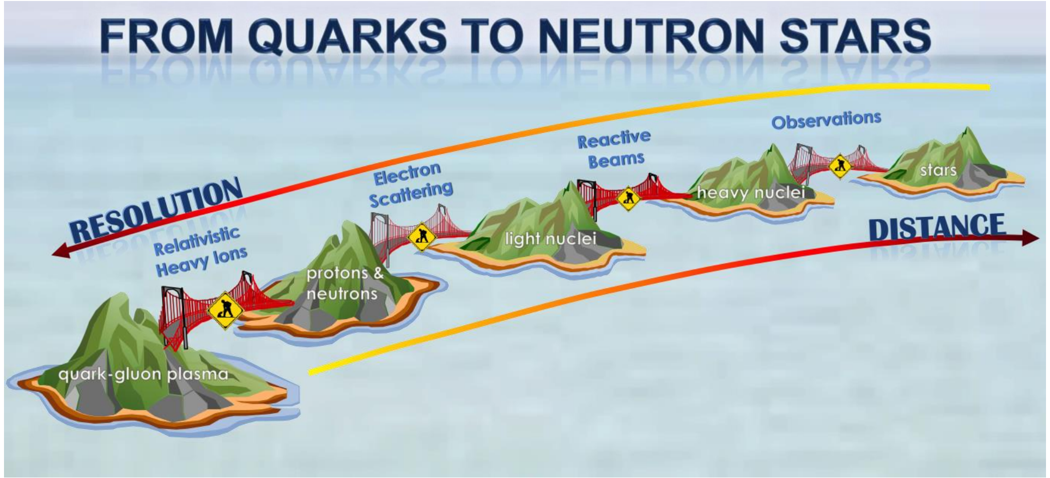
Nuclear Structure Theory: today and tomorrow

Witek Nazarewicz (MSU/ORNL)

ISOLDE Workshop 2014: 50th Anniversary Edition

ISOLDE, CERN, Dec. 15-17, 2014

- Introduction
- General principles
- Today: quantitative theory; predictive capability
- Challenges for tomorrow
- Summary



The Nuclear Landscape and the Big Questions (NAS report)

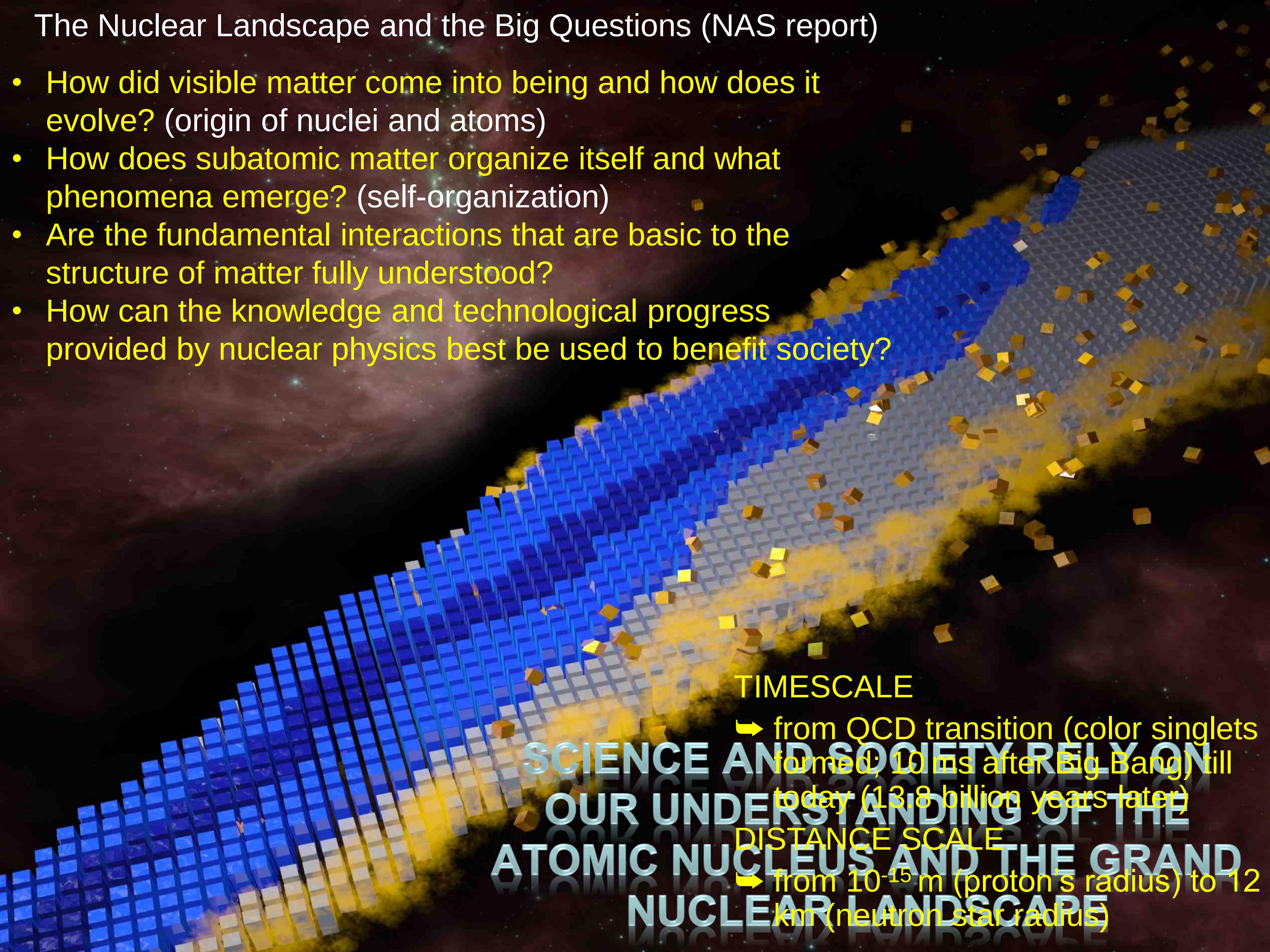
- How did visible matter come into being and how does it evolve? (origin of nuclei and atoms)
- How does subatomic matter organize itself and what phenomena emerge? (self-organization)
- Are the fundamental interactions that are basic to the structure of matter fully understood?
- How can the knowledge 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)



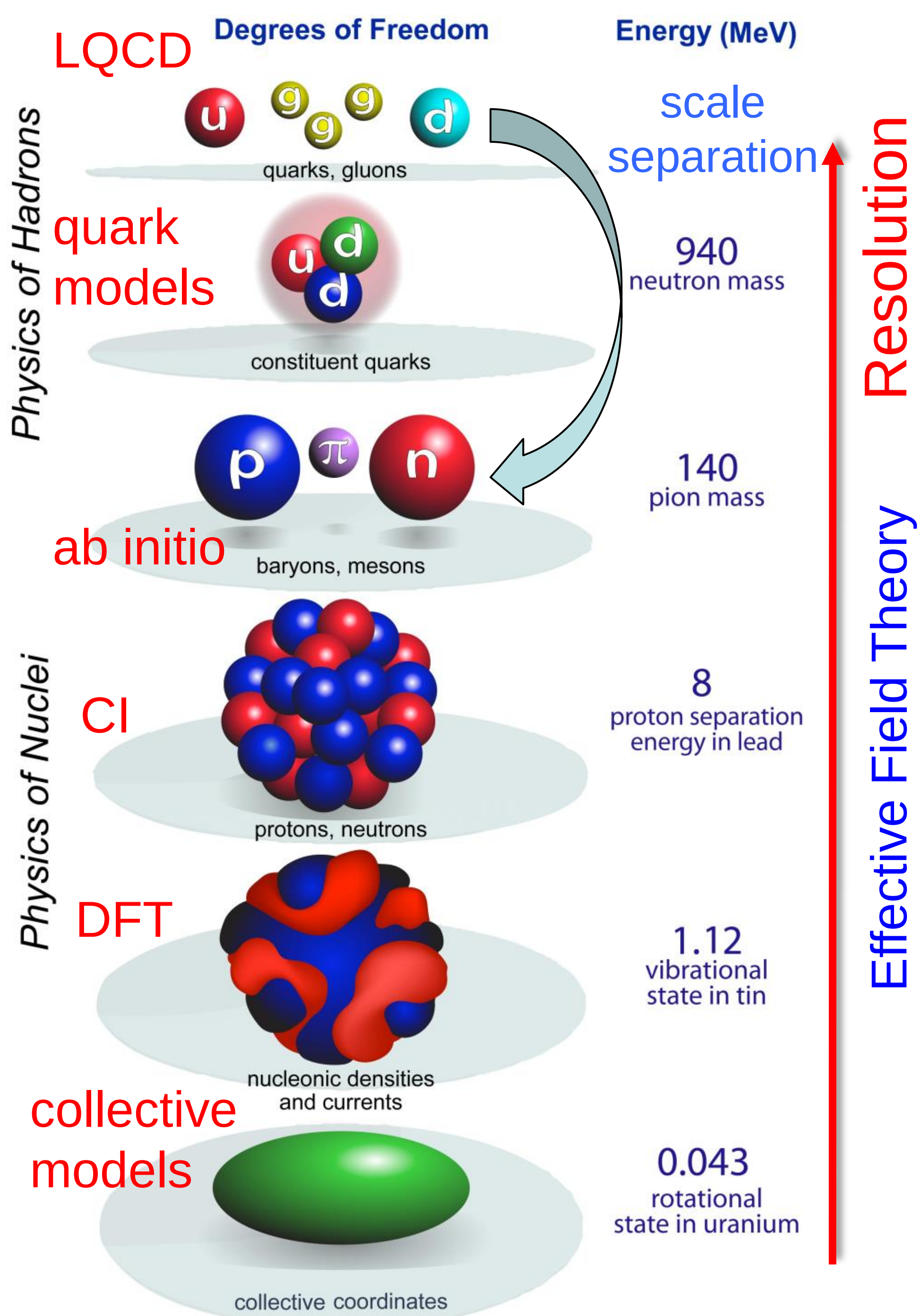
- A first rate theory predicts
- A second rate theory forbids
- A third rate theory explains after the facts

