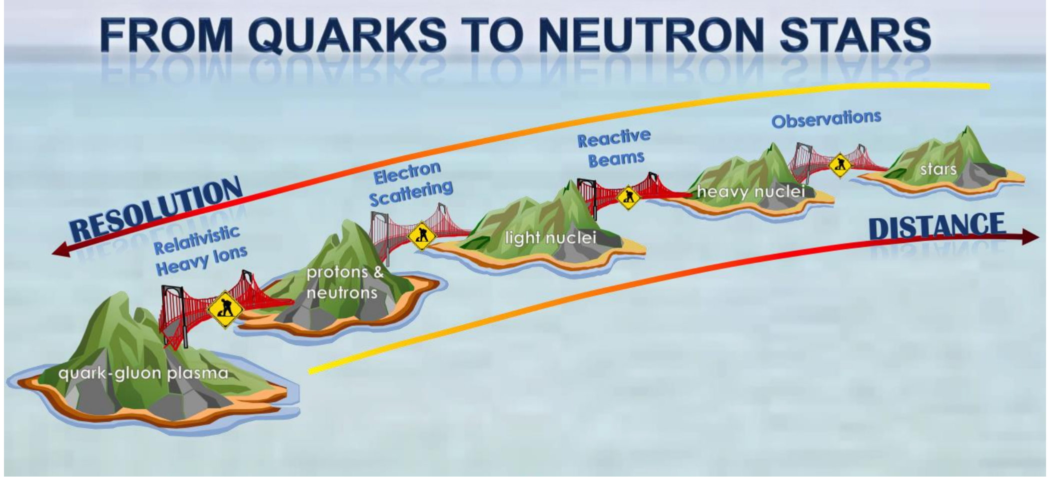
Nuclear Structure Theory: today and tomorrow

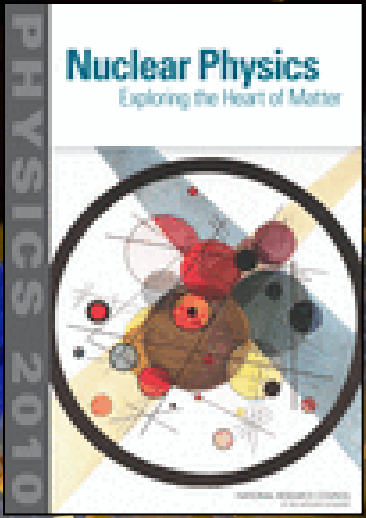
Witek Nazarewicz (MSU/ORNL)

Reflections on the Atomic Nucleus
Liverpool, July 28-30, 2015

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



The Nuclear Landscape and the Big Questions (NAS report)



- Where do nuclei and elements come from?
- How are nuclei organized?
- What are practical and scientific uses of nuclei?

BOTTOM LINE

Revolution due to major advances in accelerator technology, experimental techniques, analytic theory, and computing. This has led to a shift from phenomenological picture to nuclear theory grounded in the Standard Model. Today, we are constructing a roadmap that will lead to a predictive theory of nuclei.

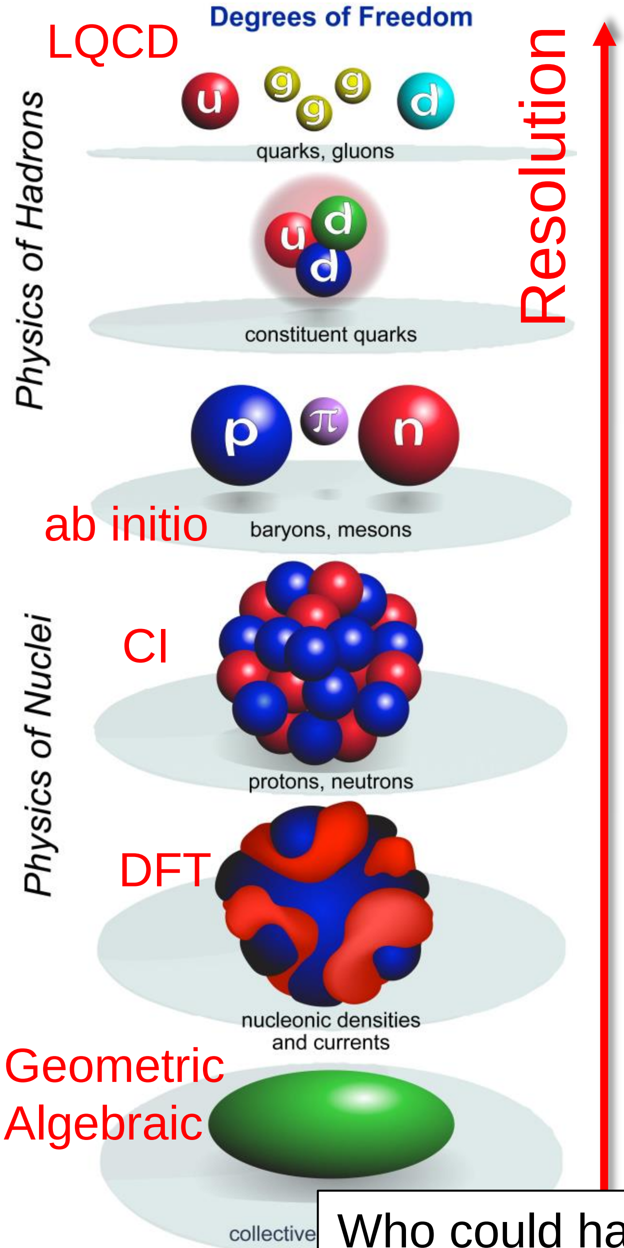
Classification of theories

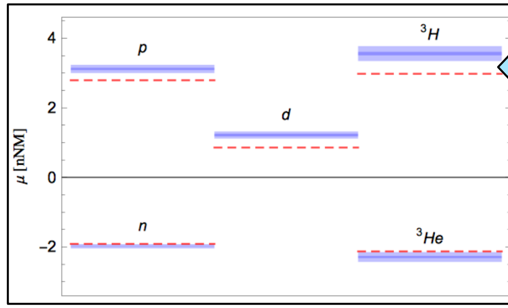
(Alexander I. Kitaigorodskii)

- A third rate theory explains after the facts (postdictive, retrodictive)
- A second rate theory forbids
- A first rate theory predicts (predictive)

How to explain the nuclear landscape from the bottom up?

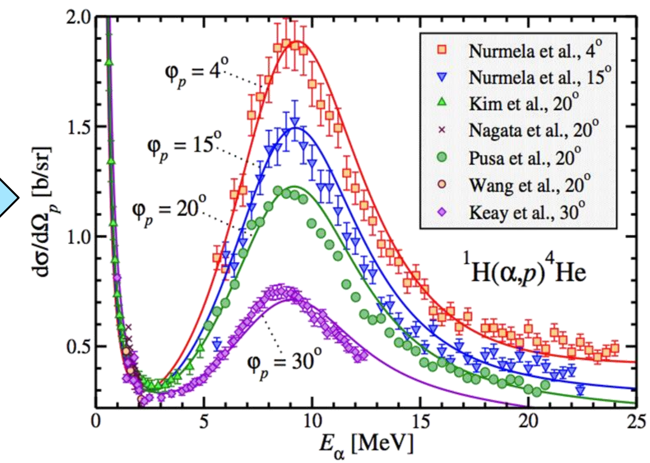
Theory revolution





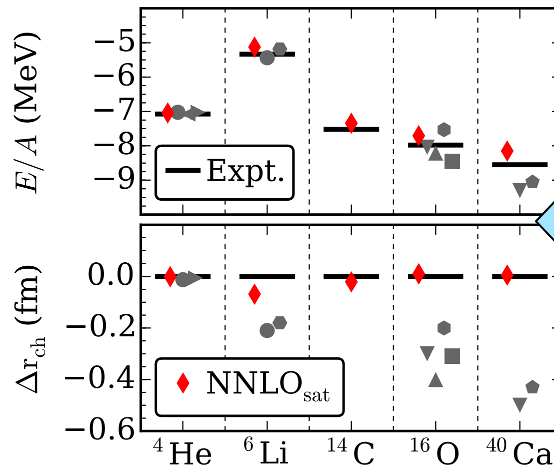
Nucleon and nuclear magnetic moments from Lattice QCD

S. Beane et al., PRL 113, 252001 (2014)



Ab-initio approach to reactions (p+^{4}He)

Hupin et al. PRC 90, 061601 (2014)

