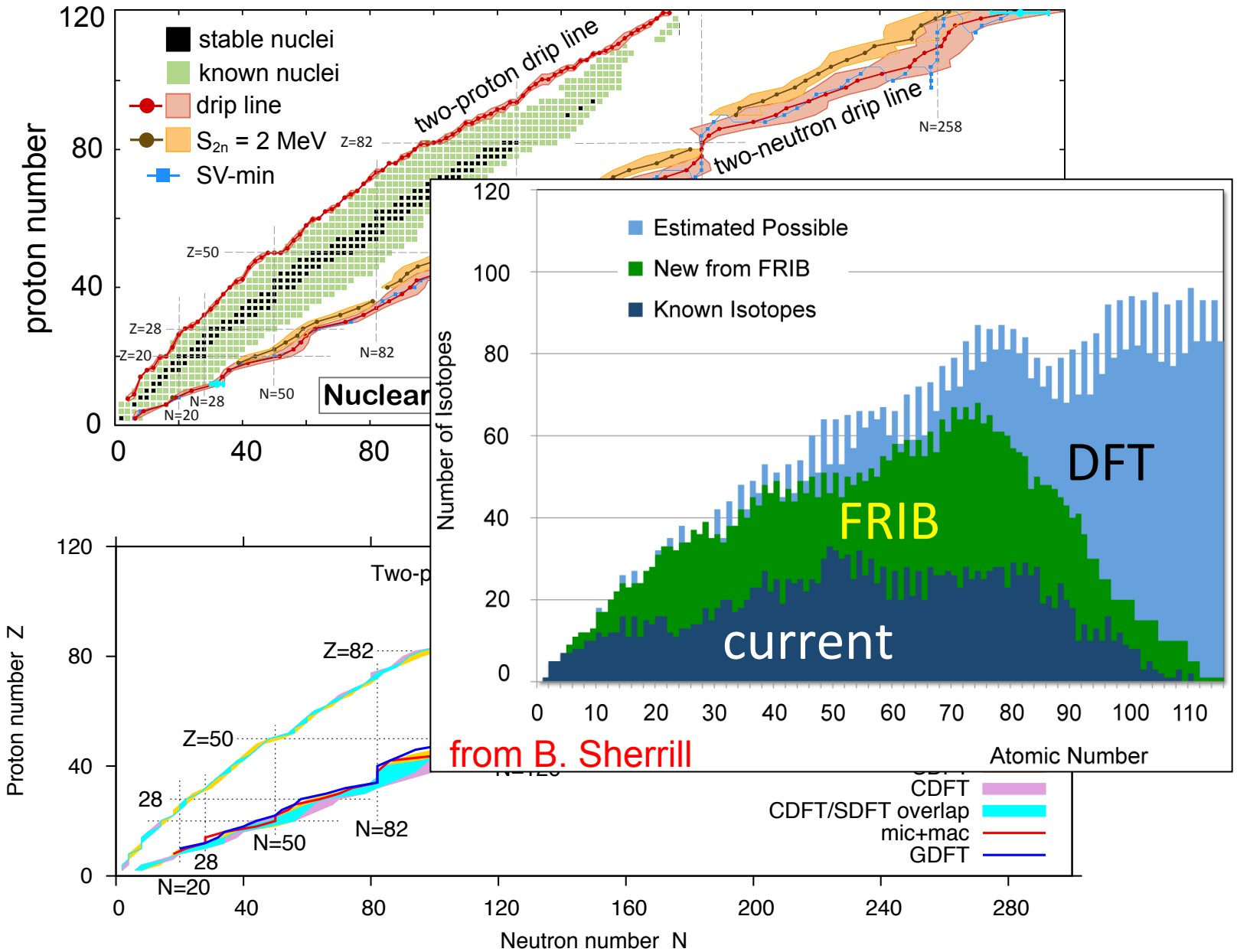


Coupled Cluster Effective Interaction (valence cluster expansion)



In-medium SRG Effective Interaction

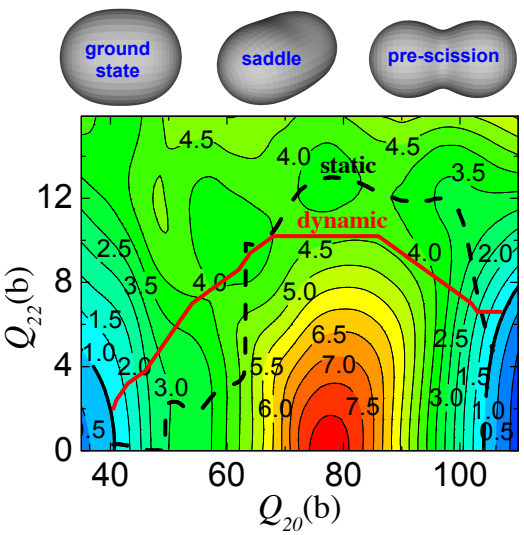
Nuclear Density Functional Theory: Large-Scale Surveys
The challenge: Universal Energy Density Functional



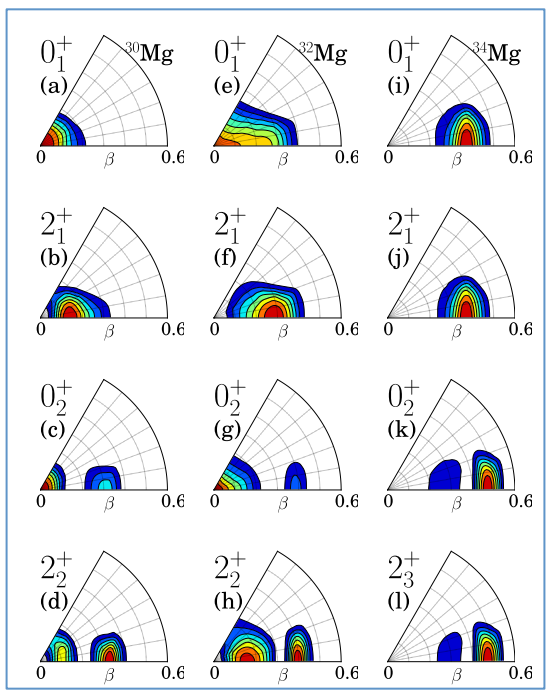
Small and Large-Amplitude Collective Motion

- New-generation computational frameworks developed
  - Time-dependent DFT and its extensions
  - Adiabatic approaches rooted in Collective Schrödinger Equation
  - Quasi-particle RPA
  - Projection techniques
- Applied to HI fusion, fission, coexistence phenomena, collective strength, superfluid modes