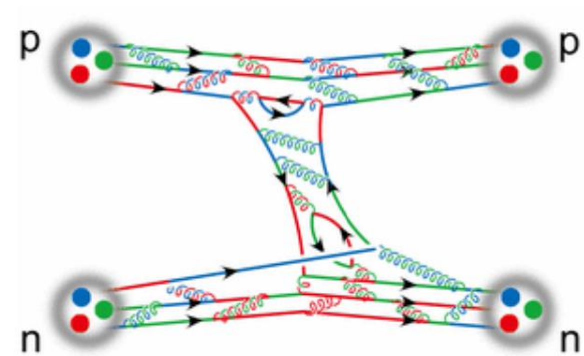
Alexander I. Kitaigorodskii

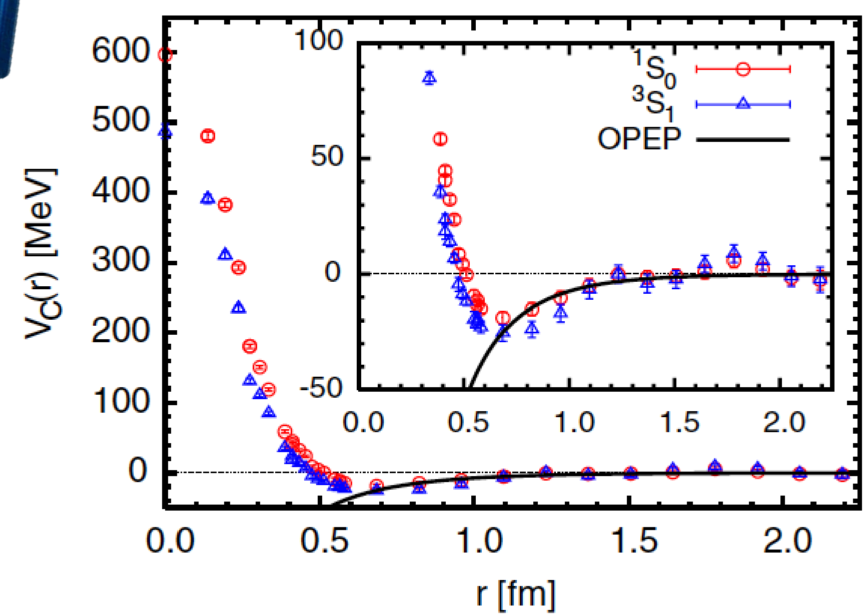
Characteristics of good theory:

- Predictive power
- Robust extrapolations
- Validation of data
- Short- and long-term guidance

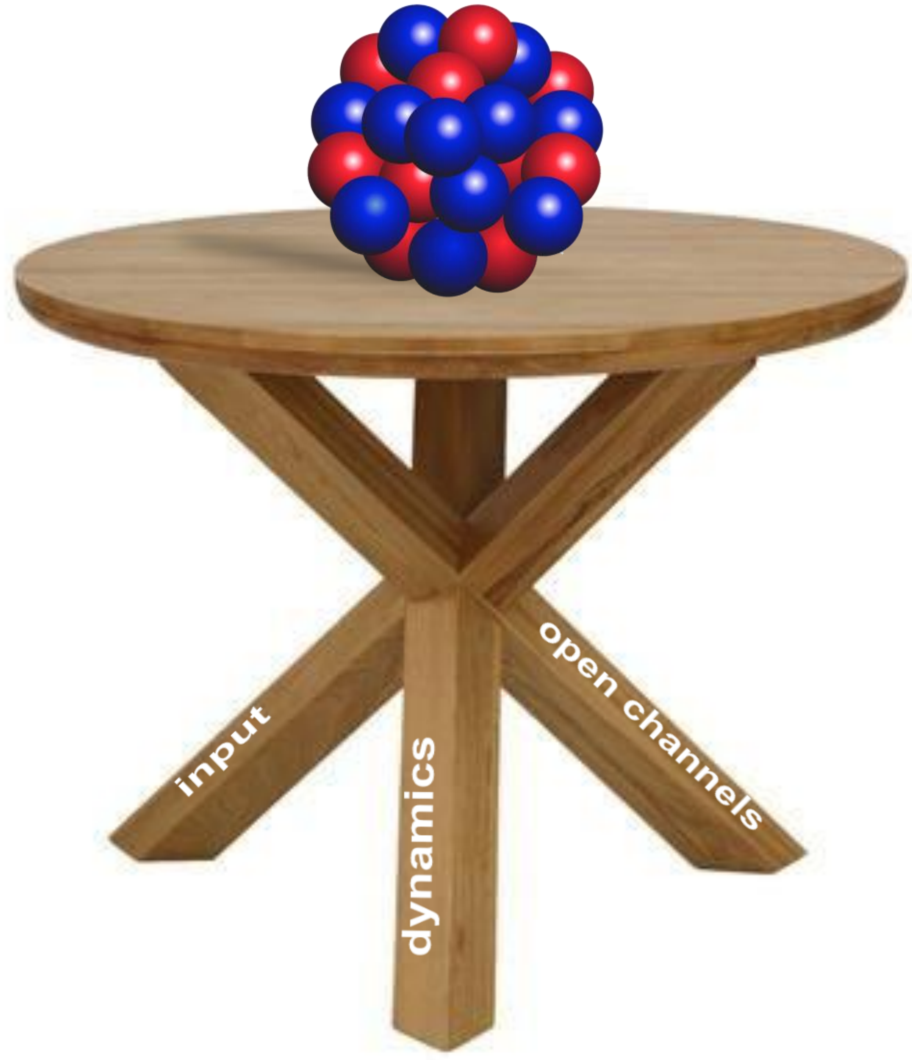
The challenge and the prospect: physics of nuclei directly from QCD