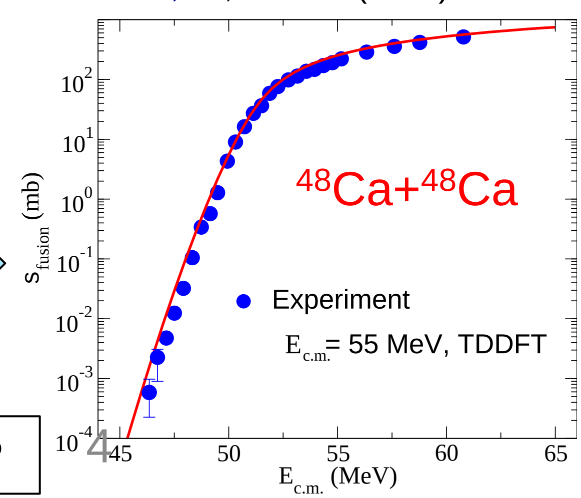


Coupled cluster description of binding energies and radii

A. Ekstrom et al., 91, 051301 (2015)

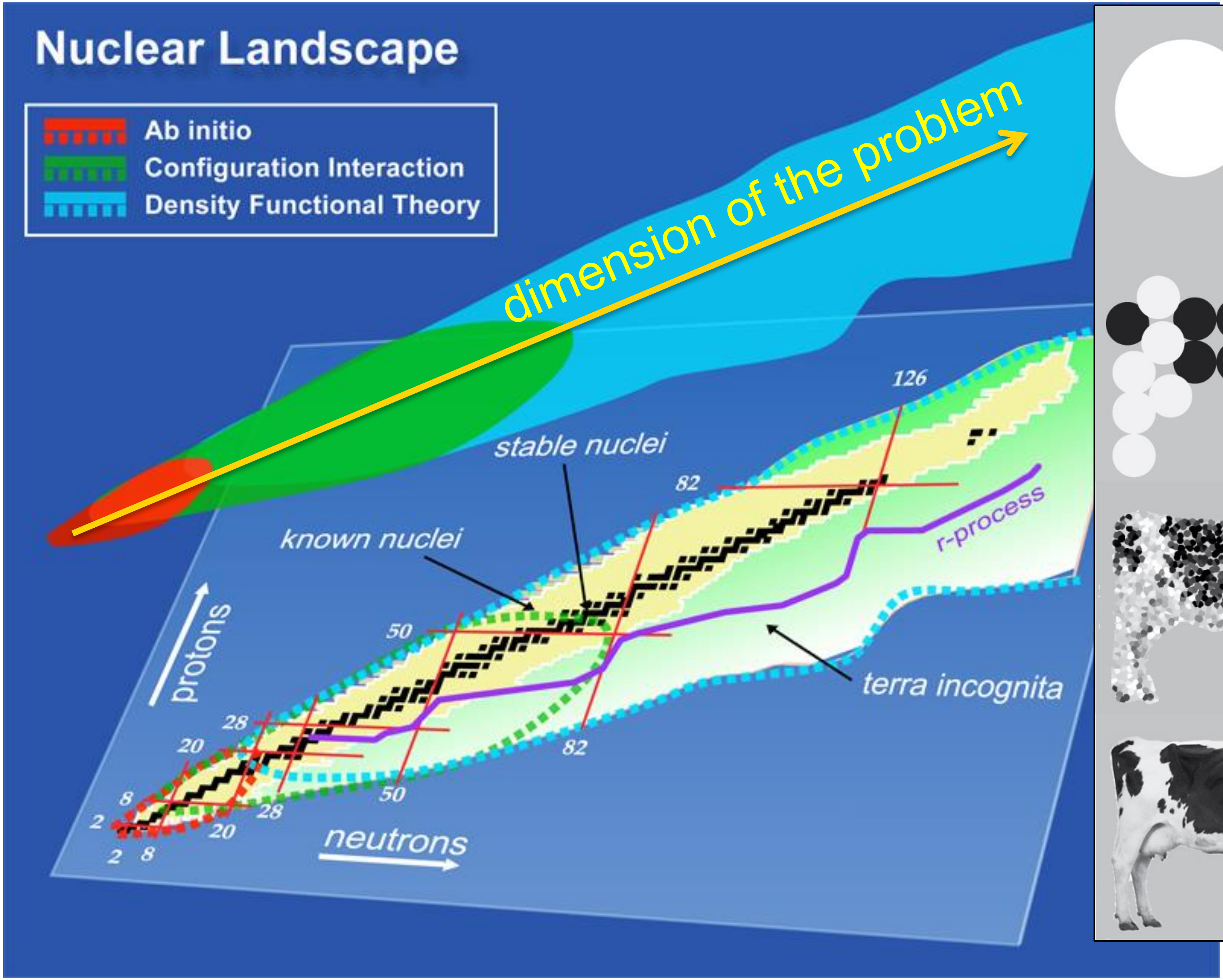
Fusion cross sections from TDDFT

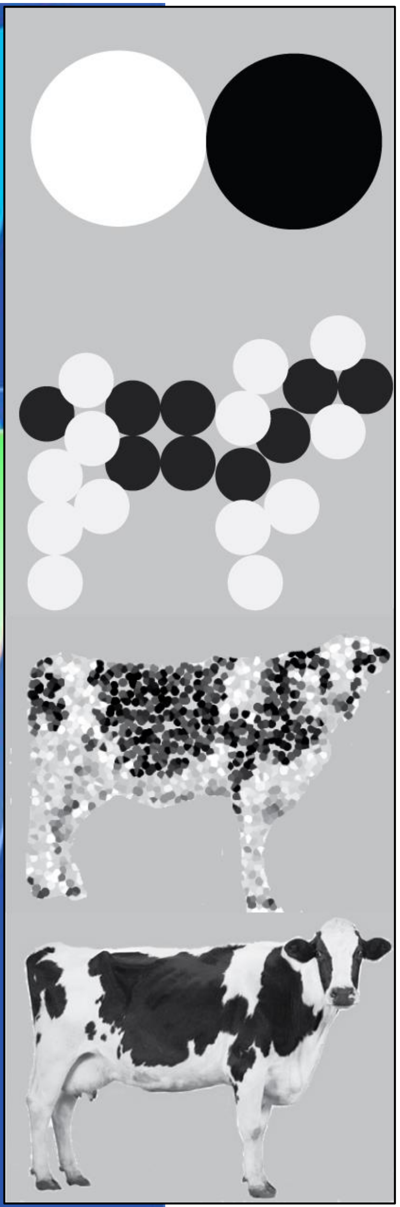
R. Keser et al., PRC 85, 044606 (2012)



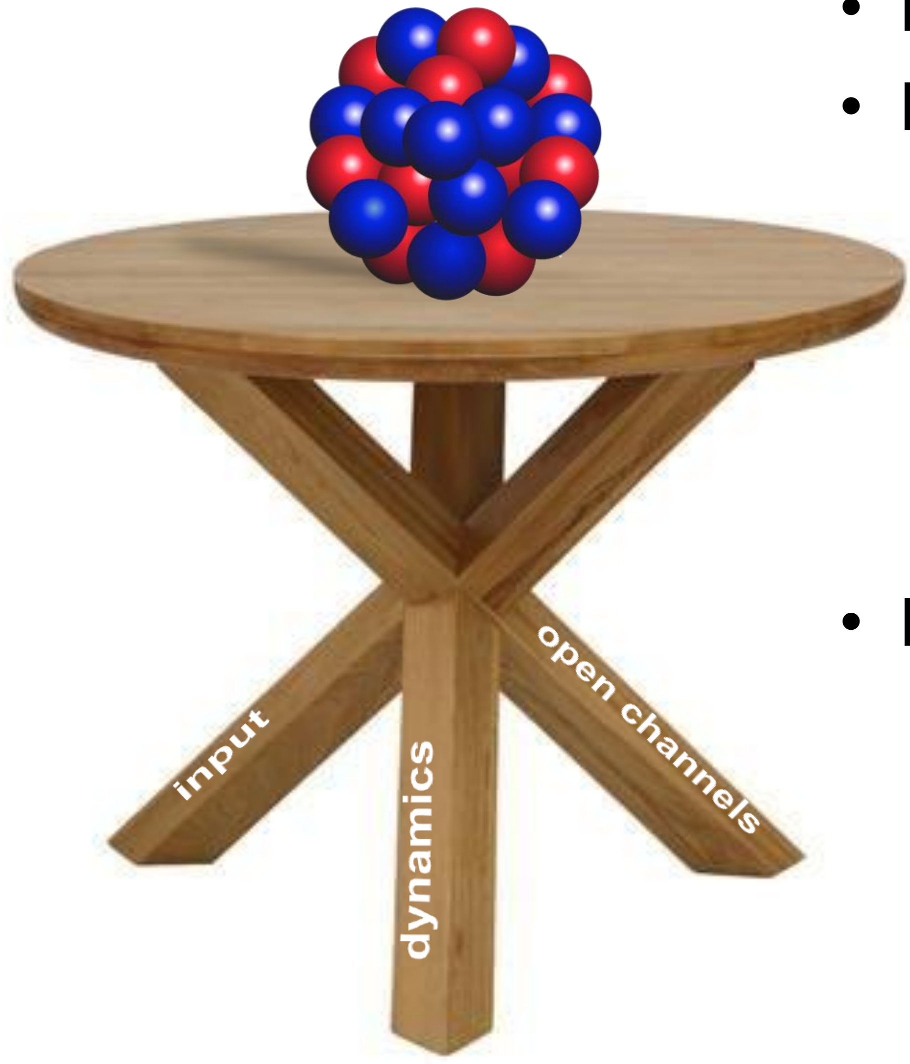
Who could have predicted this 20 years ago?