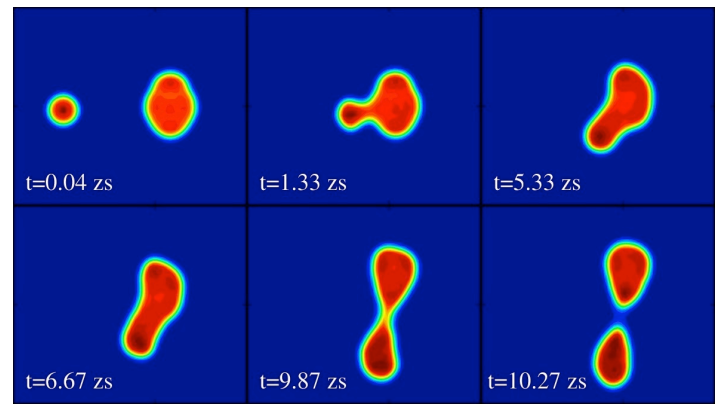
Spontaneous fission



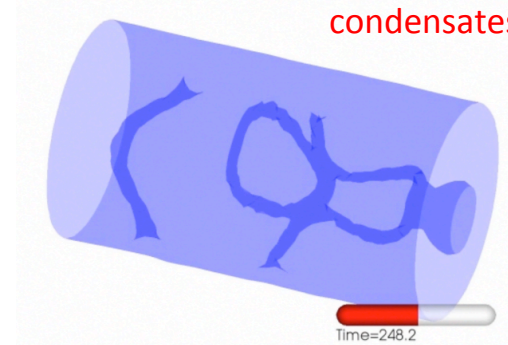
Shape coexistence



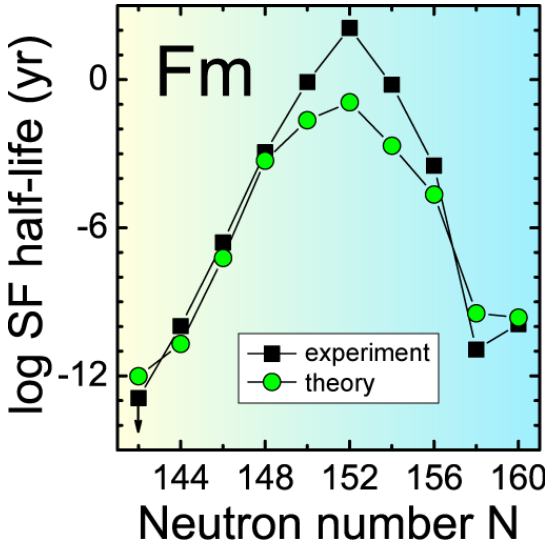
Heavy Ion fusion



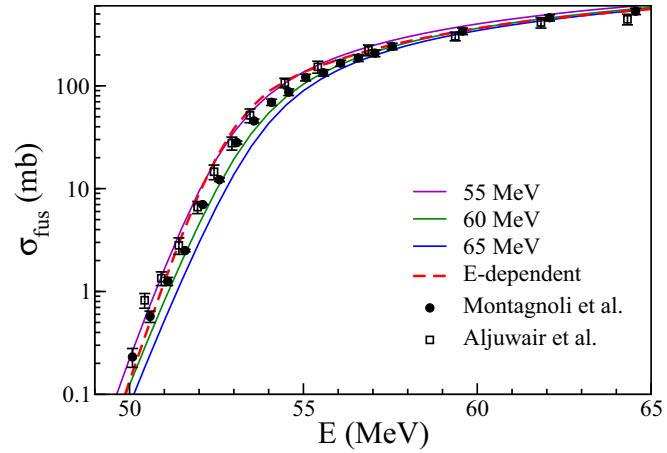
Vortex dynamics in superfluid condensates