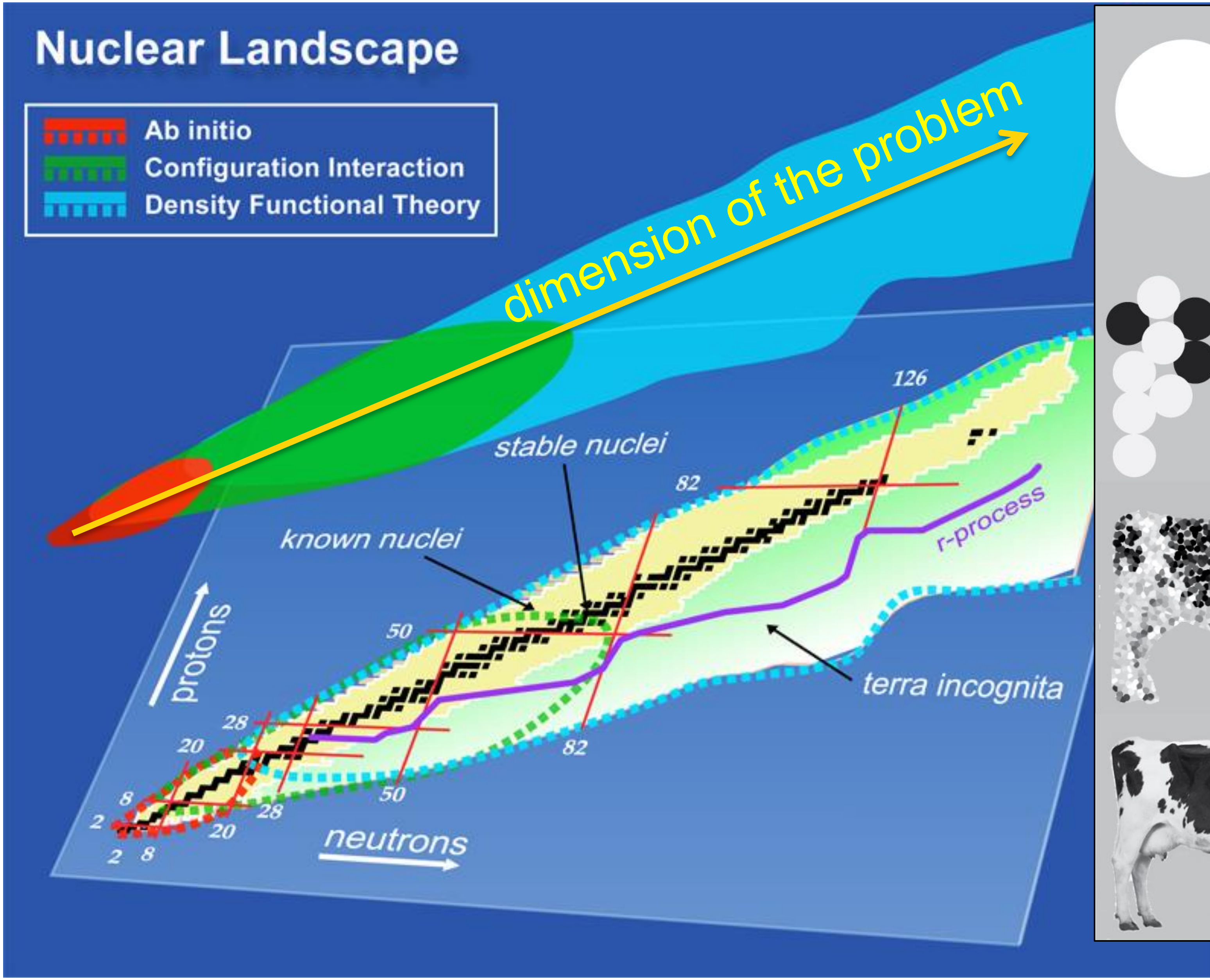
Theory of rare isotopes is demanding

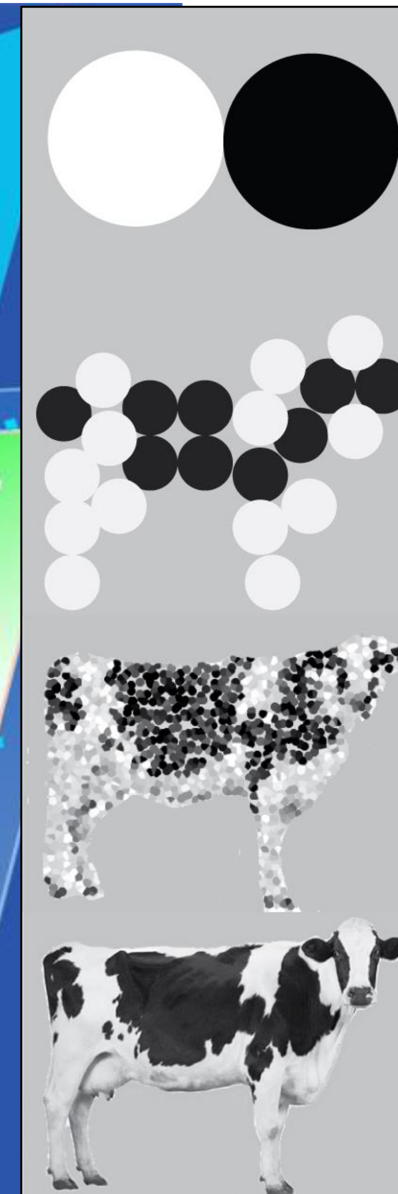


Great recent progress

- 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

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



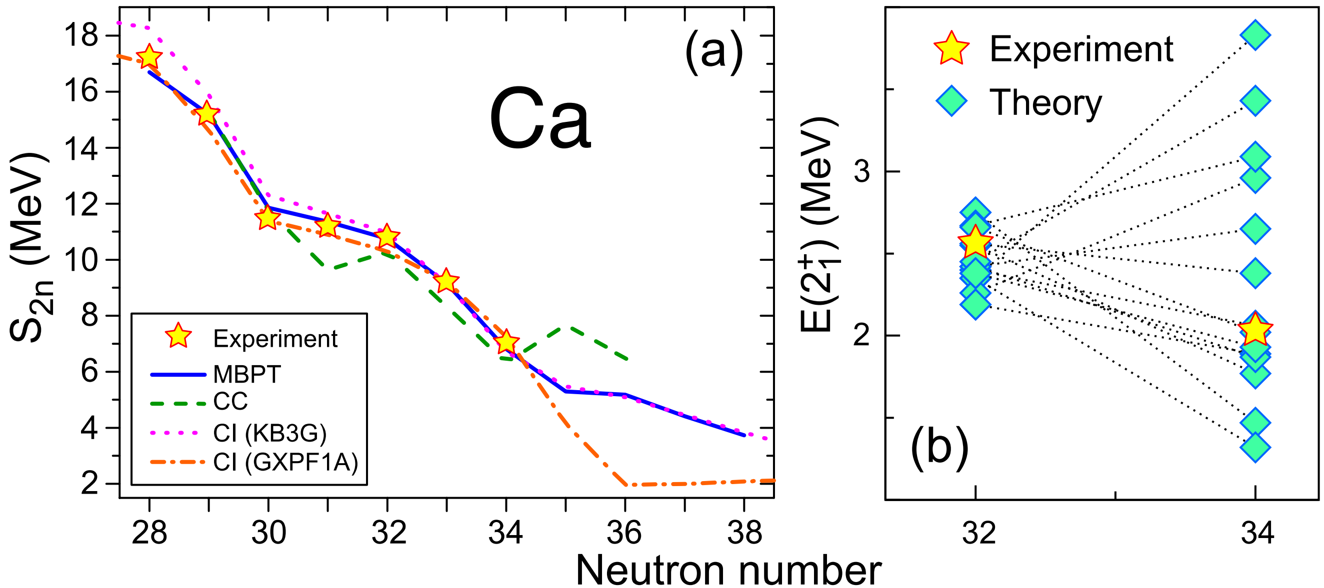


Illustrative physics examples

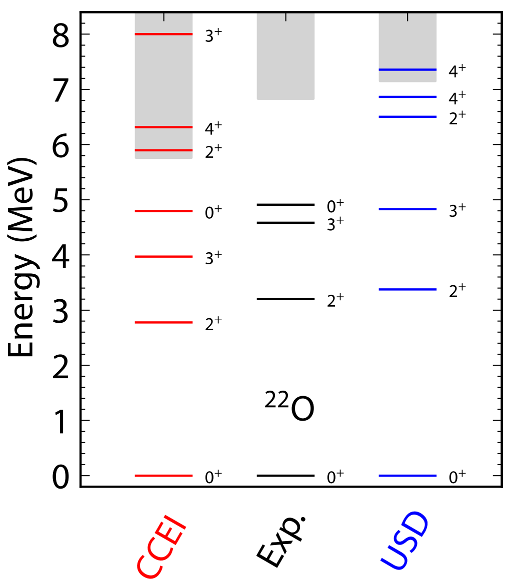
The frontier: medium-mass nuclei

ISOLTRAP@CERN
Wienholtz et al,
Nature (2013)

RIBF@RIKEN
Steppenbeck et al
Nature (2013)

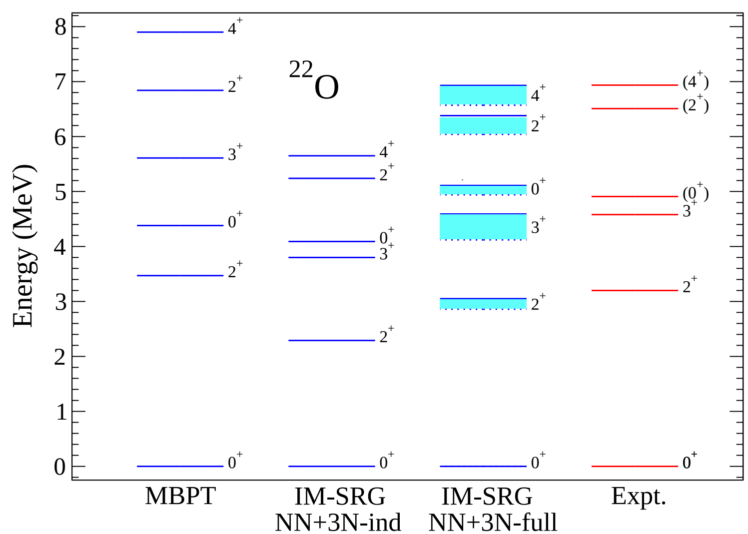


Microscopic valence-space Shell Model



Coupled Cluster
Effective
Interaction
(valence cluster
expansion)

Jansen et al.
Phys. Rev. Lett.
113, 142502
(2014)



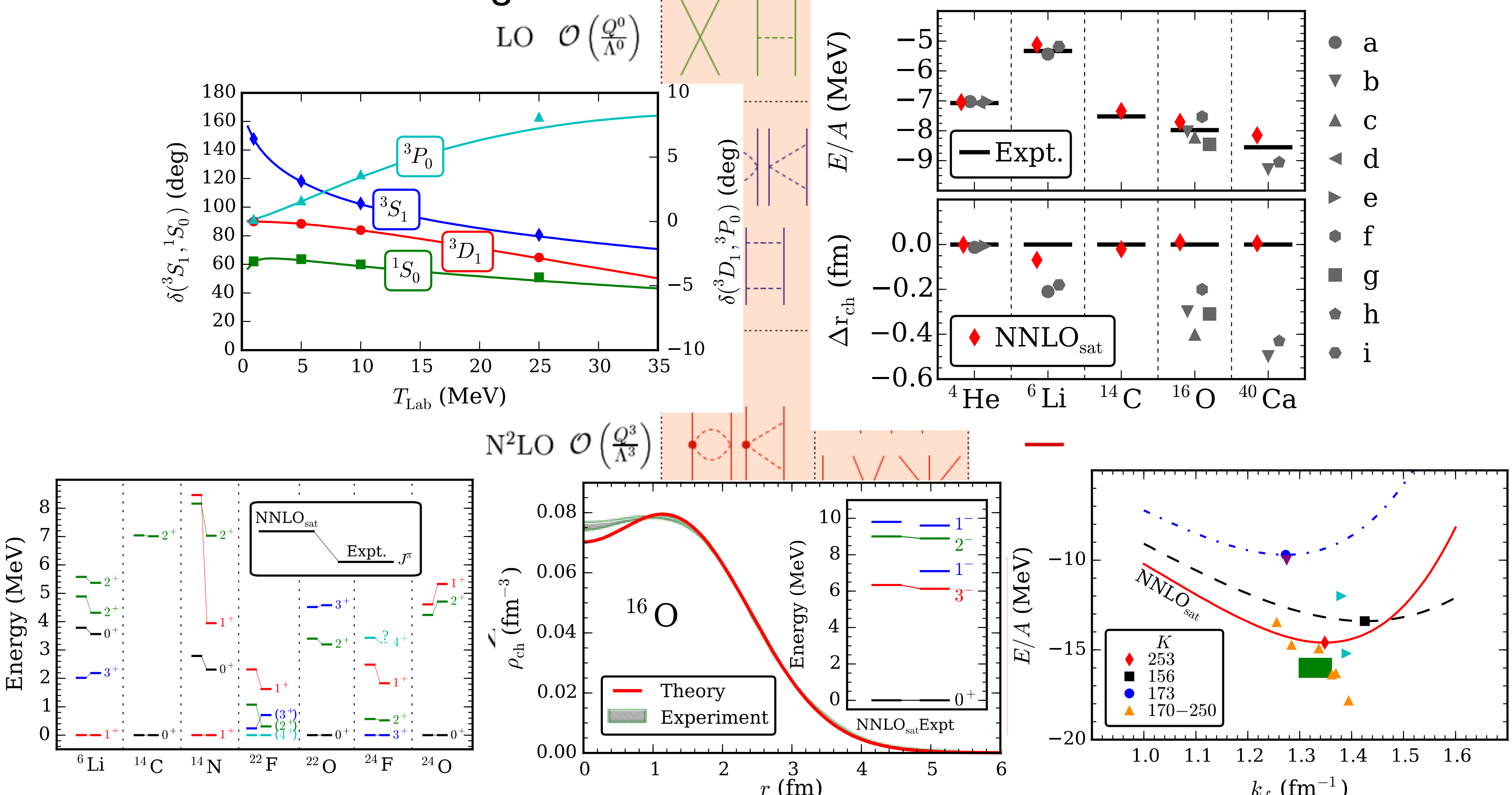
In-medium
SRG
Effective
Interaction

Bogner et al.
Phys. Rev. Lett.
113, 142501
(2014)

Accurate nuclear interaction from chiral effective field theory for nuclei and nuclear matter

A. Ekström et al, 2014

- order-by-order optimization (here: NN and NNN in N2LO)
- few-body systems and light nuclei (2,3,4, ∞ is not a good idea!)
- Focus on low energies

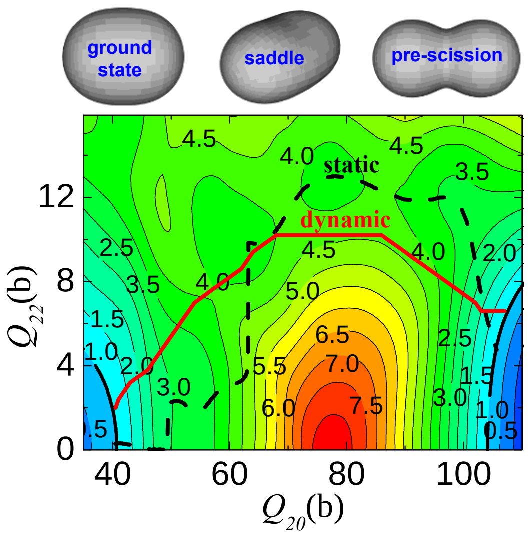


Small and Large-Amplitude Collective Motion

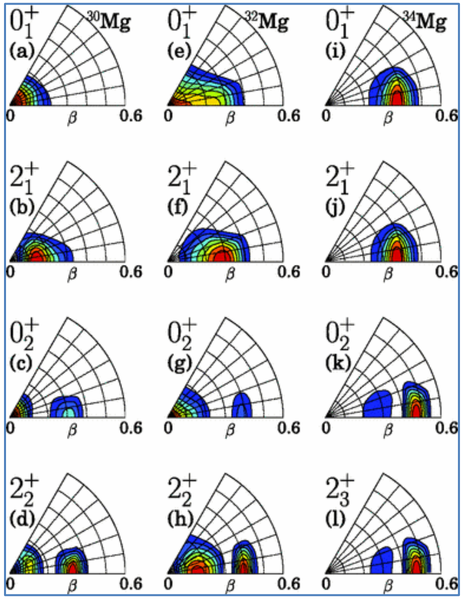
- New-generation computational frameworks developed
  - Time-dependent DFT and its extensions
  - Adiabatic approaches rooted in Collective Schrödinger Equation
  - Quasi-particle RPA
  - Projection techniques
- Applied to HI fusion, fission, coexistence phenomena, collective strength, superfluid modes

Shape coexistence

Spontaneous fission

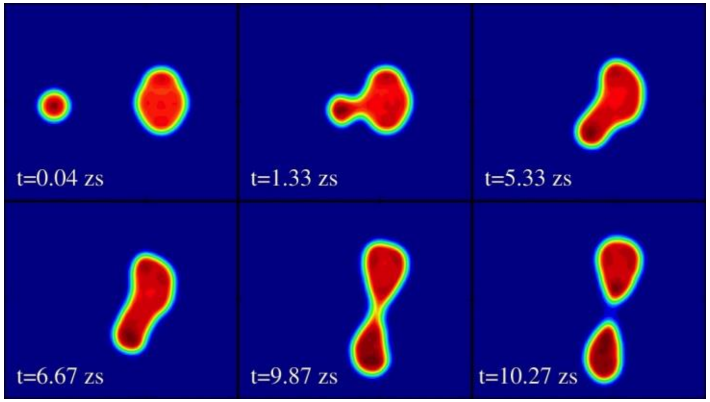


Sadhukhan et al.
Phys. Rev. C 88, 064314 (2013)