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



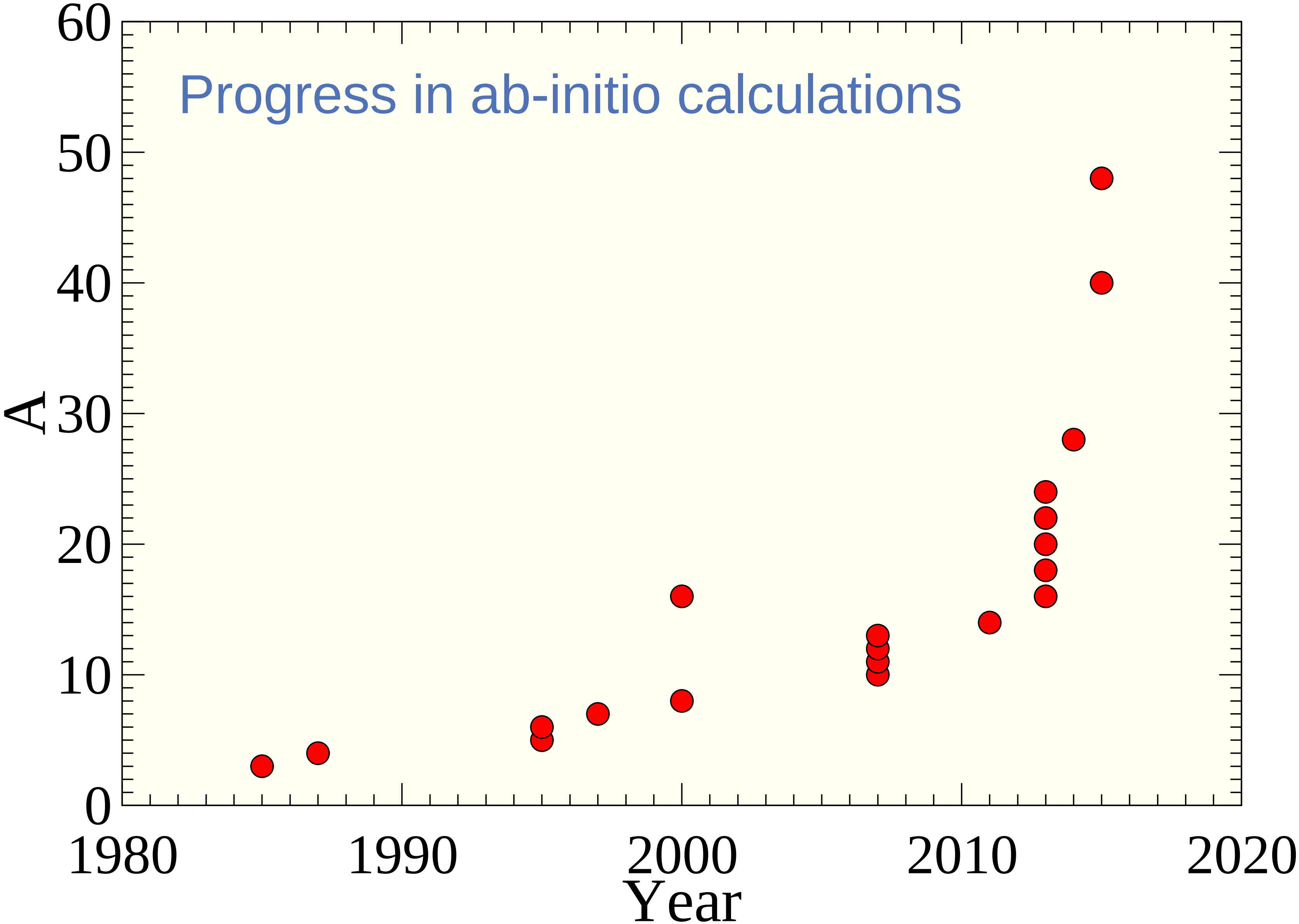


Theory of nuclei is demanding



- New insights
- 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

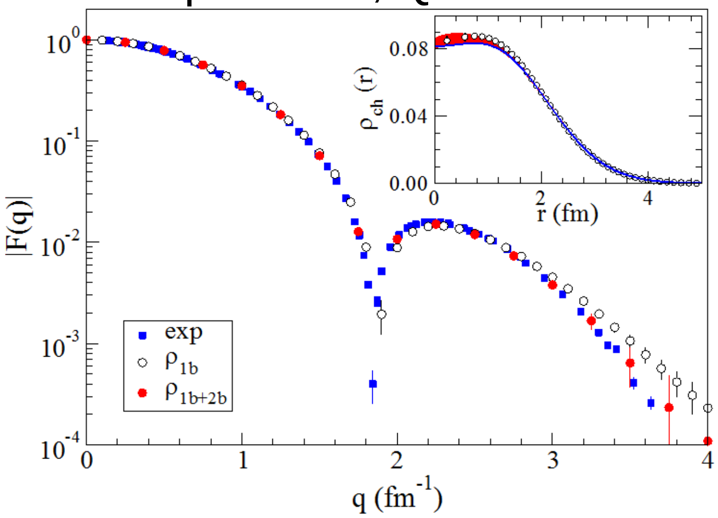


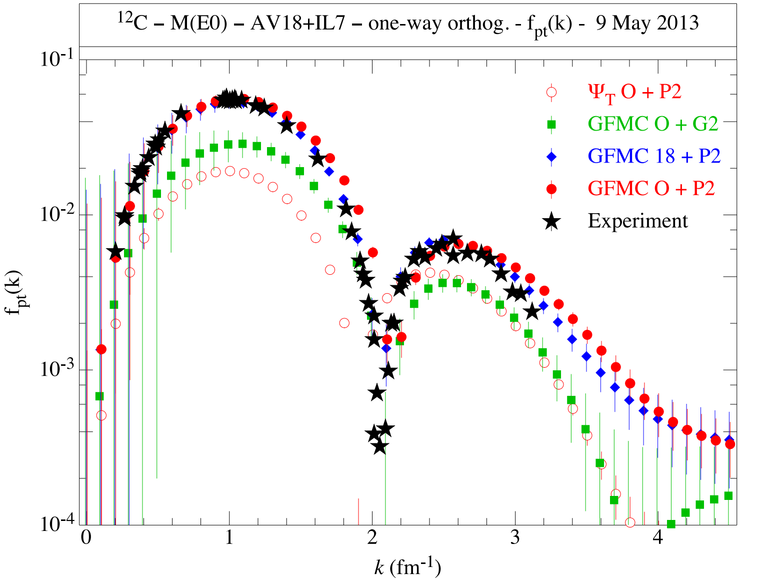
Progress in ab-initio calculations
A
Year
0
10
20
30
40
50
60
1980
1990
2000
2010
2020

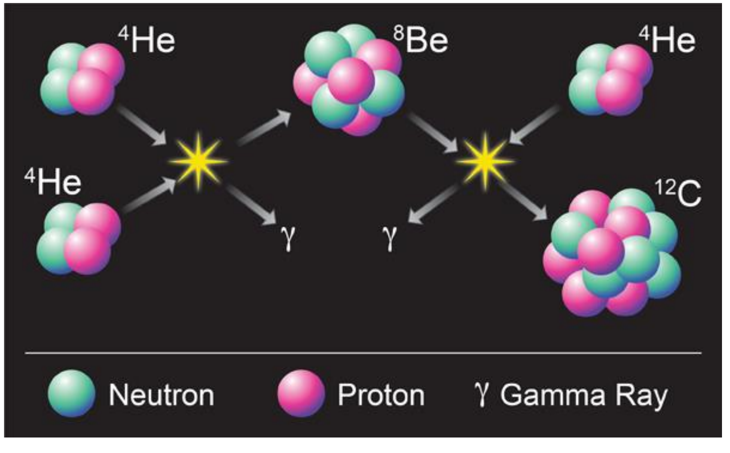
^{12}C structure

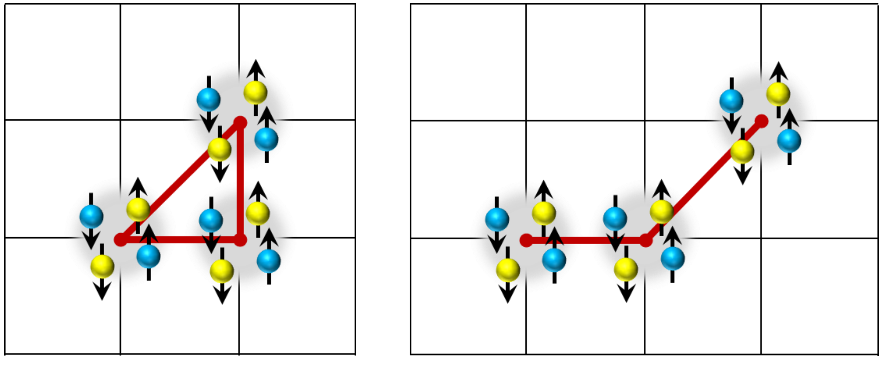
Ground-state and Hoyle-state form factor