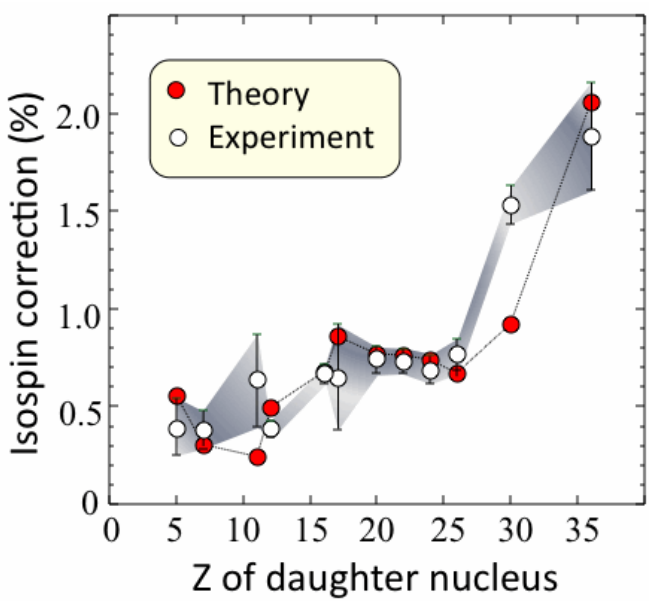
SF lifetimes



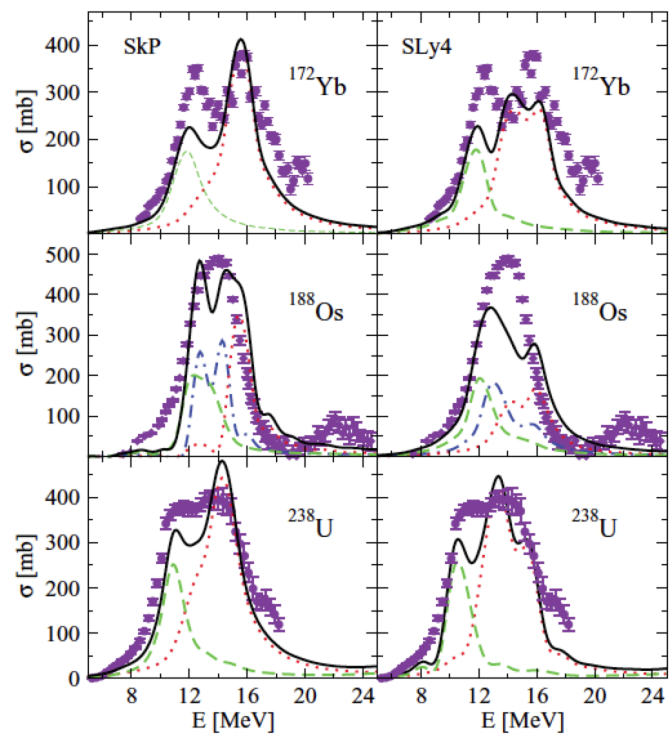
Fusion cross section



Isospin mixing

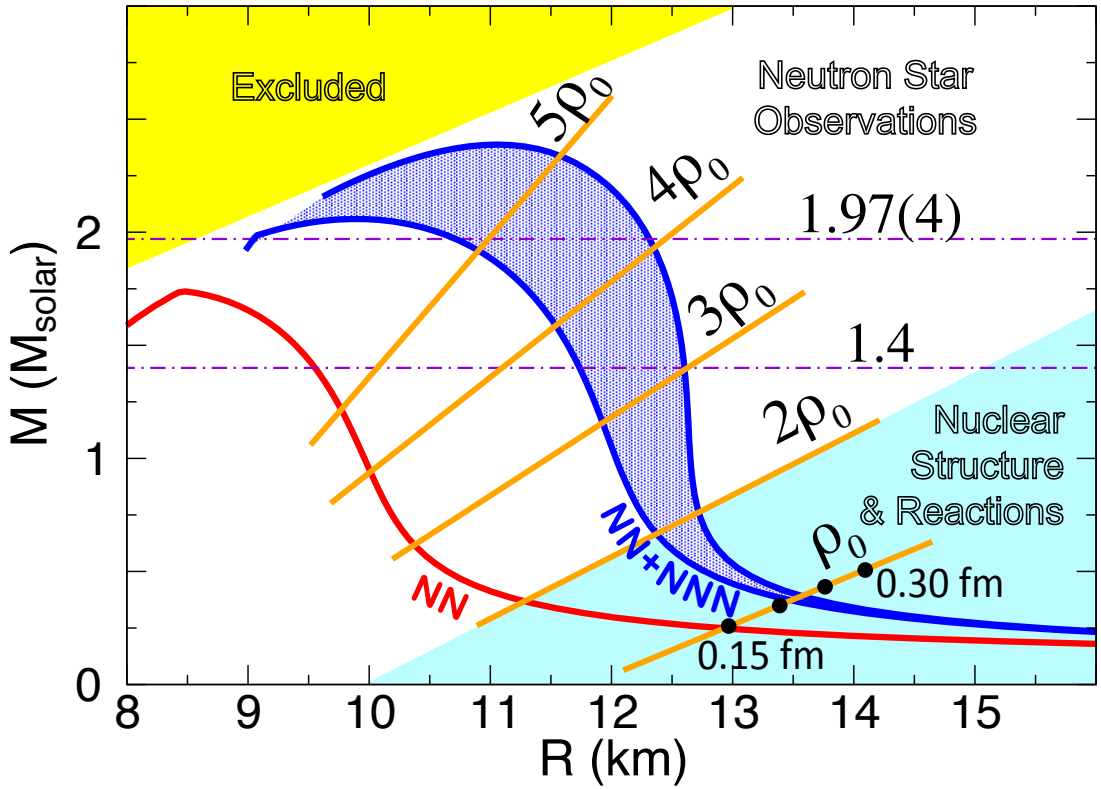


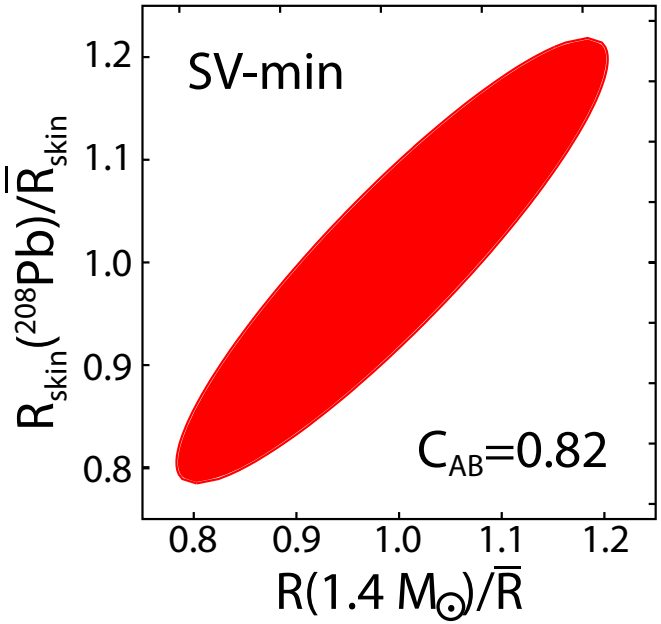
E1 strength



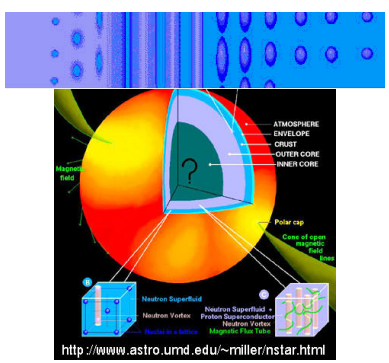
From nuclei to neutron stars (a multiscale problem)

Reddy



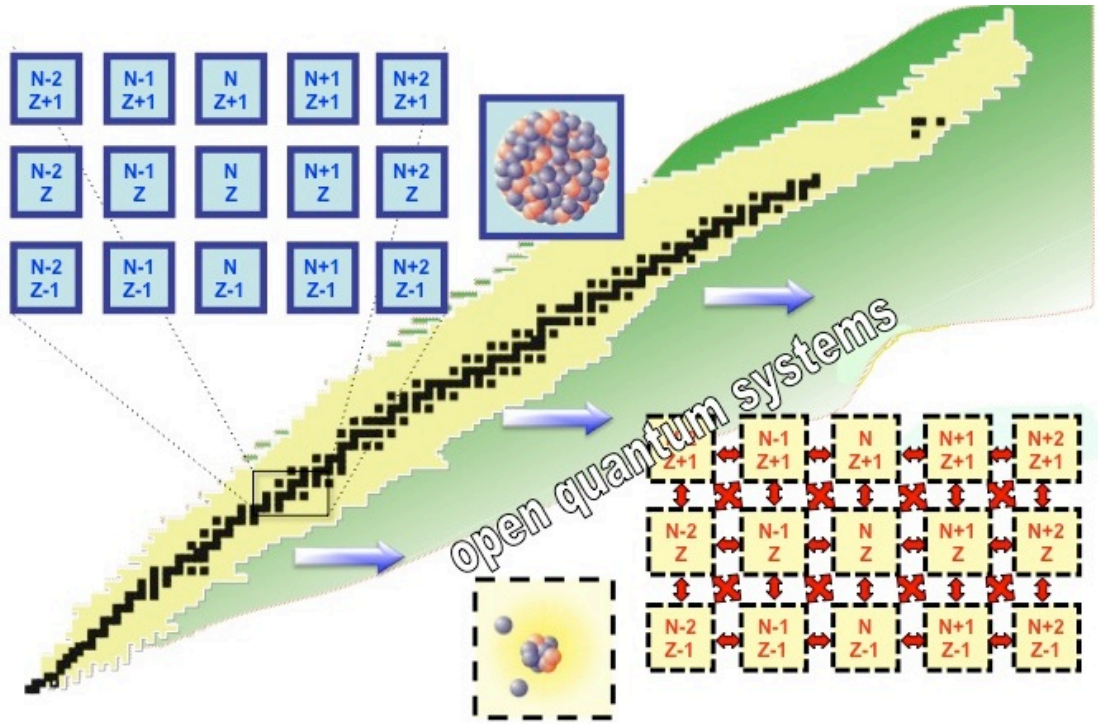


The covariance ellipsoid for the neutron skin R_{skin} in ^{208}Pb and the radius of a 1.4$M_\odot$ neutron star. The mean values are: R(1.4$M_\odot$)=12 km and R_{skin}= 0.17 fm.

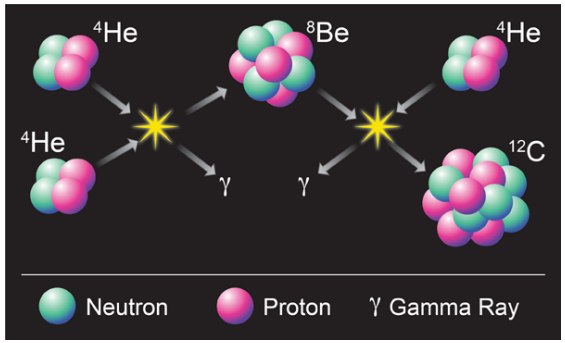


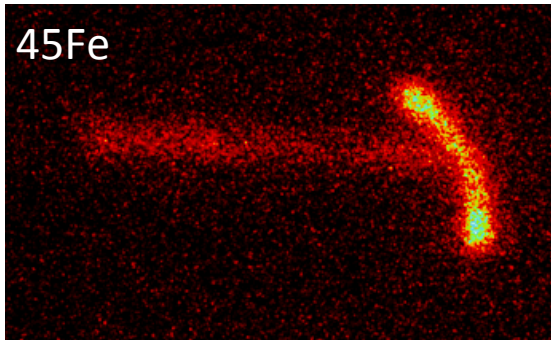
Major uncertainty: density dependence of the symmetry energy. Depends on *T=3/2* three-nucleon forces