Hinohara et al.
Phys. Rev. C 84, 061302(R) (2011)

Heavy Ion fusion



Umar et al.
Phys. Rev. C 81, 064607 (2010)

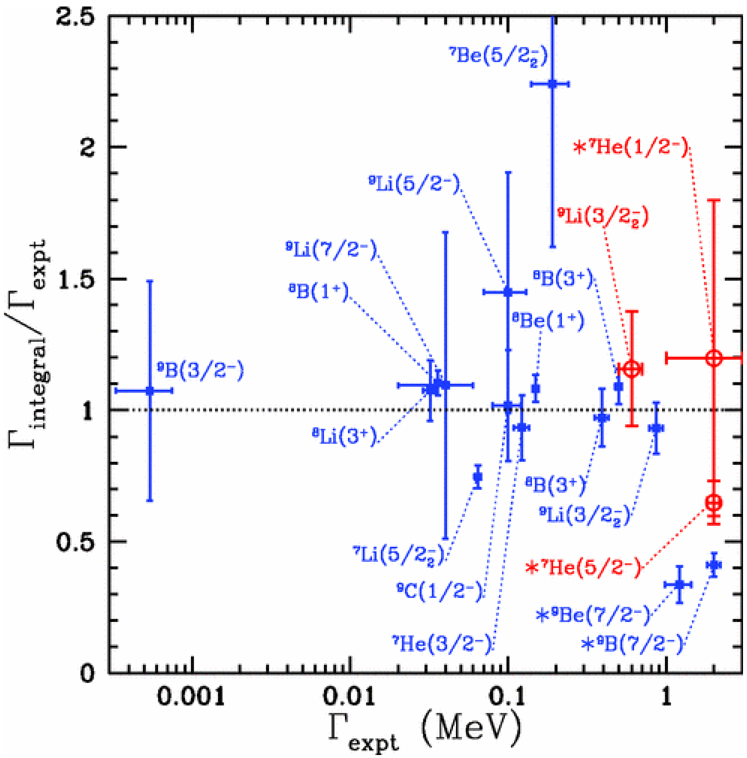
Impact of open channels on structural properties

A suite of powerful approaches developed to open nuclear systems:

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

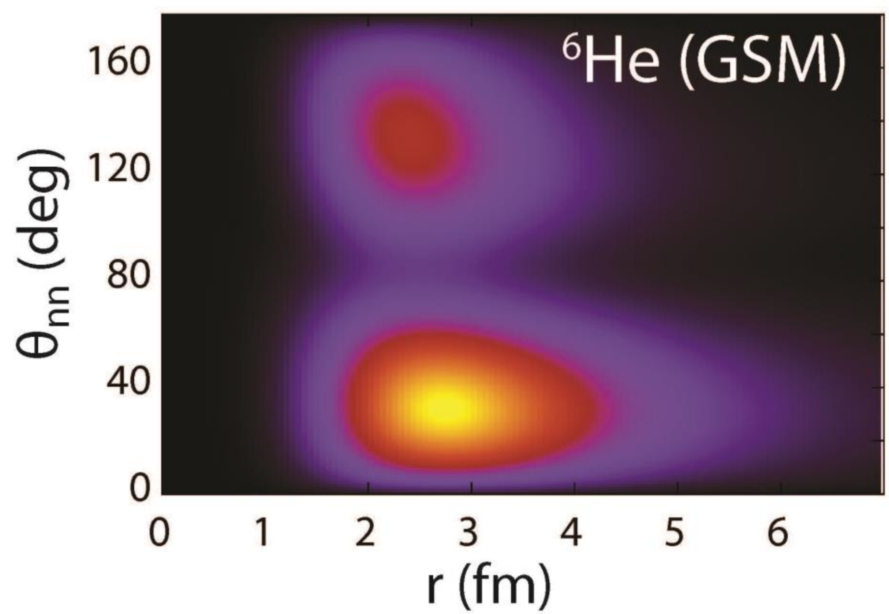
Ab initio calculations of ANCs and widths

Nollett, Phys. Rev. C 6, 044330 (2012)



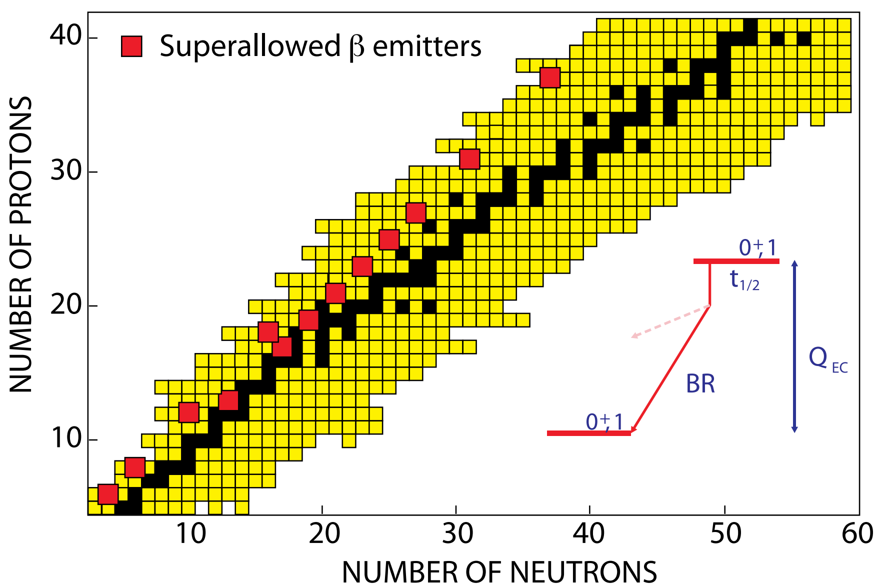
Di-neutron correlations in CS/GSM

Papadimitriou et al. Phys. Rev. C 84, 051304 (2011)

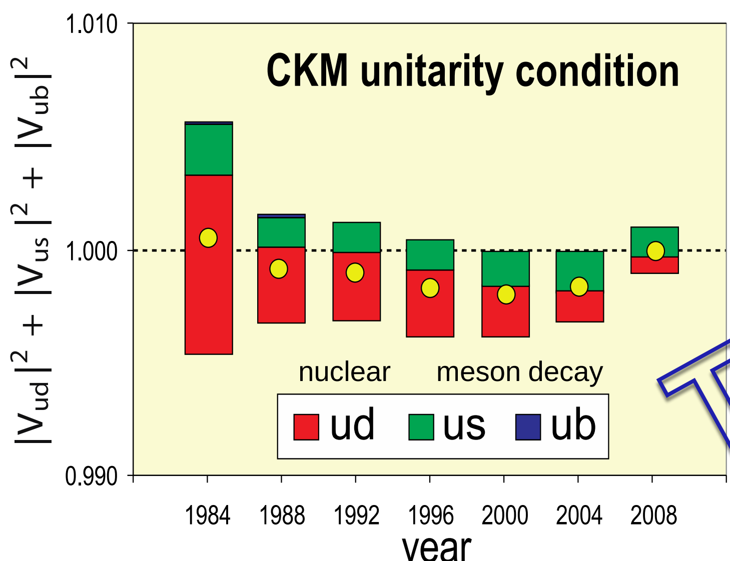


Rare Isotopes and fundamental symmetry tests

Superallowed Fermi $0^+ \rightarrow 0^+$ β-decays



ANL
ISOLDE
Jyväskylä
Munich
NSCL
TAMU
TRIUMF…
Warsaw, Tennessee..

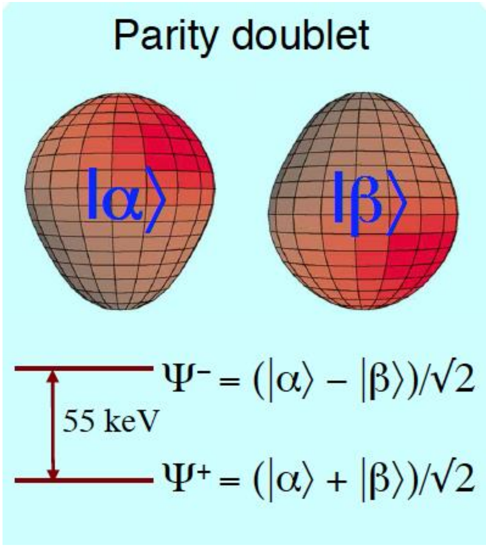


$$|V_{\mathrm{ud}}|^2 + |V_{\mathrm{us}}|^2 + |V_{\mathrm{ub}}|^2 = 0.99935(67)$$

Theory!

Atomic electric dipole moment

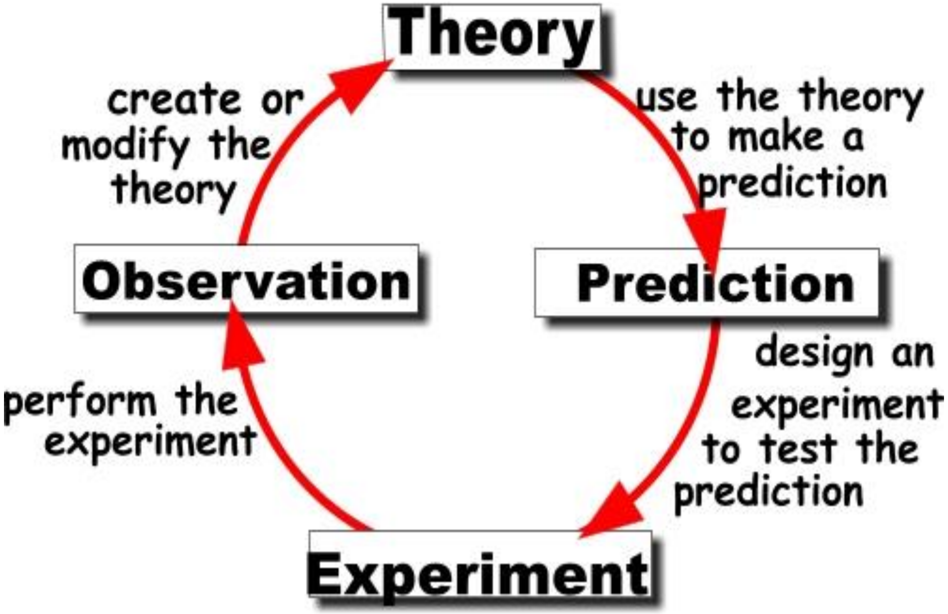
The violation of CP-symmetry is responsible for the fact that the Universe is dominated by matter over anti-matter



- Closely spaced parity doublet gives rise to enhanced electric dipole moment
- Large intrinsic Schiff moment
- ^{199}Hg (Seattle, 1980's – present)
- ^{225}Ra (Starting at ANL and KVI)
- ^{223}Rn at TRIUMF
- Potential at FRIB (10^{12}/s w ISOL target (far future); 10^{10} initially