Pieper et al., QMC





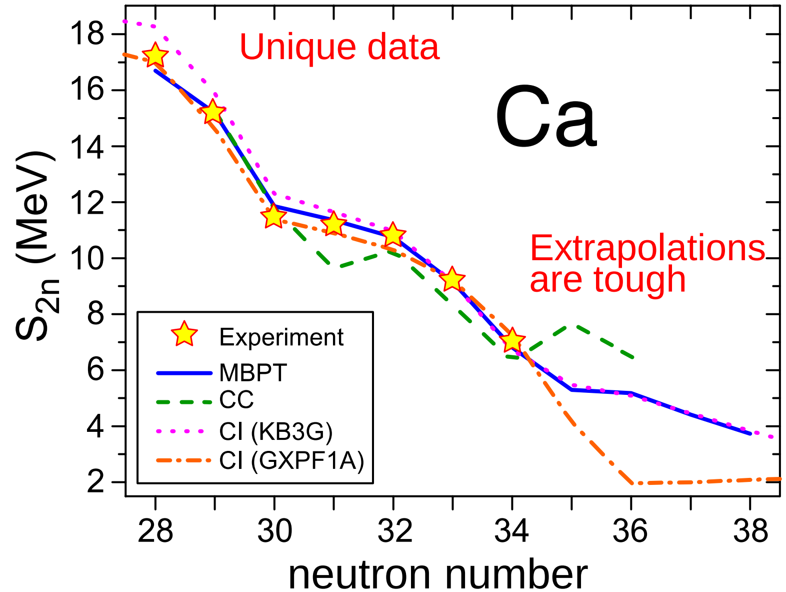




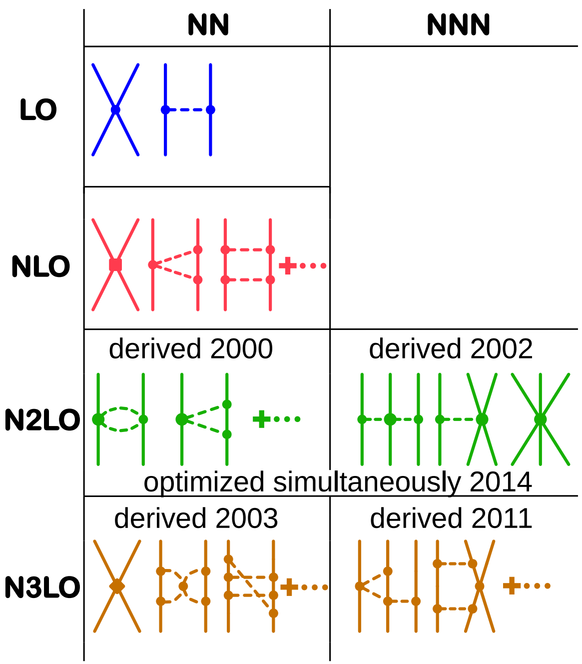
Epelbaum et al., Phys. Rev. Lett. 109, 252501 (2012). Lattice EFT

The frontier: neutron-rich calcium isotopes

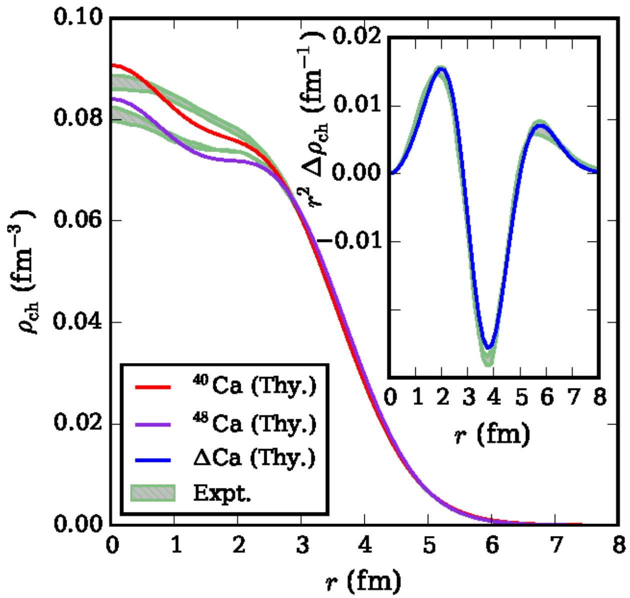
where *ab-initio* and DFT meet…

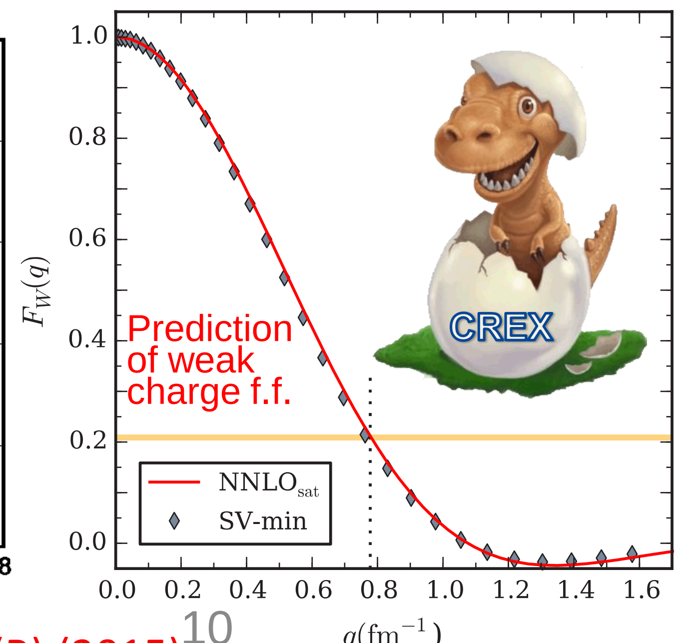


Nuclear Forces
from χEFT



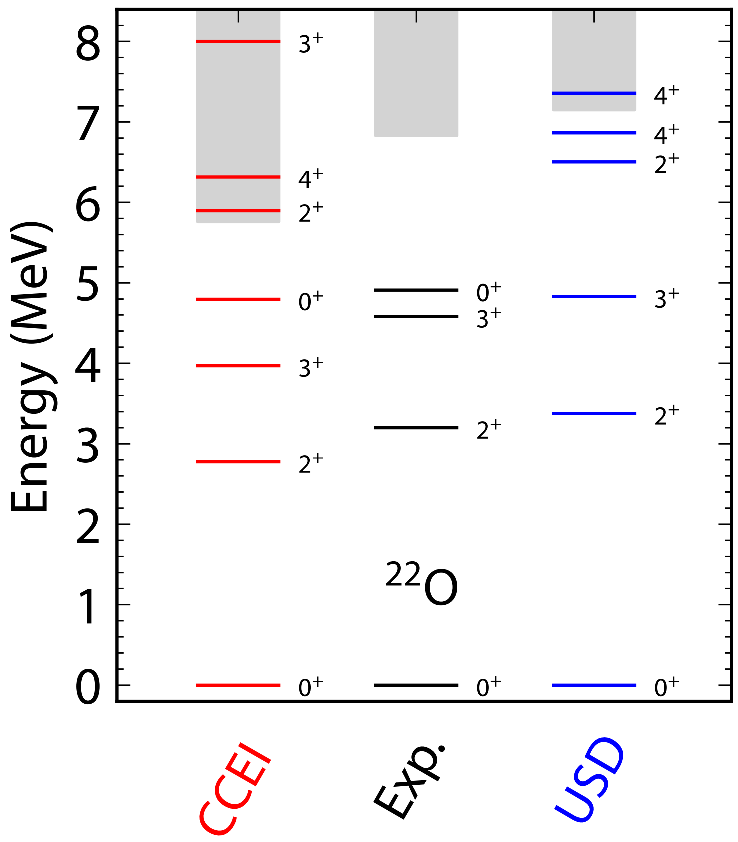
Consistency with known data



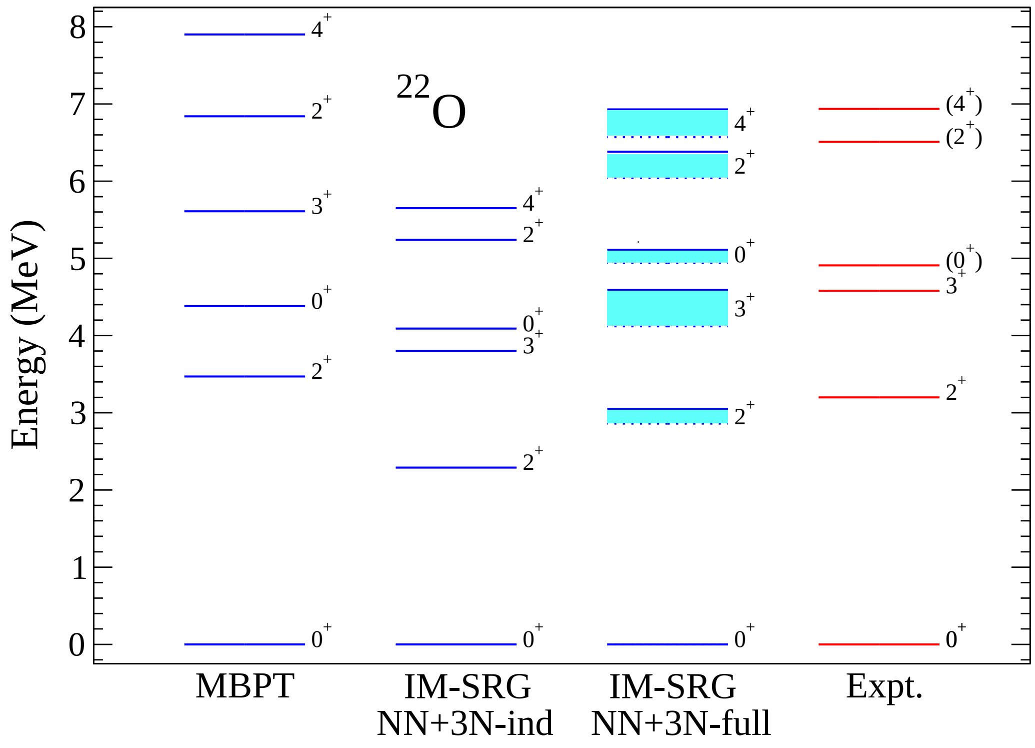


A. Ekström et al. Phys. Rev. C 91, 051301(R) (2015)

Microscopic valence-space Shell Model



Coupled Cluster Effective Interaction (valence cluster expansion)
Jansen et al. , Phys. Rev. Lett. 113, 142502 (2014)