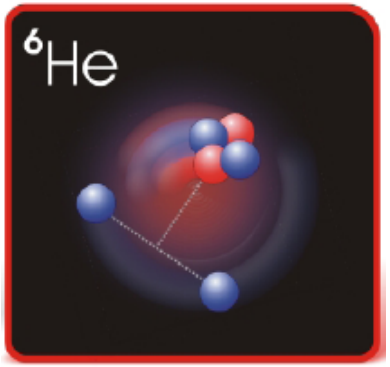
Atomic Nuclei: Many-Body Open Quantum Systems



- Facts: (i) nuclear structure is impacted by couplings to reaction and decay channels; (ii) reaction dynamics is impacted by nuclear structure
- Challenge: clustering, alpha decay, and fission still remain major challenges for theory
- Answer: unified picture of structure and reactions

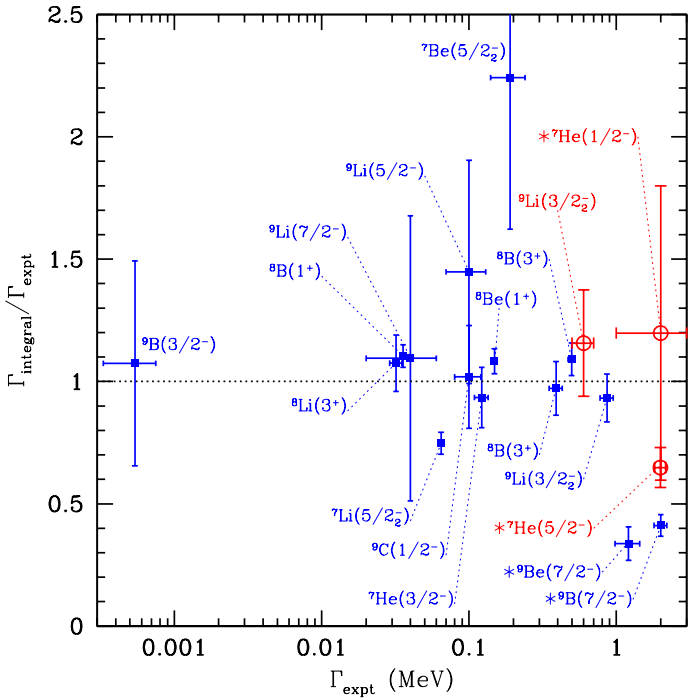




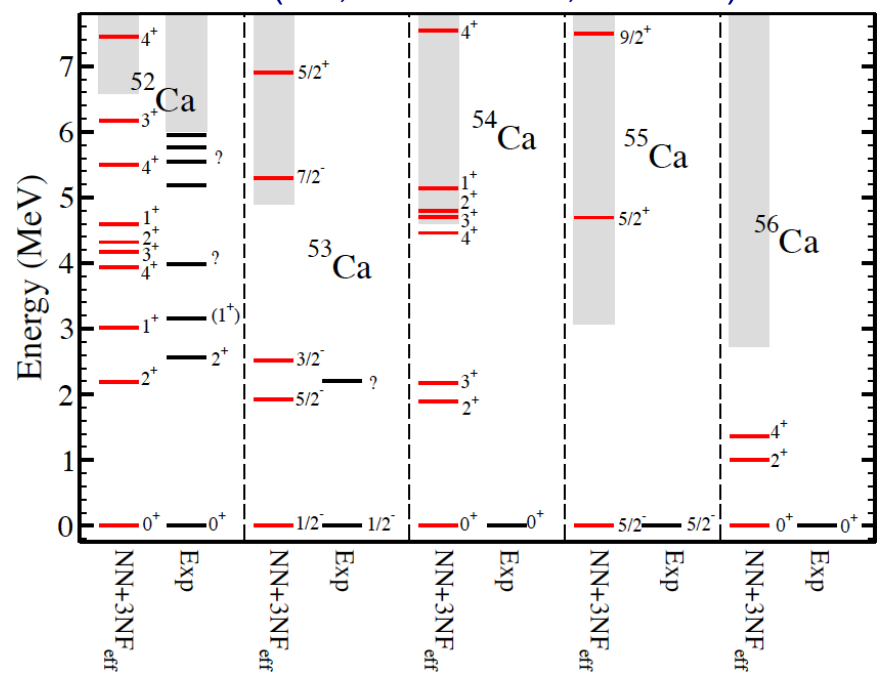


Impact of open channels on structural properties

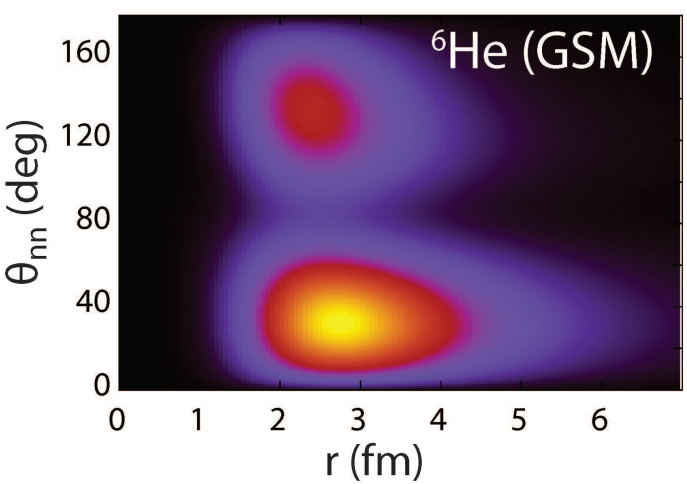
Ab initio calculations of ANCs and widths



Ab initio calculations of nuclear spectra (CC, NCSM/RGM, NCGSM)



Di-neutron correlations in CS/GSM



A suite of powerful approaches developed to open nuclear systems:

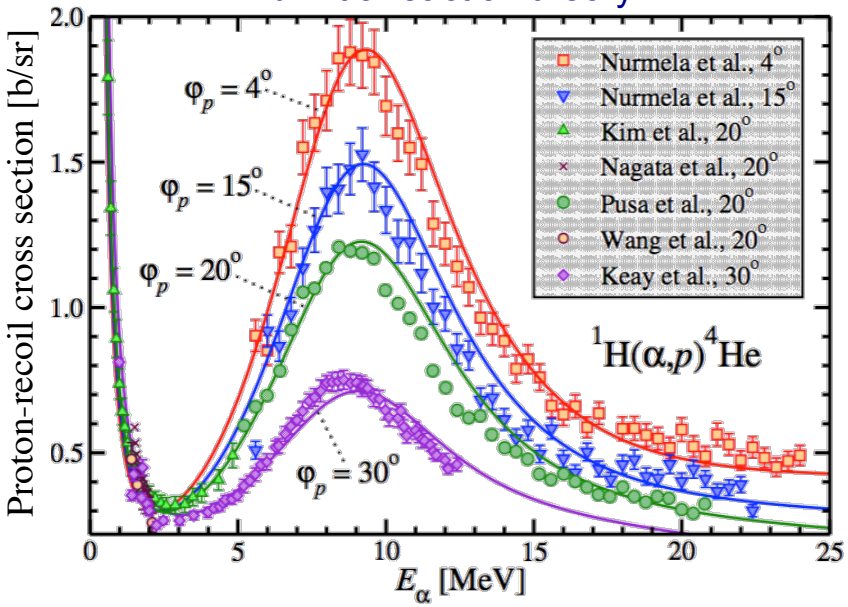
- Real-energy continuum shell model
- Complex-energy continuum shell model
- Ab-initio extensions

Profound interdisciplinary connections:

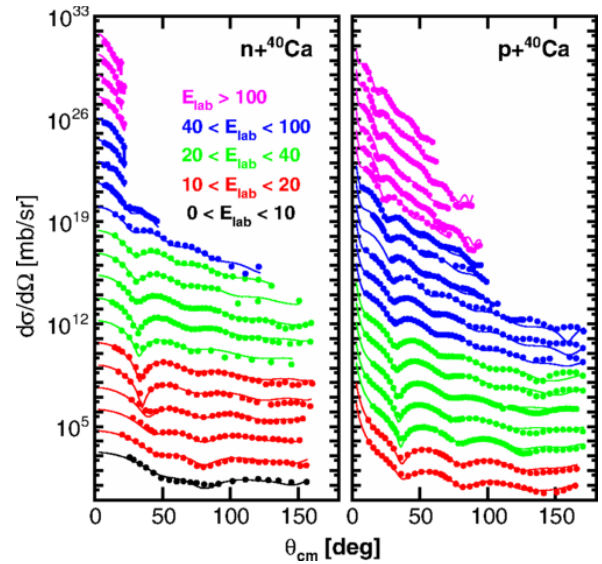
- resonance trapping and super-radiance
- threshold anomalies and channel coupling effects
- spectral fluctuations and statistics of resonances
- clusterization
- spatially extended halos and Efimov states

Microscopic reaction theory

Ab initio reaction theory



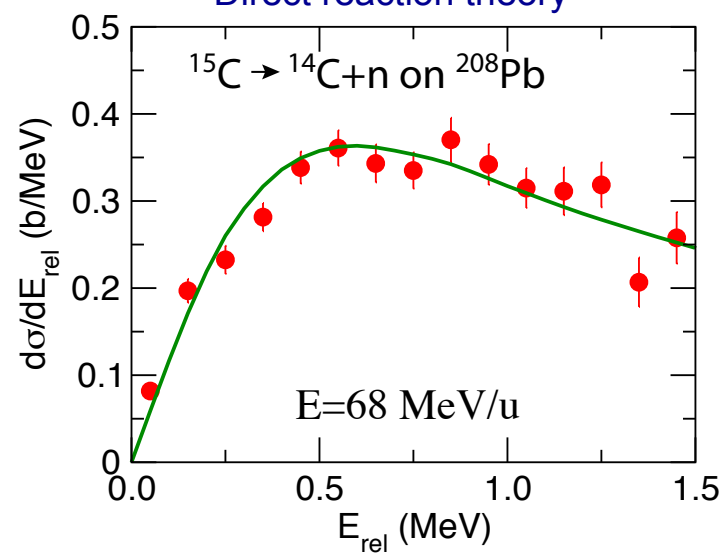
Quality input: nonlocal dispersive optical potential



Near-term prospects:

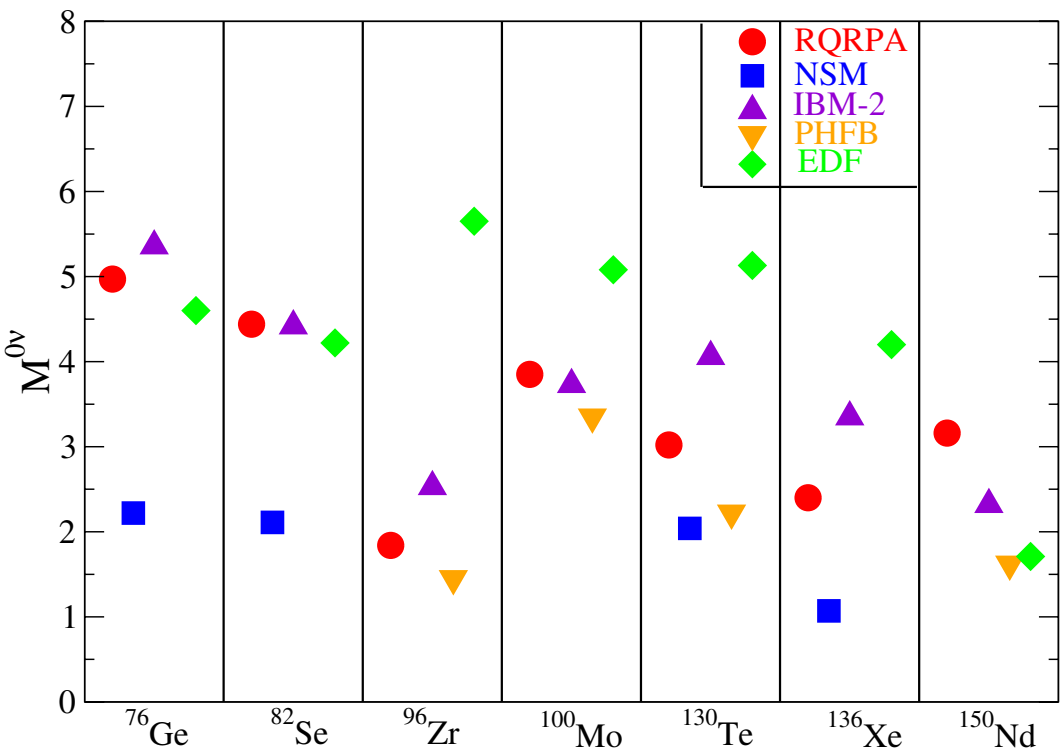
- High-fidelity simulations with NN+NNN for composite projectiles and exotic nuclei
- Nuclear reactions with *microscopic* optical potentials
- Description of direct, semi-direct, pre-equilibrium, and compound processes

Direct reaction theory



Fundamental symmetry tests and neutrino physics

- Superallowed Fermi $0^+ \rightarrow 0^+$ β-decays
- Neutrinoless double-beta decays
- Schiff moment for EDM
- Neutrino-nucleus scattering

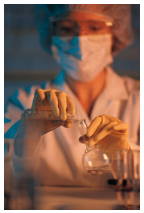


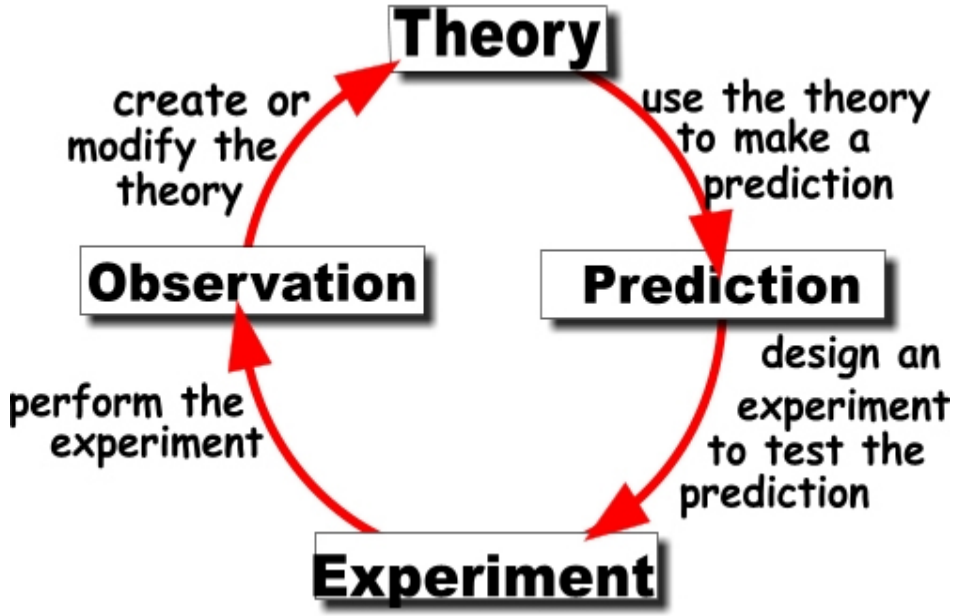
Current $0\nu\beta\beta$ predictions

"There is generally significant variation among different calculations of the nuclear matrix elements for a given isotope. For consideration of future experiments and their projected sensitivity it would be very desirable to reduce the uncertainty in these nuclear matrix elements."
(Neutrinoless Double Beta Decay NSAC Report 2014)