Prospects

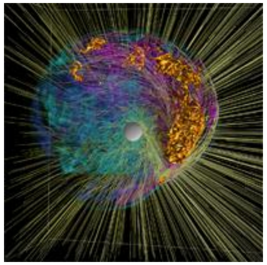
Scientific method: our paradigm

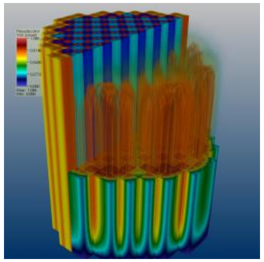


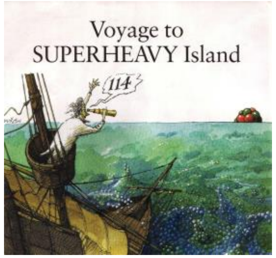
The theory-experiment cycle is repeated, continually testing and modifying the theory, until the theory describes experimental observations. *Then the theory is considered a scientific law.*

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

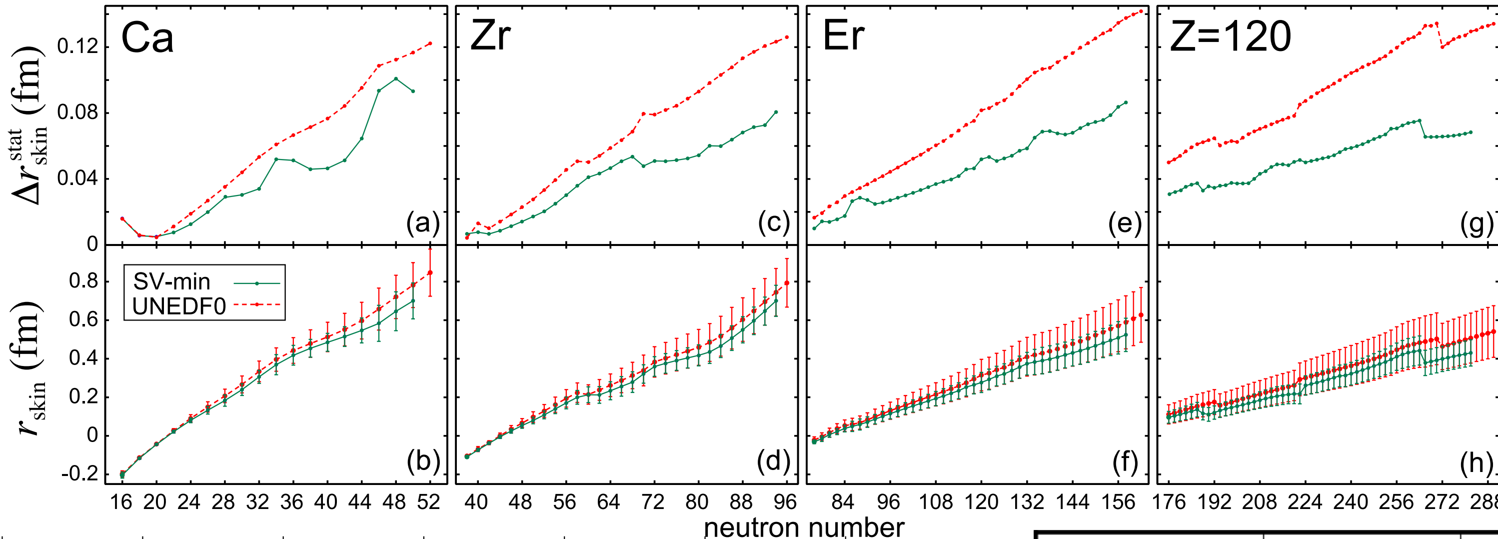
Quality control
Uncertainty quantification

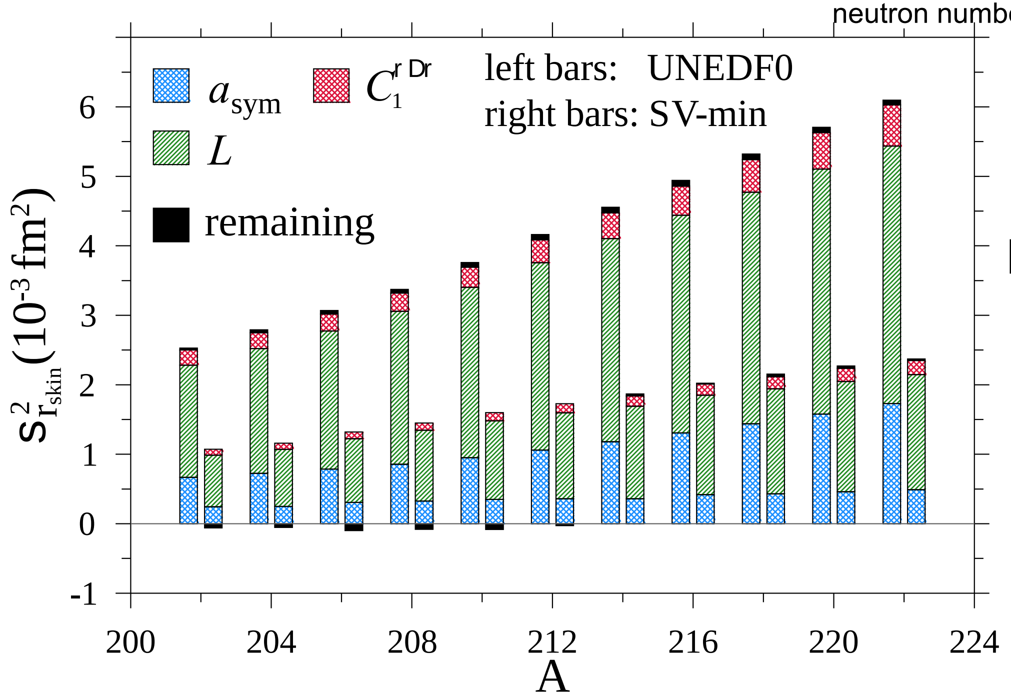
"Remember that all models are wrong; the practical question is *how wrong do they have to be to not be useful*"

(E.P. Box)

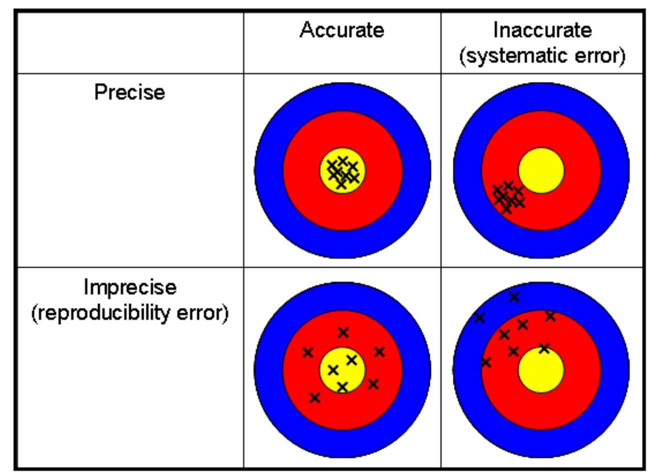
Example: Neutron-skin uncertainties of Skyrme EDF

M. Kortelainen et al., Phys. Rev. C 88, 031305 (2013)



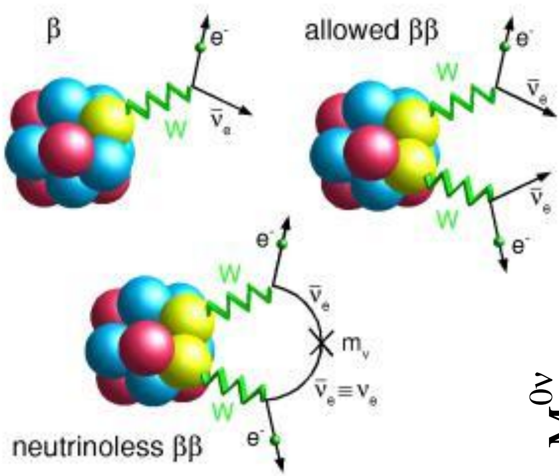


but…

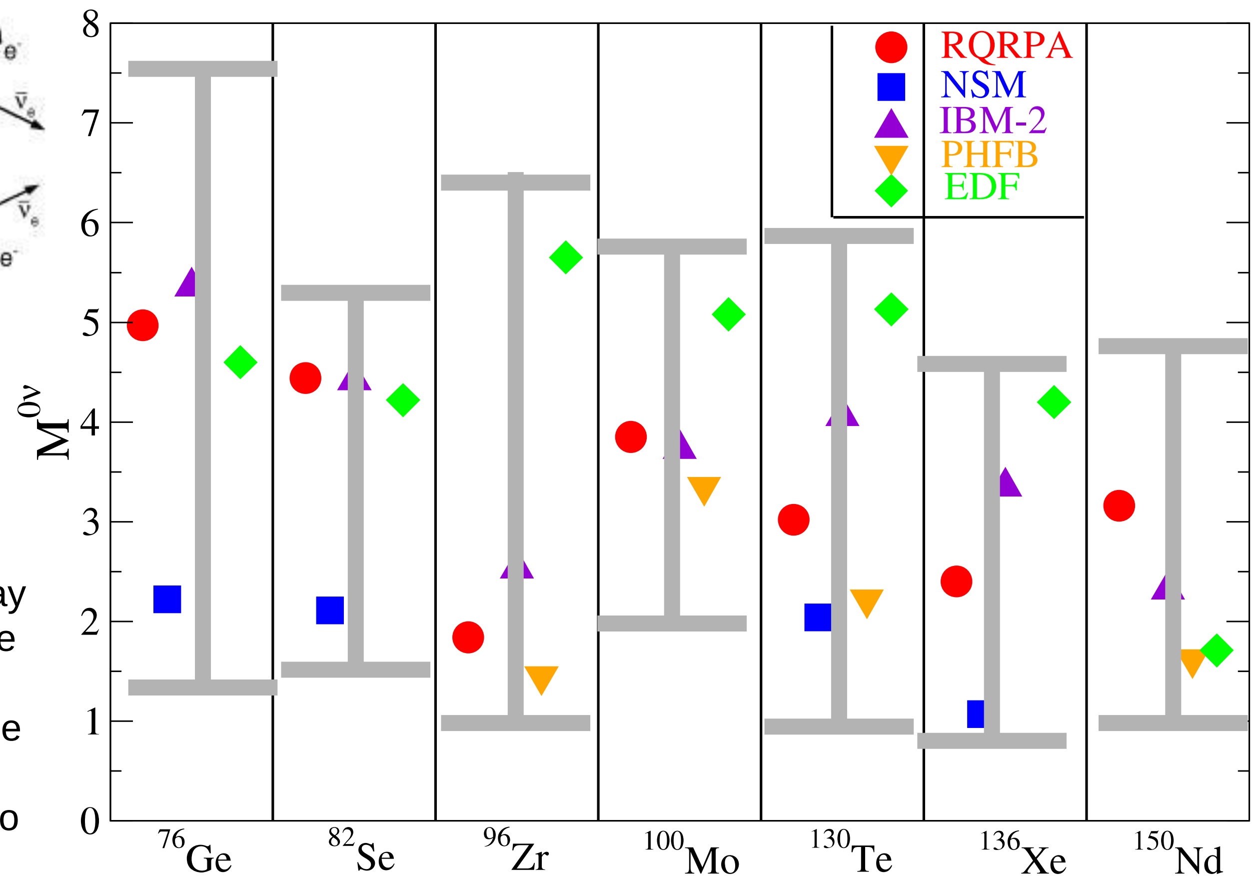


…EFT framework is designed for model independence and systematic improvement of approximations. This has a potential of enriching the experiment-theory feedback

Current 0νββ predictions



In contrast the study of neutrinoless double beta decay may shed light on the absolute mass scale. Neutrinoless double beta decay requires the neutrino to be its own anti-particle, i.e. the neutrino has to be a Majorana fermion.