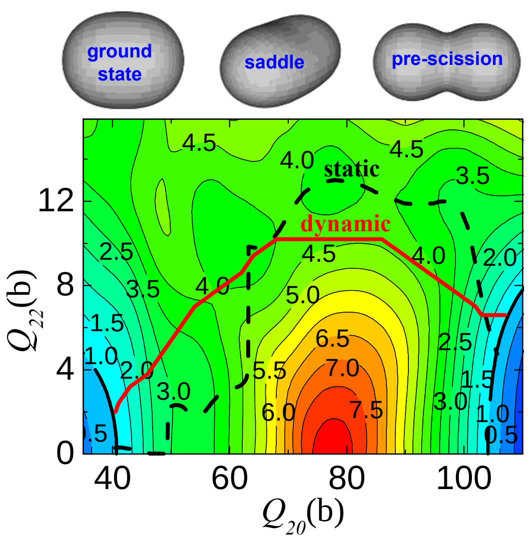
In-medium SRG Effective Interaction
Bogner et al. Phys. Rev. Lett. 113, 142501 (2014)

Small and Large-Amplitude Collective Motion

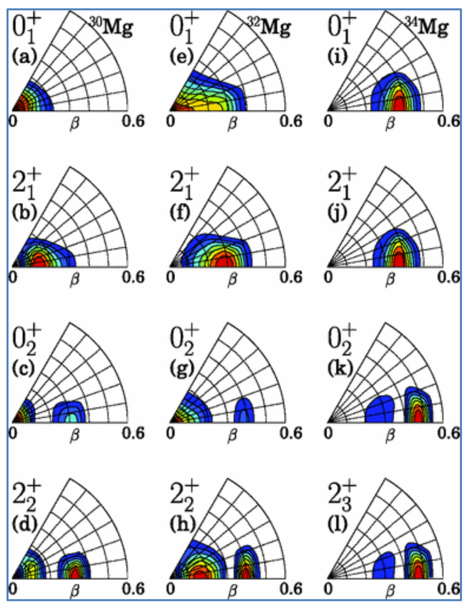
- New-generation computational frameworks developed
  - Time-dependent DFT and its extensions
  - Adiabatic approaches rooted in Collective Schrödinger Equation
  - Quasi-particle RPA
  - Projection techniques
- Applied to HI fusion, fission, coexistence phenomena, collective strength, superfluid modes

Shape coexistence

Spontaneous fission

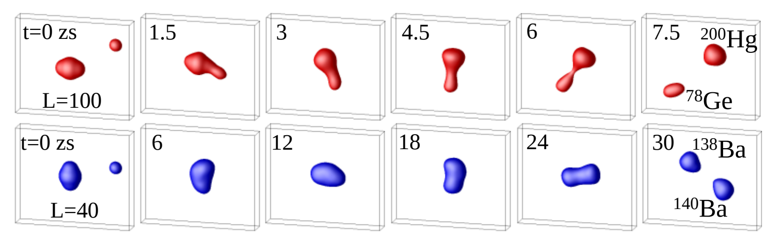


Sadhukhan et al.
Phys. Rev. C 88, 064314 (2013);
Phys. Rev. C 90 061304(R) (2014)



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

Heavy Ion fusion (^{40}Ca+^{238}U)



Wakhle et al.
PRL 113, 182502 (2014)

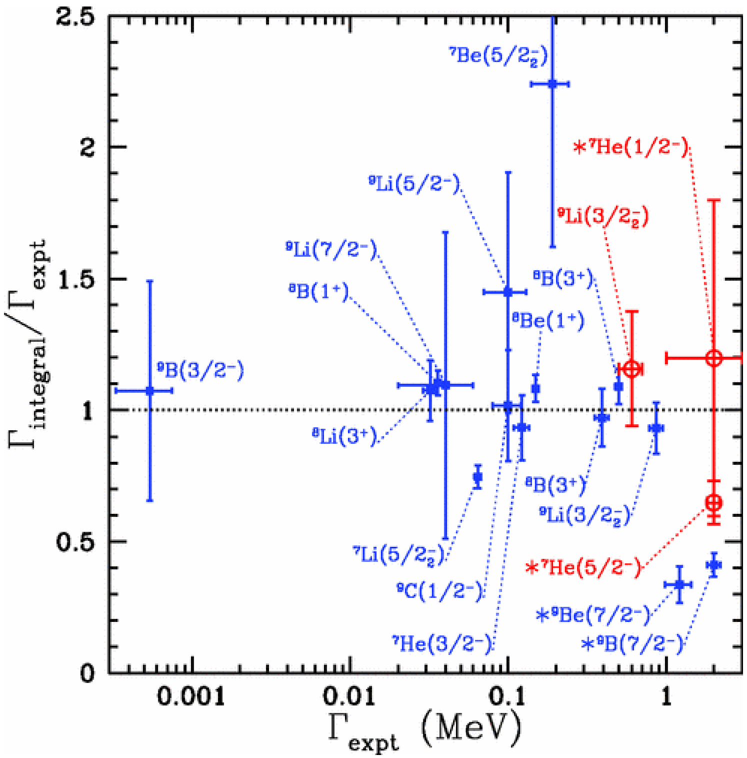
Impact of open channels on structural properties

A suite of powerful approaches developed to open nuclear systems:

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

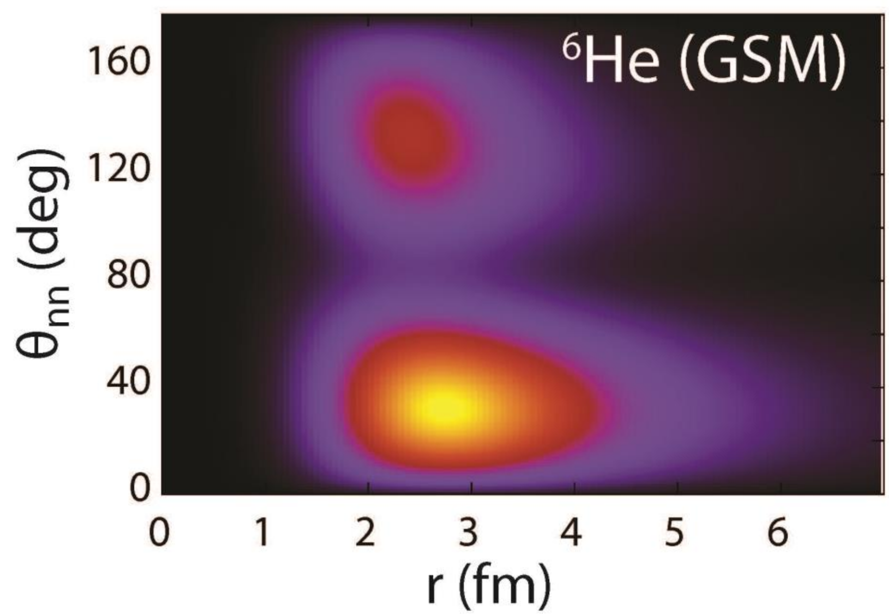
Ab initio calculations of ANCs and widths

Nollett, PRC 6, 044330 (2012)



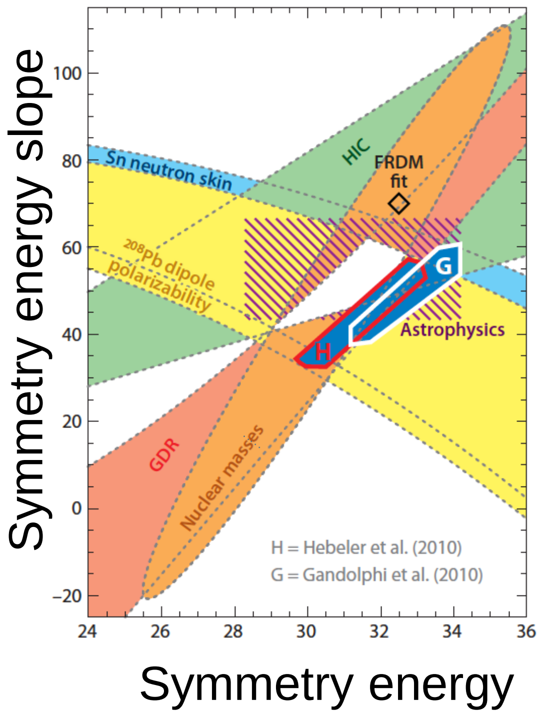
Di-neutron correlations in CS/GSM

Papadimitriou et al. PRC 84, 051304 (2011)