Prospects

Scientific method: our paradigm



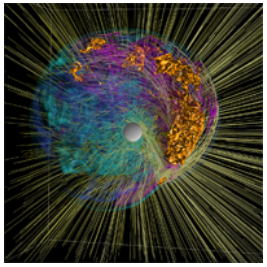


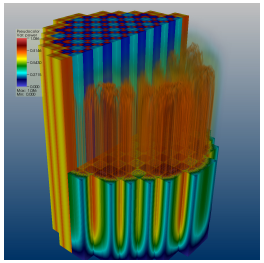
The theory-experiment cycle is repeated, continually testing and modifying the theory, until the theory describes experimental observations. *Then the theory is considered a scientific law.*

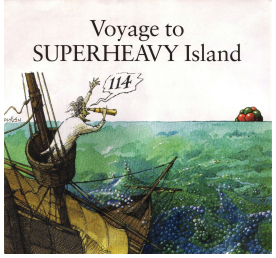
Yin and yang can be thought of as complementary (rather than opposing) forces that interact to form a dynamic system in which the whole is greater than the assembled parts.

Experimental context: some thoughts…

- **Beam time and cycles are difficult to get and expensive.** Experiment keeps theory honest. Theory could help by being more involved in assessing the impact of planned runs and projects.
  - What is the information content of measured observables?
  - Are estimated errors of measured observables meaningful?
  - What experimental data are crucial for better constraining current nuclear models?
- New technologies are essential for providing predictive capability, to estimate uncertainties, and to assess extrapolations
  - Theoretical models are often applied to entirely new nuclear systems and conditions that are not accessible to experiment

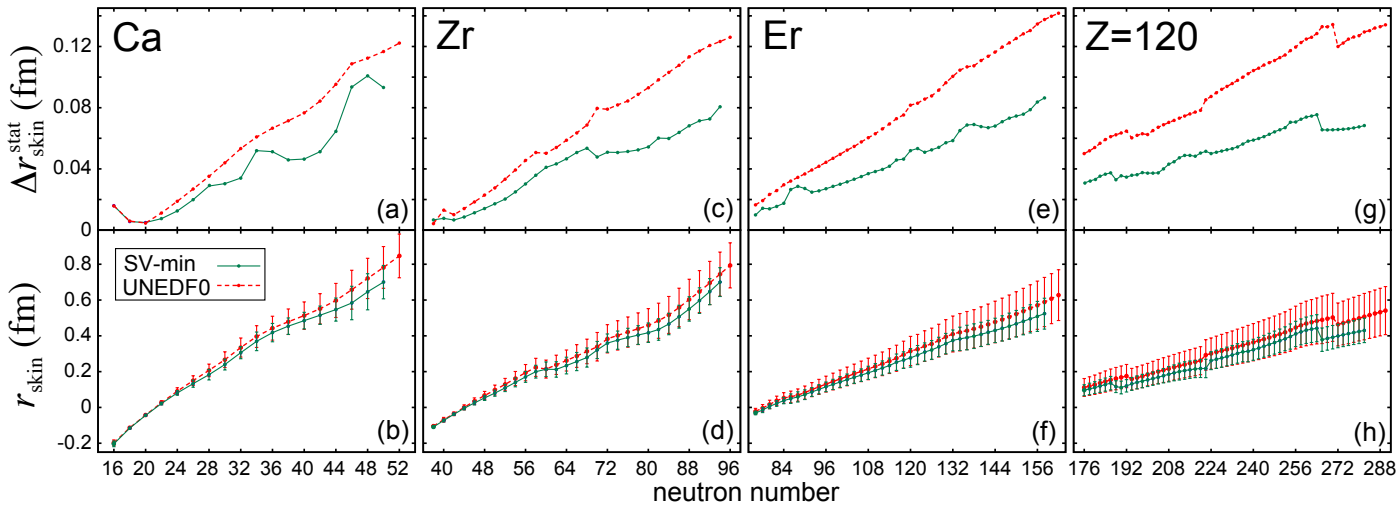


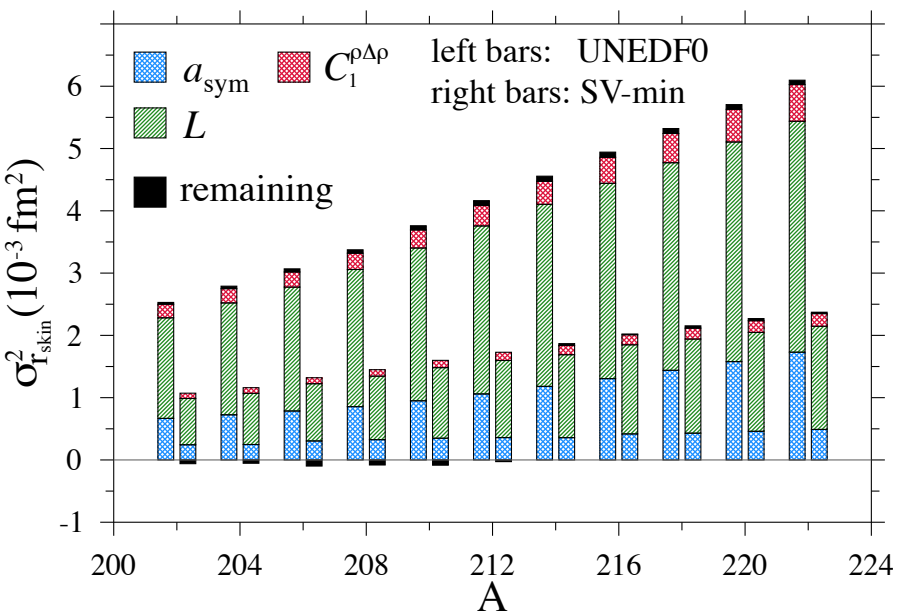




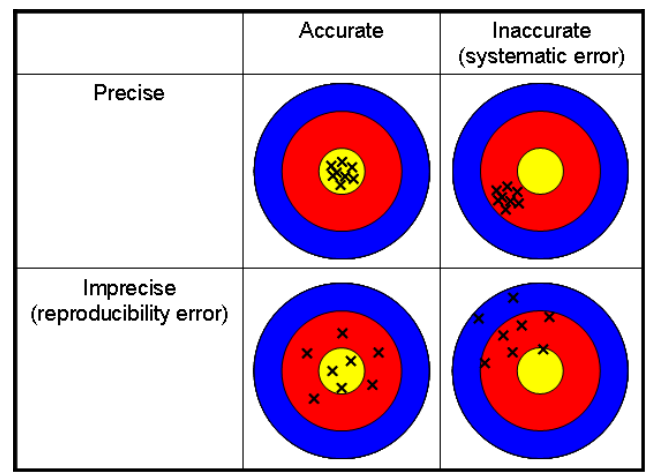
A paradigm shift is needed to enhance the coupling between theory and experiment