"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)

Error estimates of theoretical models: a guide

J Dobaczewski, W Nazarewicz and P-G Reinhard, *J. Phys.G* **41** 074001 (2014)

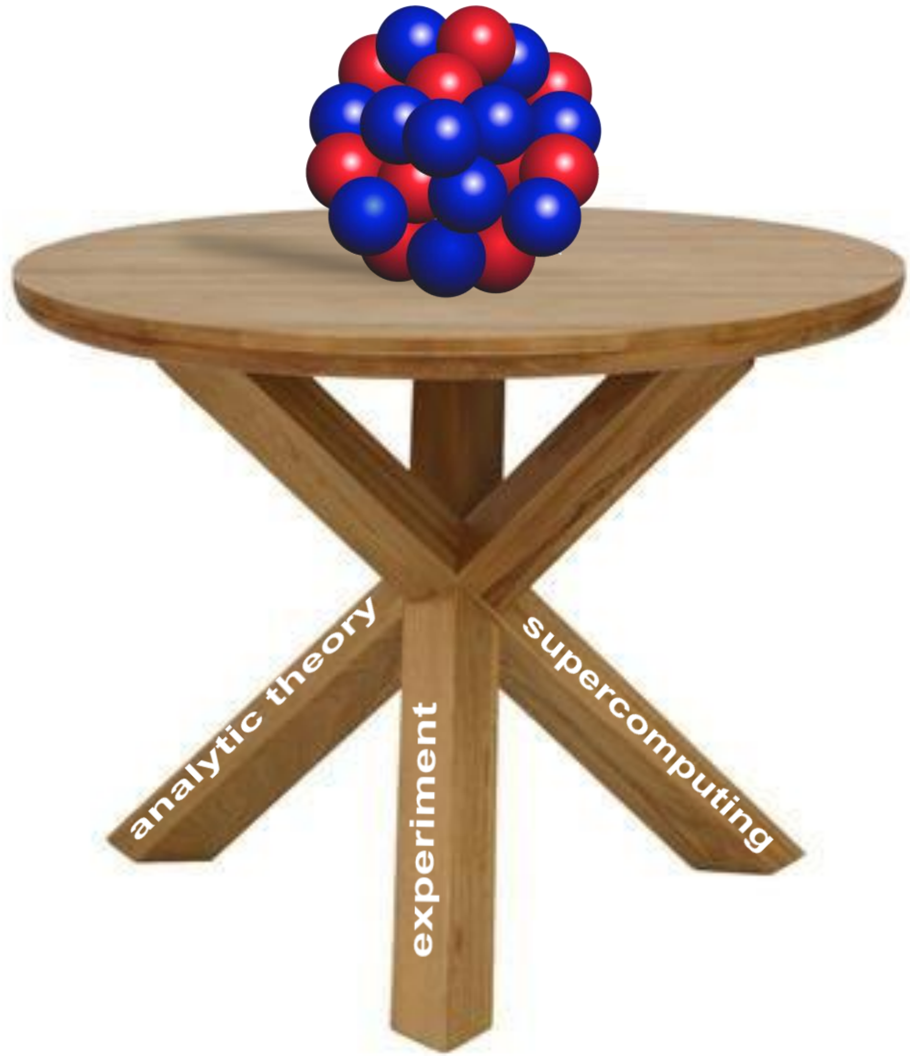
JPG Focus Issue on “Enhancing the interaction between nuclear experiment and theory through information and statistics”

http://iopscience.iop.org/0954-3899/page/ISNET

Around 35 papers (nuclear structure, reactions, nuclear astrophysics, medium energy physics, statistical methods…)

"This Focus Issue draws from a range of topics within nuclear physics, from studies of individual nucleons to the heaviest of nuclei. The unifying theme, however, is to illustrate the extent to which uncertainty is a key quantity, and to showcase applications of the latest computational methodologies. It is our assertion that a paradigm shift is needed in nuclear physics to enhance the coupling between theory and experiment, and we hope that this collection of articles is a good start."

High Performance Computing and Nuclear Theory



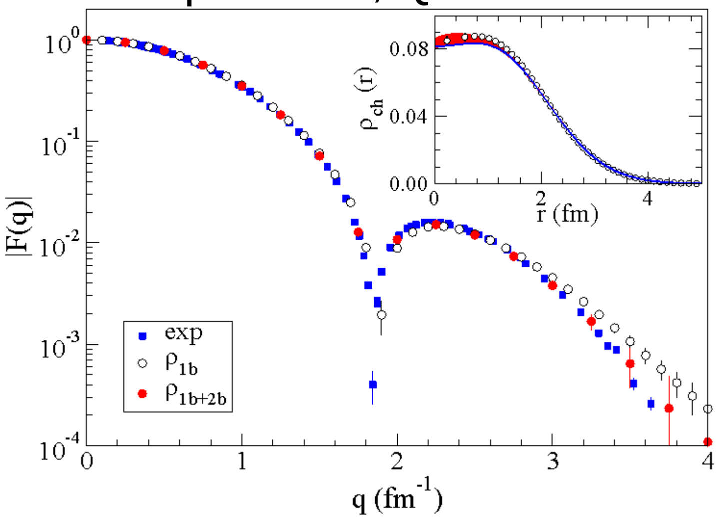
"High performance computing provides answers to questions that neither experiment nor analytic theory can address; hence, *it becomes a third leg supporting the field of nuclear physics*." (NAC Decadal Study Report)

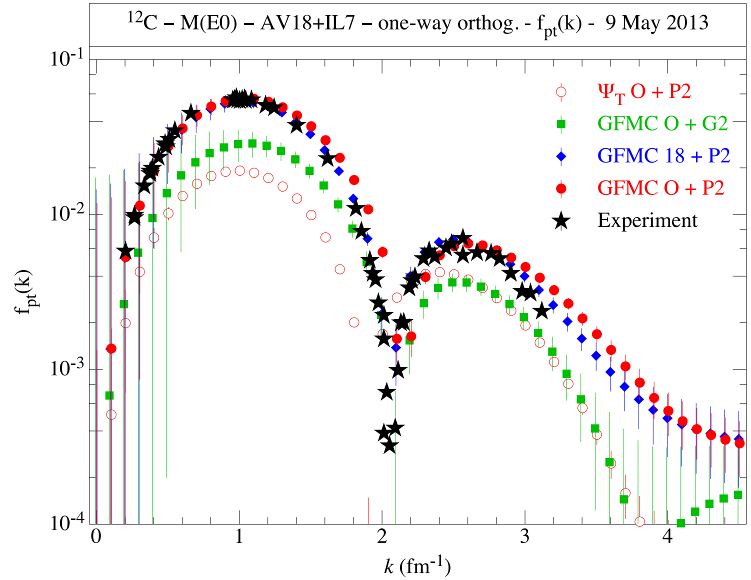
Future: large multi-institutional efforts involving strong coupling between physics, computer science, and applied math

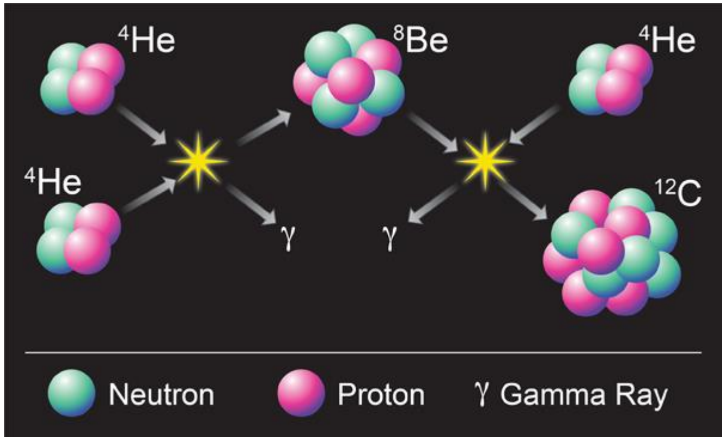
^{12}C Electron Scattering

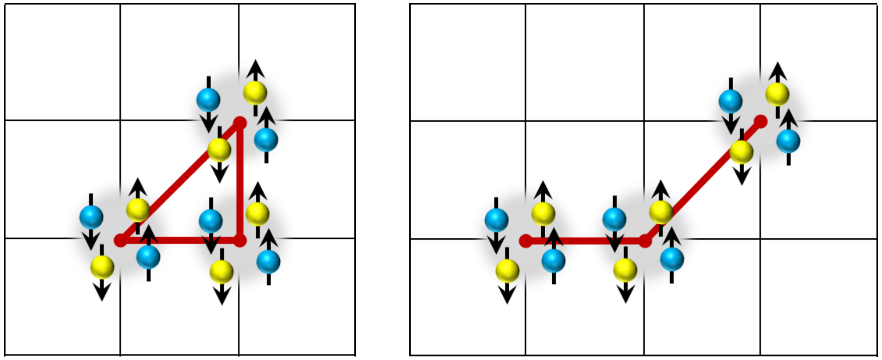
Ground-state and Hoyle-state form factor