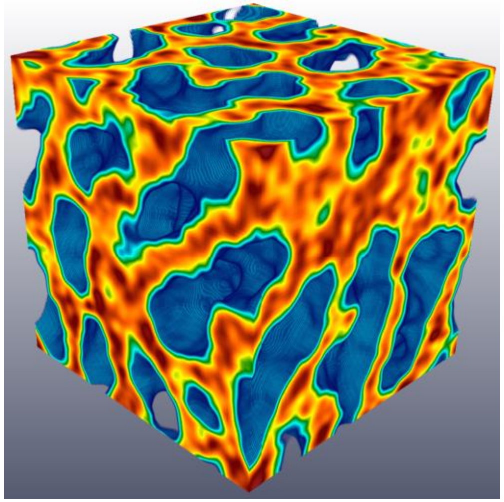


Quest for understanding the neutron-rich matter on Earth and in the Cosmos

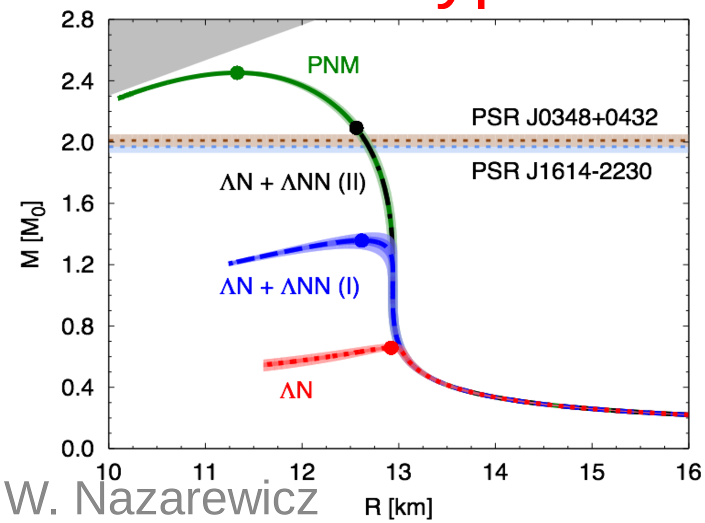
Bounds on EOS



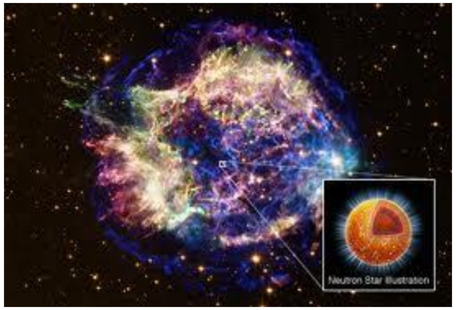
Crustal structures

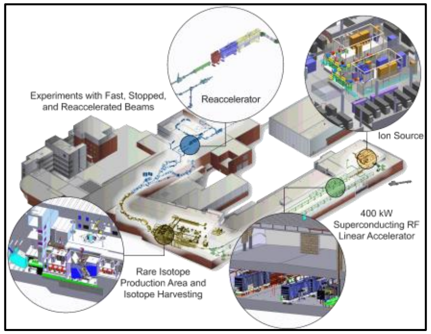


EOS with hyperons



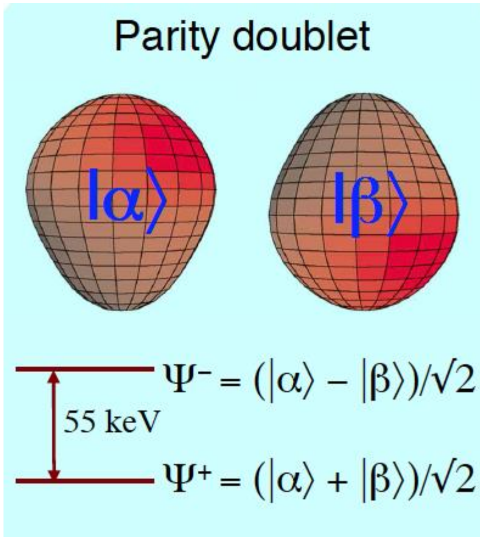
Data





Rare Isotopes and fundamental symmetry tests

Atomic electric dipole moment: The violation of CP-symmetry is responsible for the fact that the Universe is dominated by matter over anti-matter

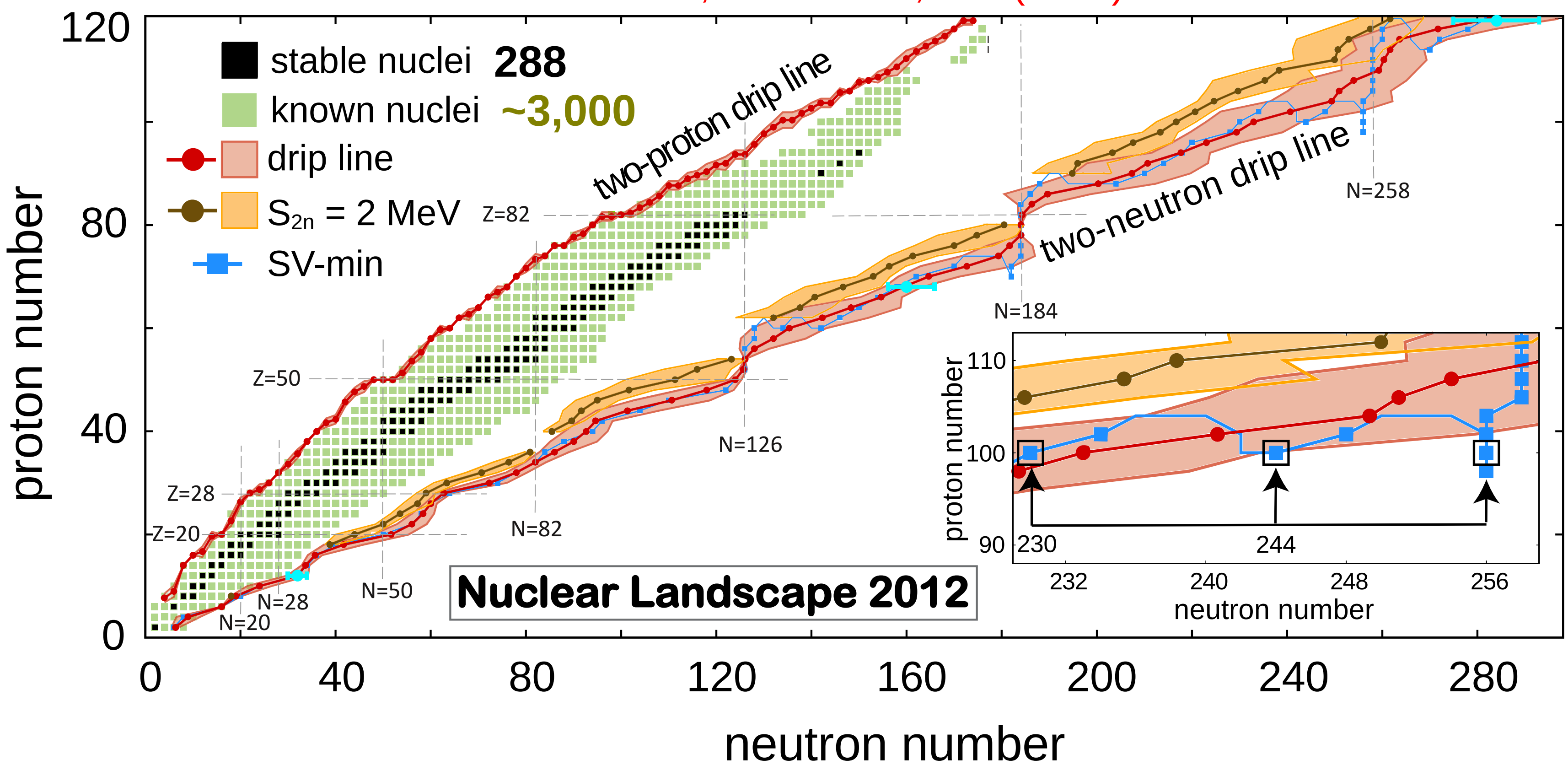


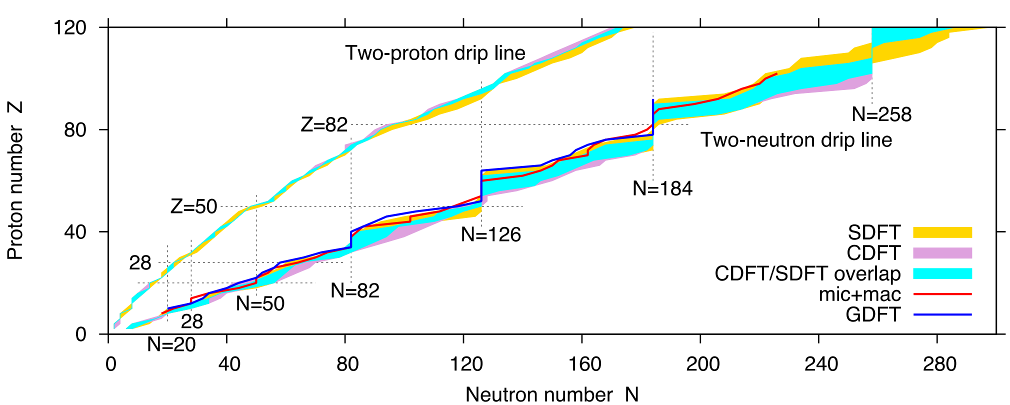
- Closely spaced parity doublet gives rise to enhanced electric dipole moment
- Large intrinsic Schiff moment:
  Dobaczewski & Engel, PRL 94, 232502 (2005)
- ^{199}Hg (Seattle, 1980's – present)
- ^{225}Ra (Starting at ANL and KVI)
- ^{223}Rn at TRIUMF
- Potential at FRIB (10^{12}/s w ISOL target (far future); 10^{10} initially