Quality control through Uncertainty Quantification



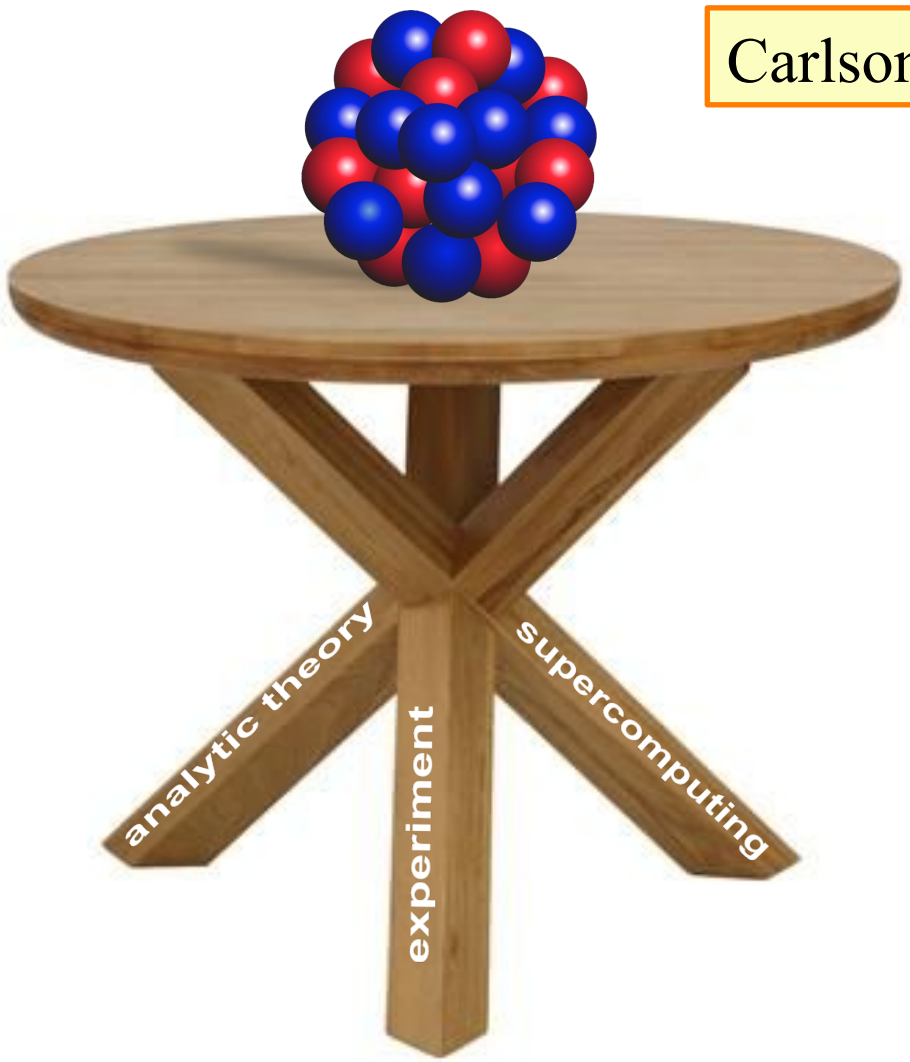


but…



…EFT framework is designed for model independence and systematic improvement of approximations. This has a potential of enriching the experiment-theory feedback

High Performance Computing and Nuclear Theory



Carlson

"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*." (NAC Decadal Study Report)

Future: large multi-institutional efforts involving strong coupling between physics, computer science, and applied math

Theory needs FRIB; FRIB needs Theory

⇒ New Initiative: FRIB Theory Center

It will enhance the national low-energy nuclear physics effort by:

- Delivering excellent research in theory relevant to the big science questions;
- Serving as a focal point for stimulating continuous interactions between theory and experiment;
- Rejuvenating the field by creating (bridge/joint) permanent positions in FRIB theory *across the country*;
- Attracting young talent through the *national* FRIB theory fellow program;
- Strengthening theory in areas of most need;
- Fostering interdisciplinary collaborations and build scientific bridges to wider theory communities;
- Coordinating a sustainable educational program in advanced; low-energy nuclear theory (TALENT!!!);
- Coordinating international initiatives in theory of rare isotopes. Building on success of J/F/C-USTIPEN.

Summary (1): Challenges for LE Nuclear Theory

- Describe the lightest nuclei in terms of lattice QCD
- Develop first-principles framework for light, medium-mass nuclei, and nuclear matter from 0.1 to twice the saturation density
- Develop predictive and quantified nuclear energy density functional rooted in first-principles theory
- Unify the fields of nuclear structure and reactions: we must free ourselves from limitations imposed by (physical) boundary conditions
- Achieve a comprehensive description of direct, semi-direct, pre-equilibrium, and compound processes for a variety of reactions
- Provide the microscopic underpinning of observed, and new, (partial-) dynamical symmetries and simple patterns
- Develop predictive microscopic model of fusion and fission that will provide the missing data for astrophysics, nuclear security, and energy research
- Carry out predictive and quantified calculations of nuclear matrix elements for fundamental symmetry tests in nuclei and for neutrino physics. Explore the role of correlations and currents.

  - Develop and utilize tools of uncertainty quantification
  - Enhance the coupling between theory and experiment
  - Take the full advantage of high performance computing

Summary (2): The LRP 2014 Request

Our field

- Establish the FRIB Theory Center. Theory centers were crucial for RHIC and Jlab communities
- Support TALENT educational initiative