Pieper et al., QMC



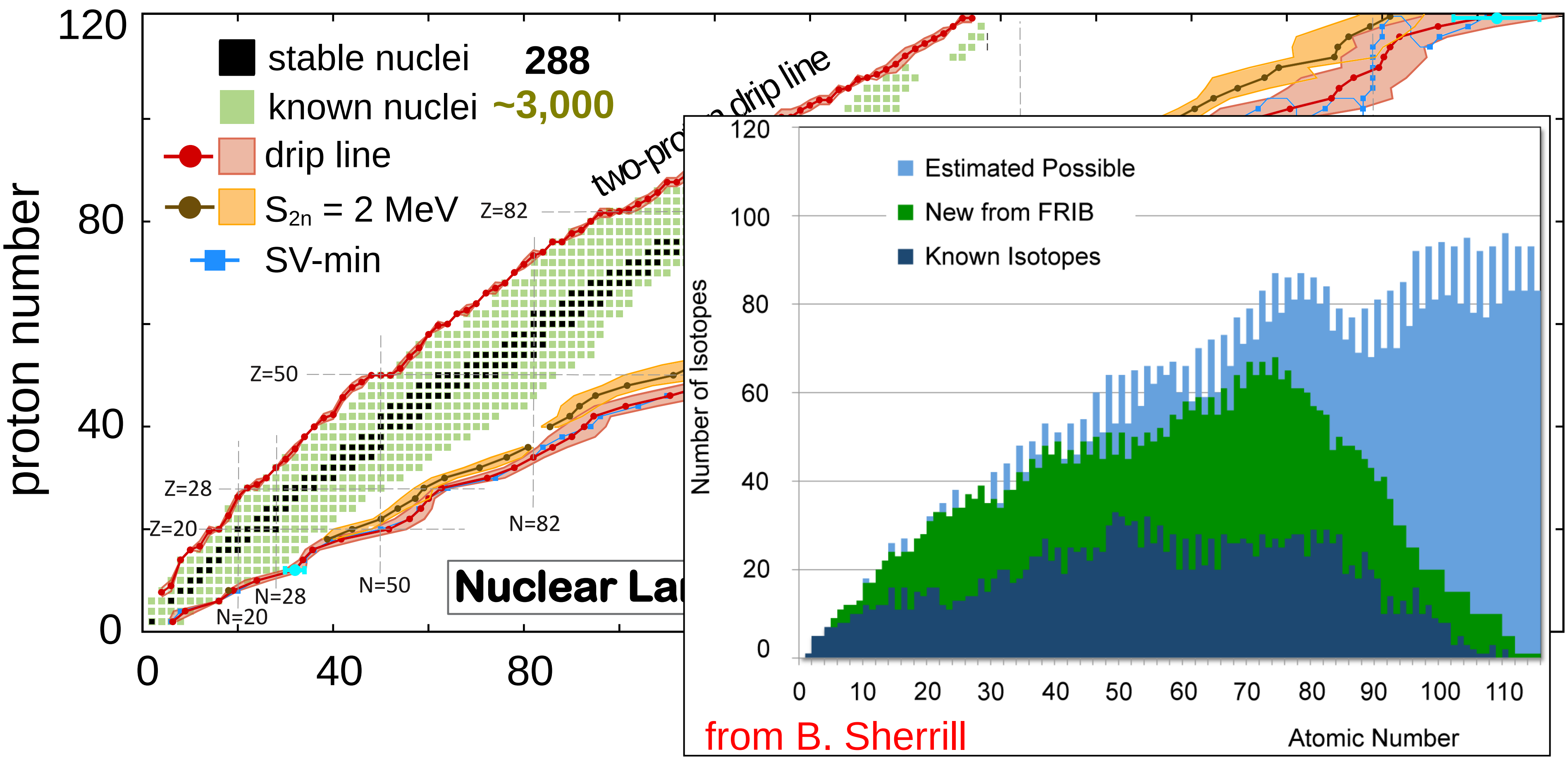






Epelbaum et al., Phys. Rev. Lett. 109, 252501 (2012). Lattice EFT

The limits: Skyrme-DFT Benchmark 2012



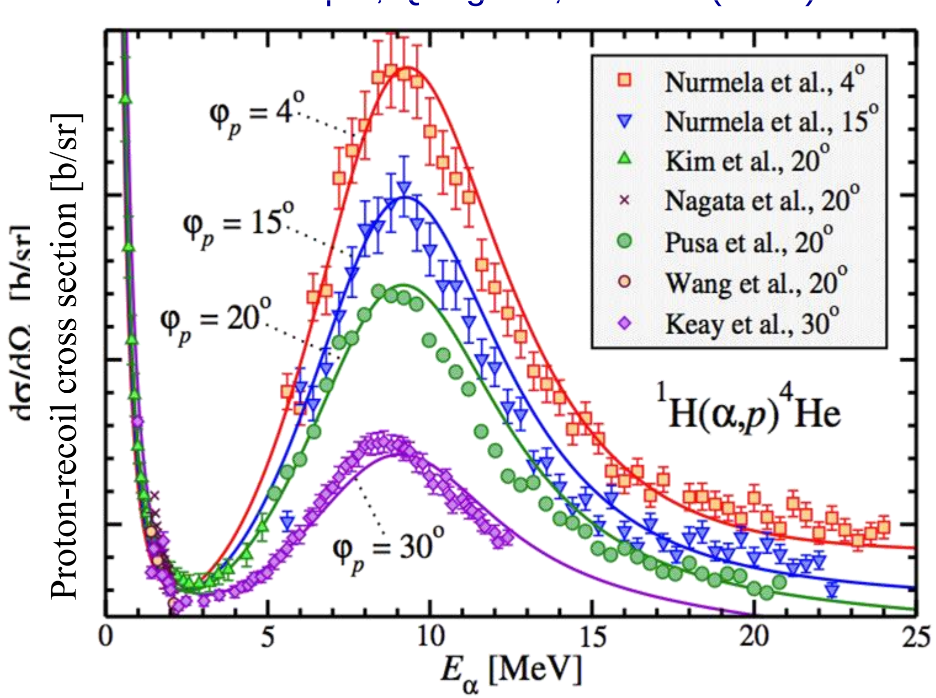
How many protons and neutrons can be bound in a nucleus?

Skyrme-DFT: 6,900±500$_{syst}$

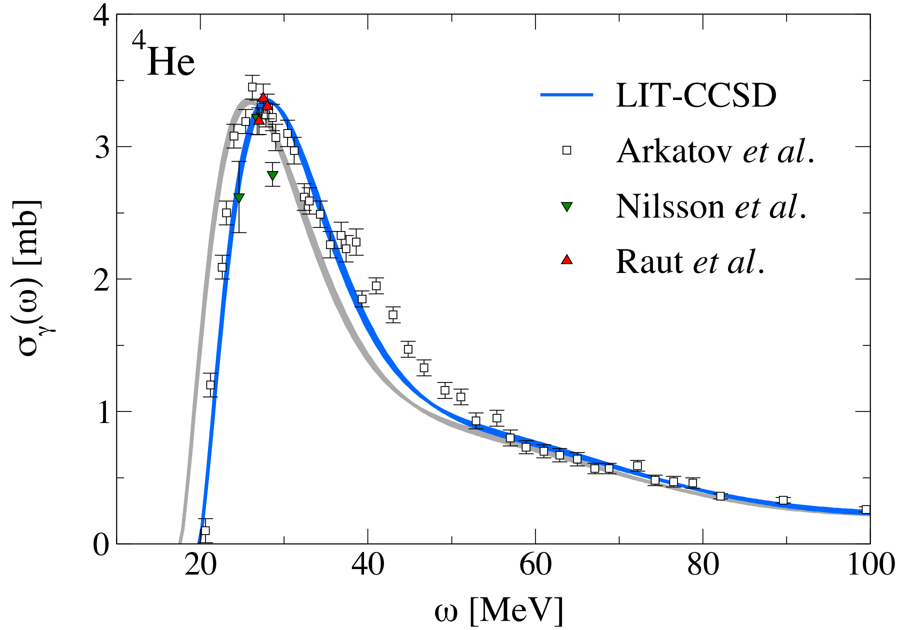
Erler et al, Nature (2012)

Microscopic reaction theory

Hupin, Quaglioni, Navratil (2014)



Bacca et al. (2014)



Near-term prospect: high-fidelity simulations with NN+NNN for composite projectiles and exotic nuclei

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 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

... and Thank You!

BACKUP

Theoretical Tools and Connections to Computational Science

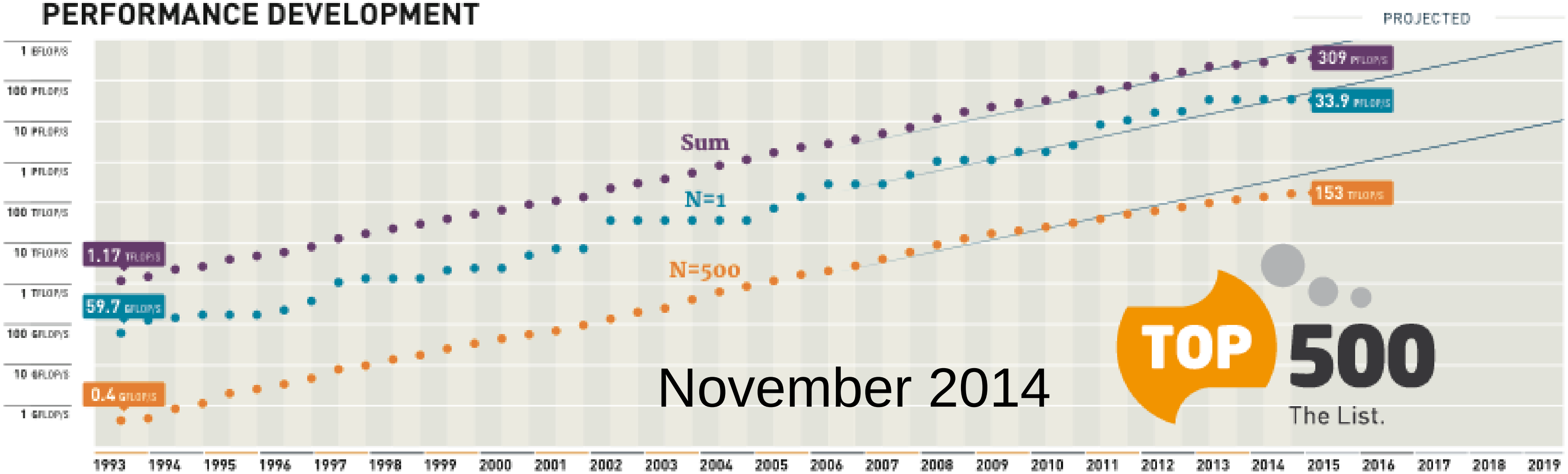
1teraflop=10^{12} flops
1peta=10^{15} flops (today)
1exa=10^{18} flops (next 10 years)

Tremendous opportunities for nuclear theory!