Gaffney et al., Nature 199, 497 (2013)

The limits: Skyrme-DFT Benchmark 2012

Erler et al, Nature 486, 509 (2012)



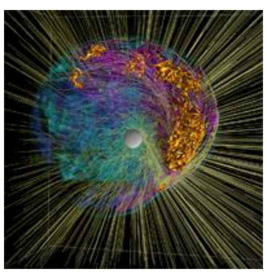
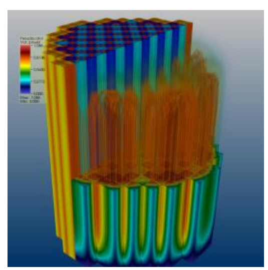


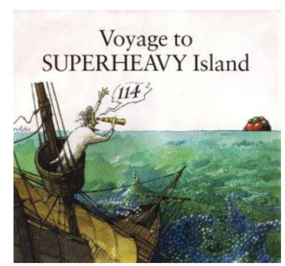
A.V. Afanasjev, et al. Phys. Lett. B (2013)

Prospects

Experimental context: some thoughts…

- Beam time and cycles are difficult to get and expensive.
- 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?
- Theoretical models are often applied to entirely new nuclear systems and conditions that are not accessible to experiment. New technologies are essential for providing predictive capability, to estimate uncertainties, and to assess extrapolations



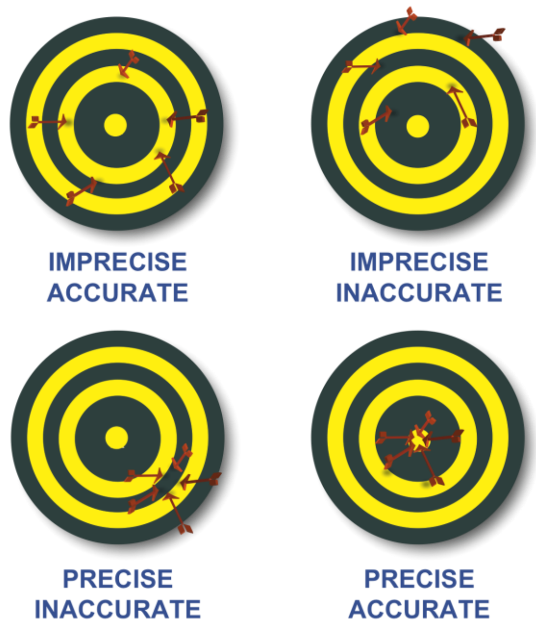
A paradigm shift is needed to enhance the coupling between theory and experiment

ISNET: Enhancing the interaction between nuclear experiment and theory through information and statistics

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

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

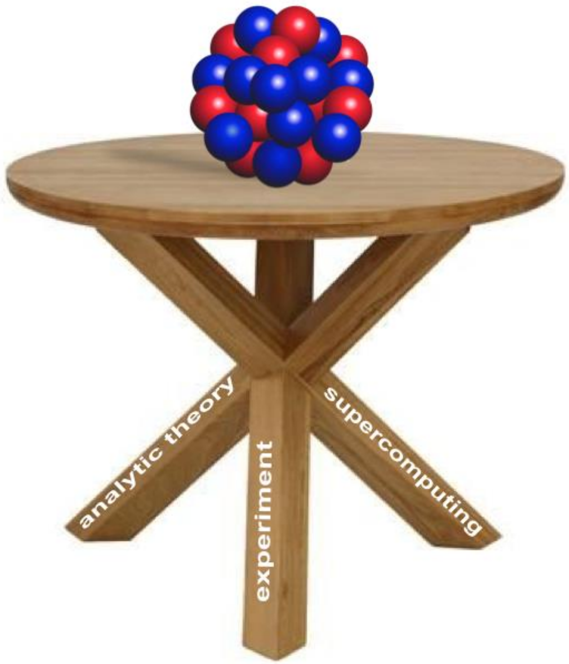
"Remember that all models are wrong; the practical question is *how wrong do they have to be to not be useful*" (E.P. Box)

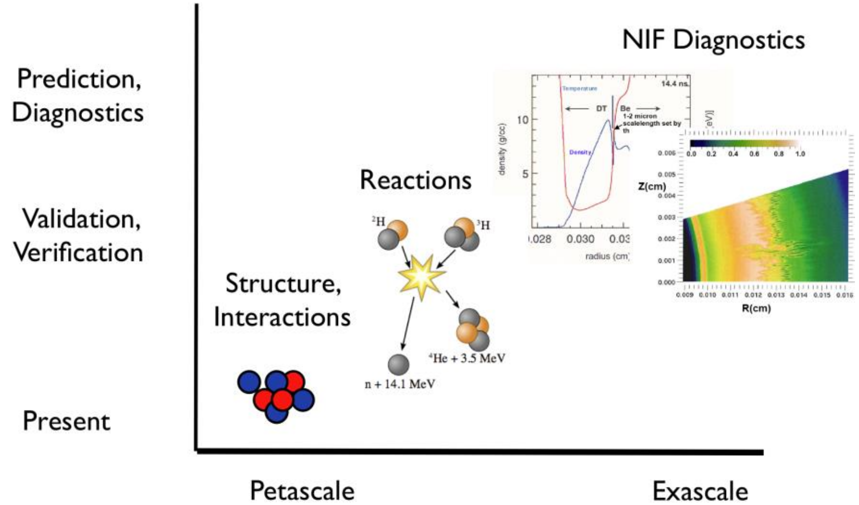


Error estimates of theoretical models: a guide

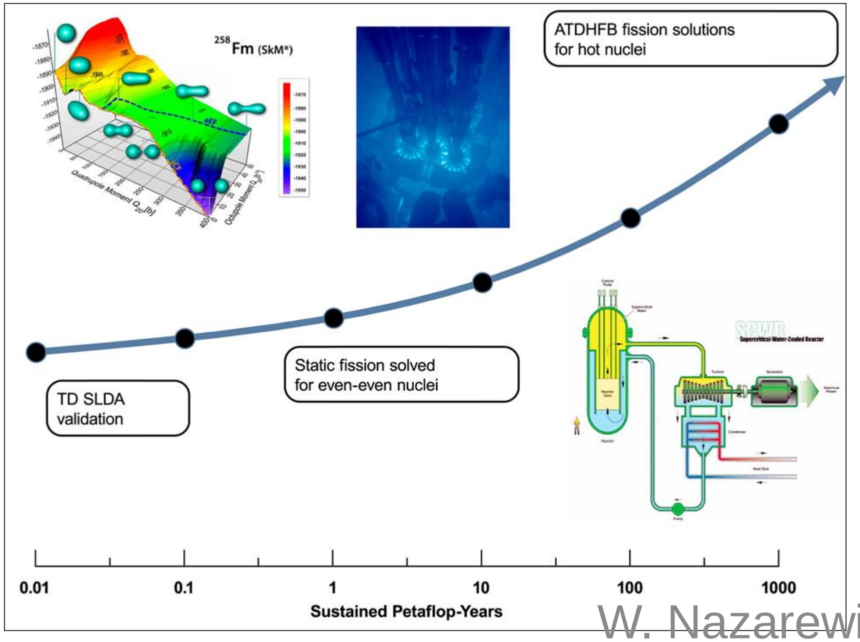
J. Phys. G **41** 074001 (2014)