Nuclear Theory in general

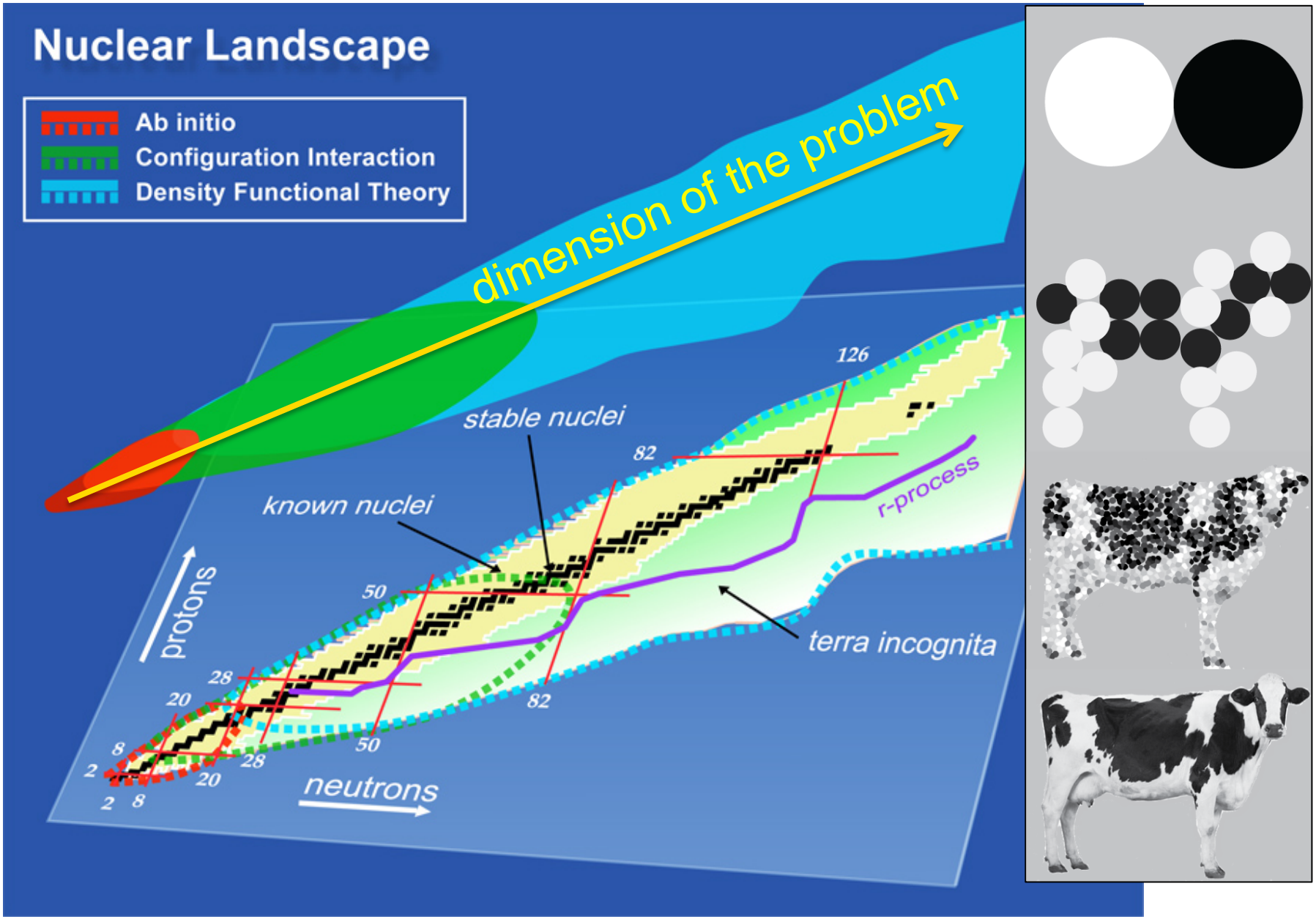
- Enhanced support for nuclear theory to realize the full scientific promise enabled by experimental investments
- Computational initiative: new investments in people, advanced software, and complementary capacity computing directed toward nuclear theory
- Continuation of Topical Collaborations: a very effective way to target specific science questions
- Adequate support for INT: a resource belonging to the entire nuclear theory community

Summary (3, final)

- The nuclear many-body problem is very complex, computationally difficult, and interdisciplinary.
- With a fundamental picture of nuclei based on the correct microphysics, we can remove the empiricism inherent today, thereby giving us greater confidence in the science we deliver and predictions we make
- For reliable model-based extrapolations, we need to improve predictive capability by developing methods to quantify uncertainties
- We need a paradigm shift to optimize a theory-experiment loop
- New-generation computers will continue to provide unprecedented opportunities for nuclear theory
- New theory initiatives for the LRP 2014

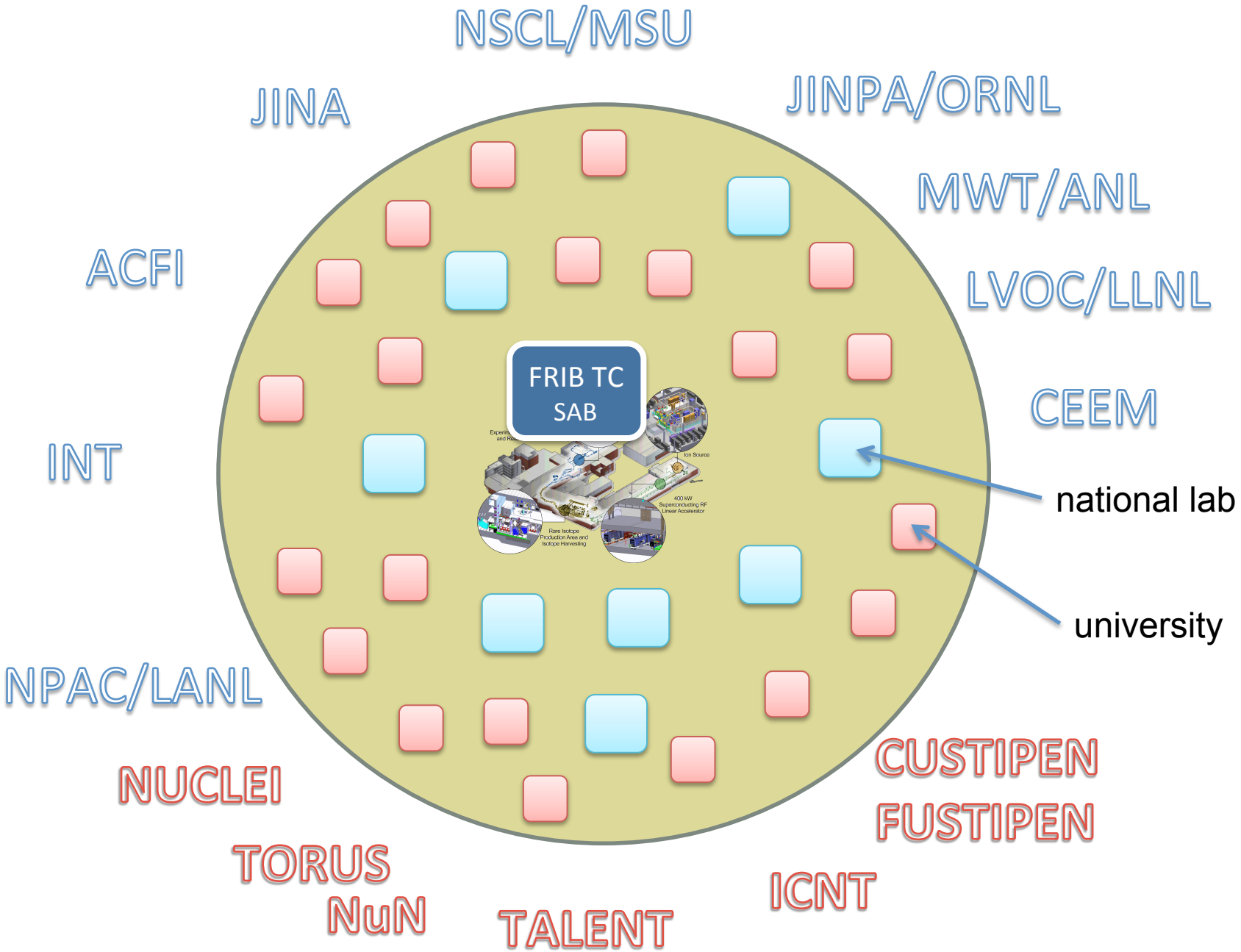
BACKUP

How to explain the nuclear landscape from the bottom up? **Theory roadmap**



- A first rate theory predicts
- A second rate theory forbids
- A third rate theory explains after the facts

Alexander I. Kitaigorodskii


NSCL/MSU
JINA
JINPA/ORNL
MWT/ANL
ACFI
LVOC/LLNL
FRIB TC
SAB
CEEM
INT
national lab
university
NPAC/LANL
NUCLEI
CUSTIPEN
FUSTIPEN
TORUS
NuN
TALENT
ICNT

INSTITUTE for NUCLEAR THEORY

A resource belonging to the entire nuclear theory community

- NP community-originated scientific programs with~400 participants per year on a tremendous diversity of topics
- INT provides a pipeline for our students and post-docs into tenure track University and permanent lab positions…over 40 to date
- INT promotes nuclear theory education, administering the National Nuclear Physics Summer School, offering TALENT courses & topical summer schools for advanced students