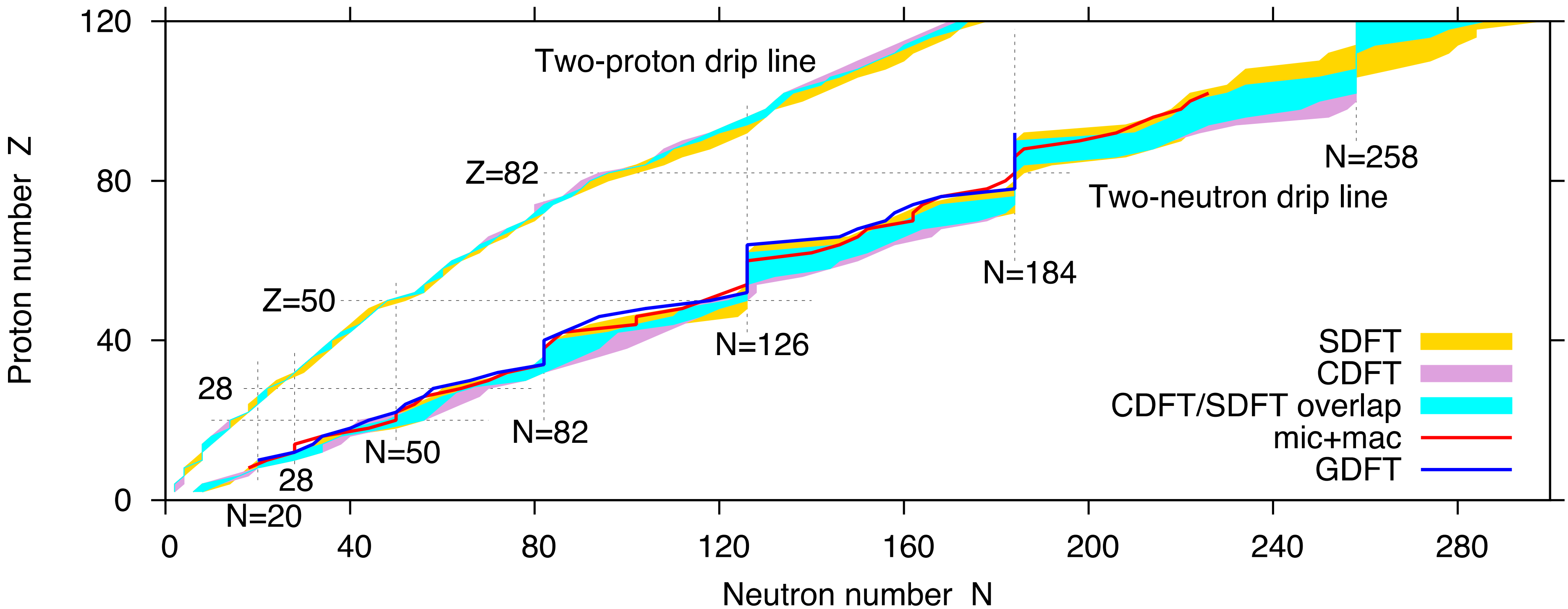
33.9 pflops

	NAME	SPECS	SITE	COUNTRY	CORES	RMAX PFLOP/S	POWER MW
1	Tianhe-2 (Milkyway-2)	NUDT, Intel Ivy Bridge (12C, 2.2 GHz) & Xeon Phi (57C, 1.1 GHz), Custom interconnect	NSCC Guangzhou	China	3,120,000	33.9	17.8
2	Titan	Cray XK7, Opteron 6274 (16C 2.2 GHz) + Nvidia Kepler GPU, Custom interconnect	DOE/SC/ORNL	USA	560,640	17.6	8.2
3	Sequoia	IBM BlueGene/Q, Power BQC (16C 1.60 GHz), Custom interconnect	DOE/NNSA/LLNL	USA	1,572,864	17.2	7.9
4	K computer	Fujitsu SPARC64 VIIIfx (8C, 2.0GHz), Custom interconnect	RIKEN AICS	Japan	705,024	10.5	12.7
5	Mira	IBM BlueGene/Q, Power BQC (16C, 1.60 GHz), Custom interconnect	DOE/SC/ANL	USA	786,432	8.59	3.95

PERFORMANCE DEVELOPMENT



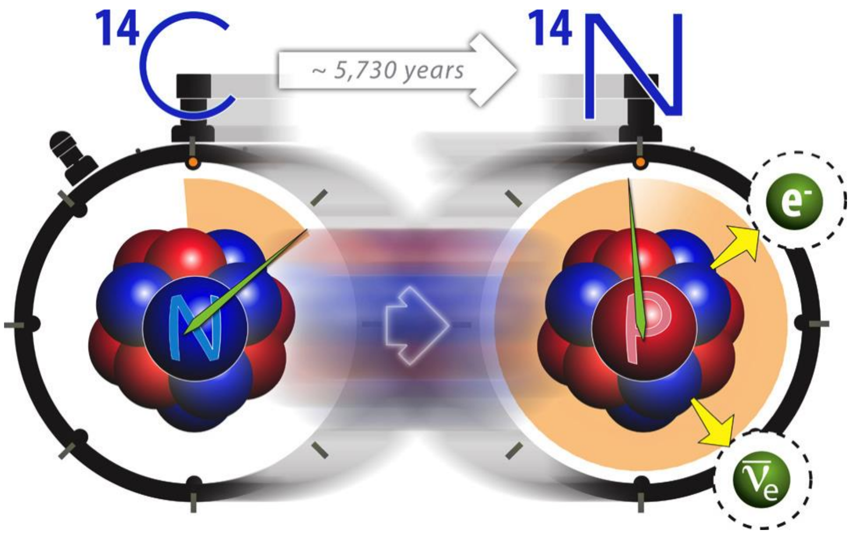
Quantified Nuclear Landscape (2)

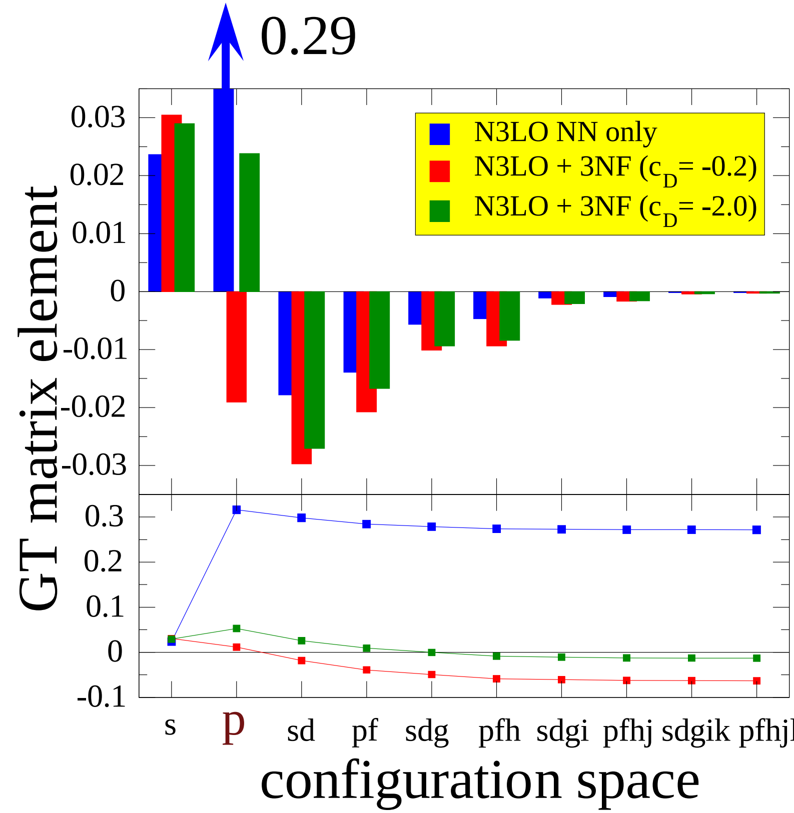


A.V. Afanasjev et al., Phys. Lett. B 726, 680 (2013)

Anomalous Long Lifetime of ^{14}C

Determine the microscopic origin of the suppressed β-decay rate: 3N force



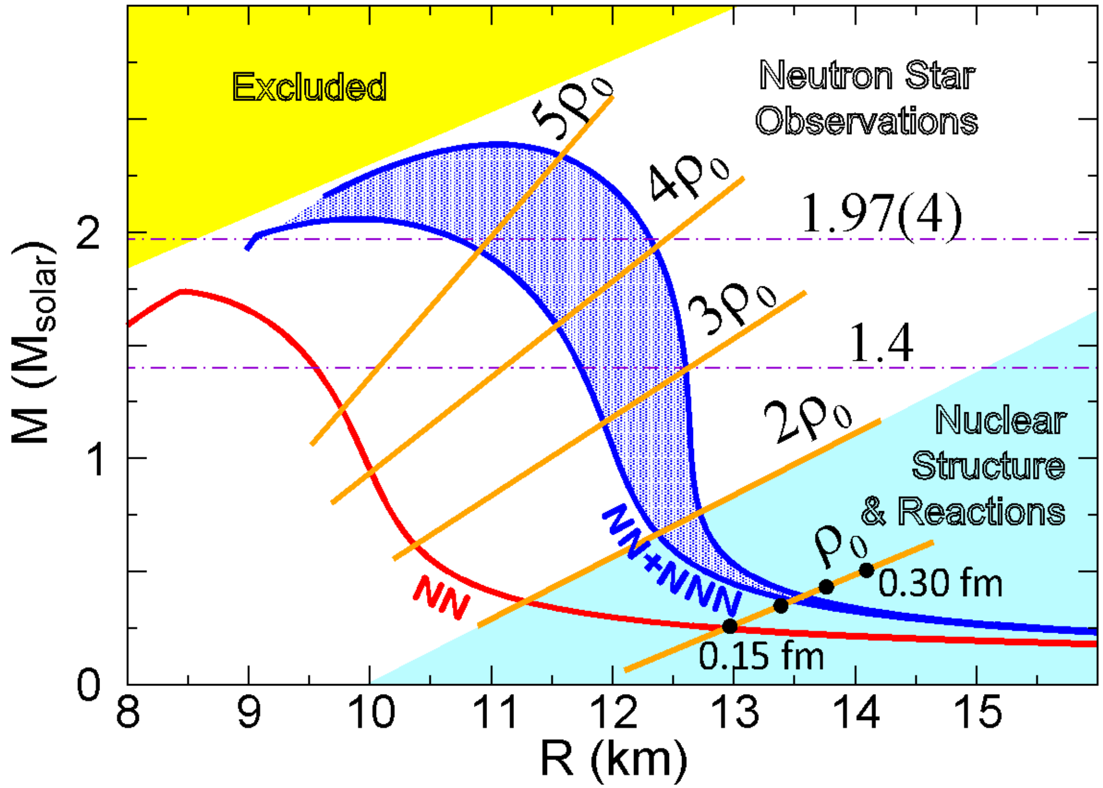


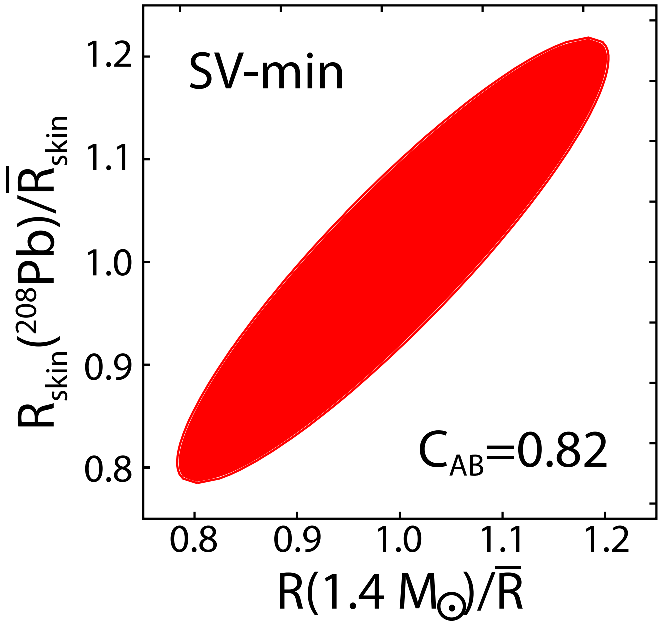
Maris et al., PRL 106, 202502 (2011)

Dimension of matrix solved for 8 lowest states ~ 10^9

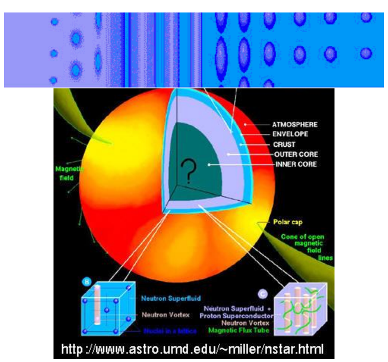
Solution took ~ 6 hours on 215,000 cores on Cray XT5 Jaguar at ORNL

From nuclei to neutron stars (a multiscale problem)





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



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