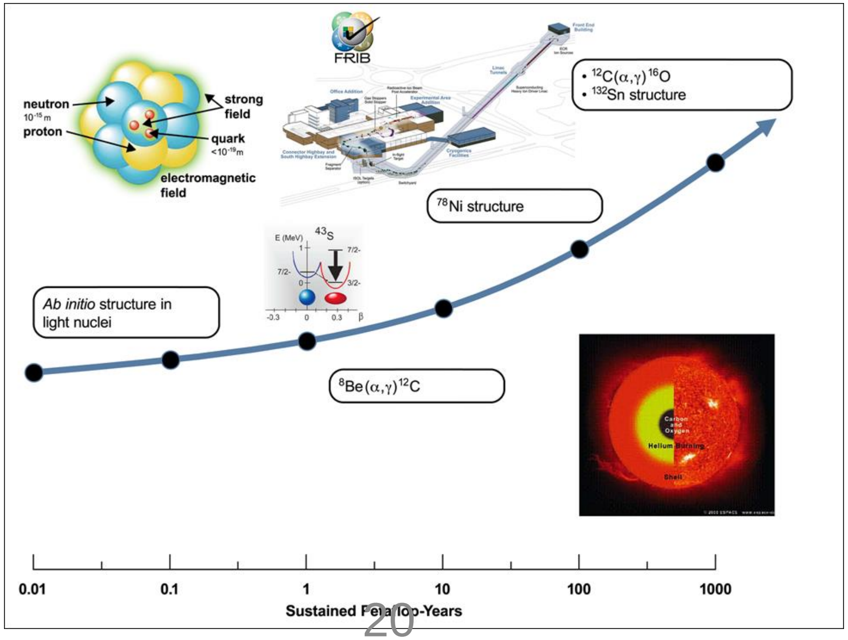
The crucial role of HPC





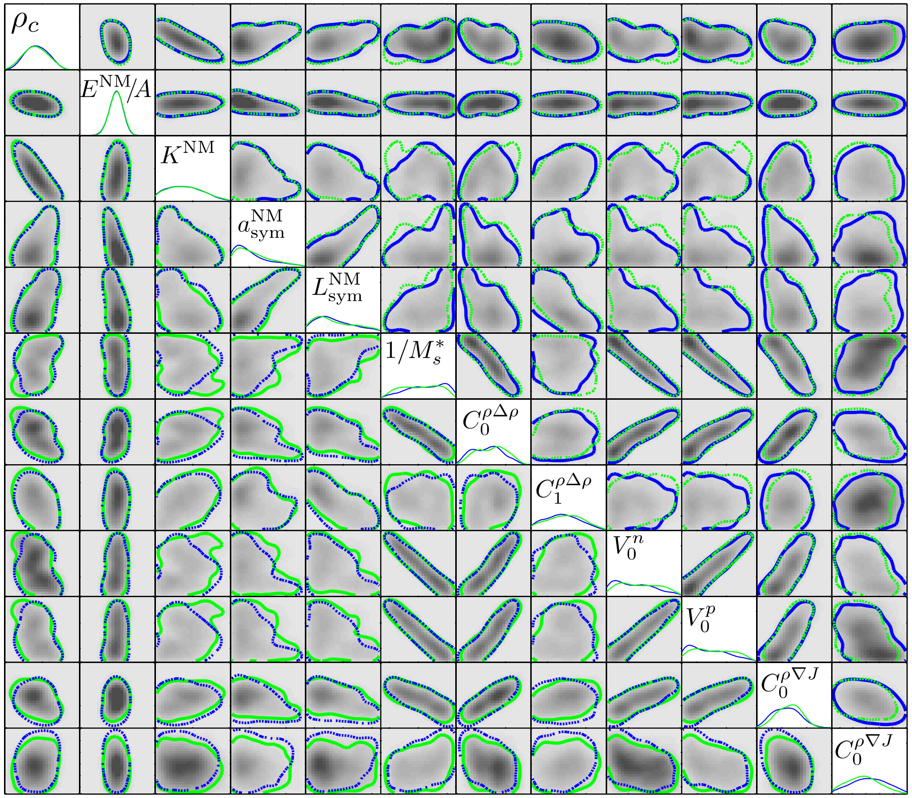
Towards predictive capability





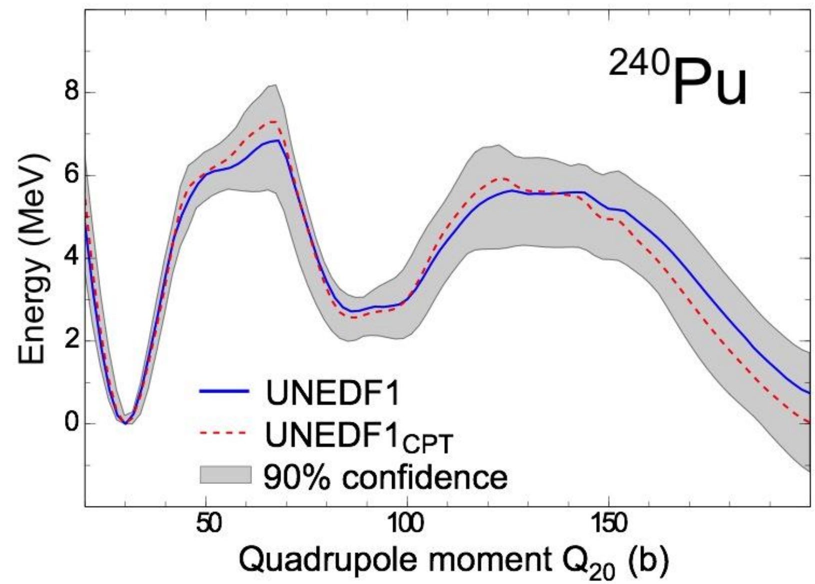
Information Content of New Measurements

J. McDonnell et al. Phys. Rev. Lett. 114, 122501 (2015)



Bivariate marginal estimates of the posterior distribution for the 12-dimensional DFT UNEDF$_1$ parameterization.

- Developed a Bayesian framework to quantify and propagate statistical uncertainties of EDFs.
- Showed that new precise mass measurements do not impose sufficient constraints to lead to significant changes in the current DFT models (models are not precise enough)



We can quantify the statement:
"New data will provide stringent constraints on theory"

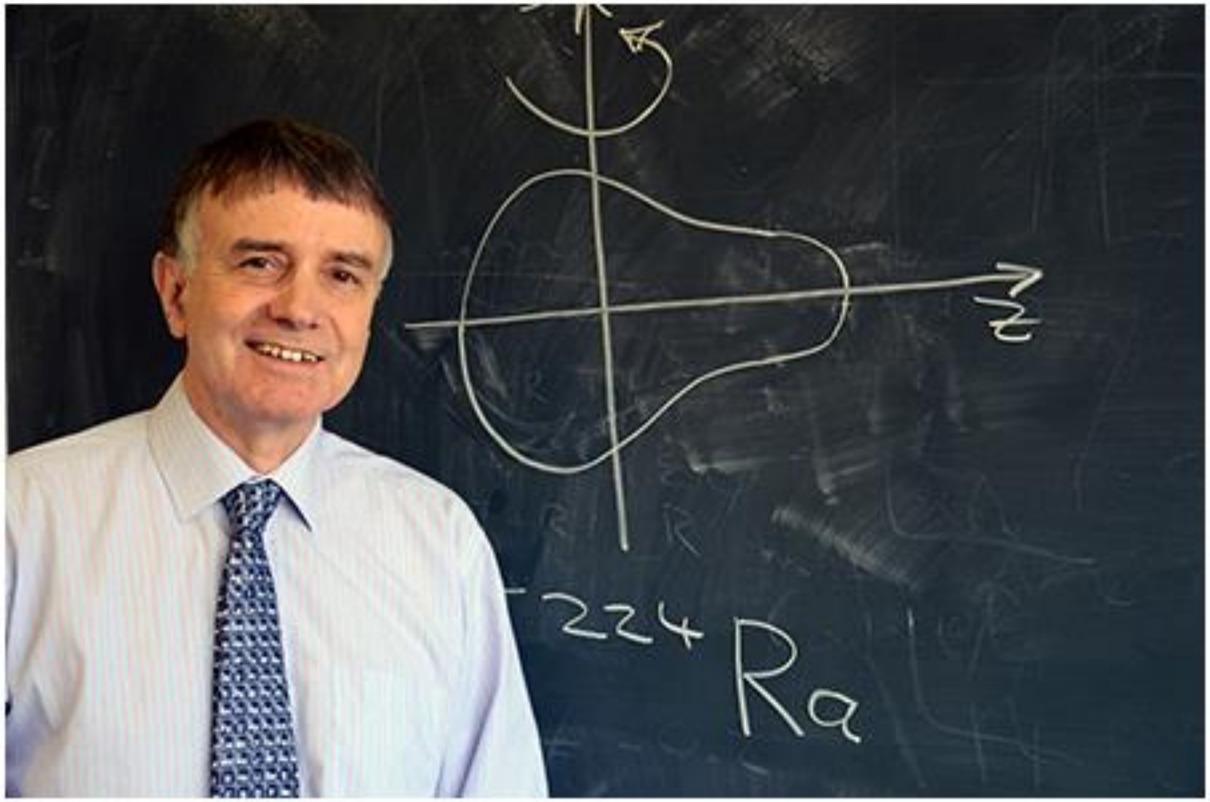
Summary (1): Challenges for LE Nuclear Theory

- 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
- Provide the microscopic underpinning of dynamical symmetries and simple patterns
- Develop predictive microscopic model of fusion and fission that will provide the missing data for astrophysics and energy research
- Carry out predictive and quantified calculations of nuclear matrix elements for fundamental symmetry tests in nuclei and for neutrino physics.

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

Scientists demonstrate pear shaped atomic nuclei



Professor Peter Butler: “Our findings contradict some nuclear theories and will help refine others”
(UoL News, May 9, 2013)

"I wish he'd been that lively when he was working."

Thank You!