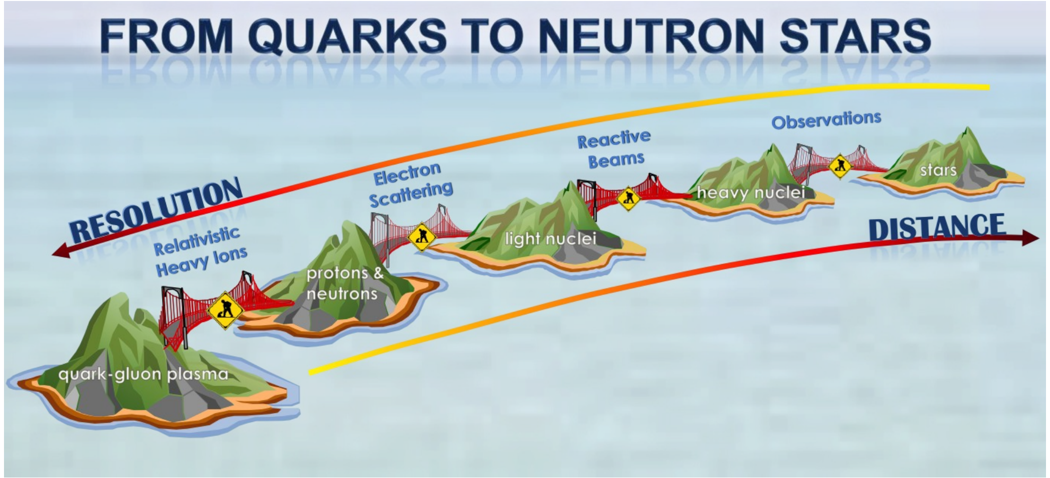
Nuclear structure III (theory)

Witek Nazarewicz (UTK/ORNL)

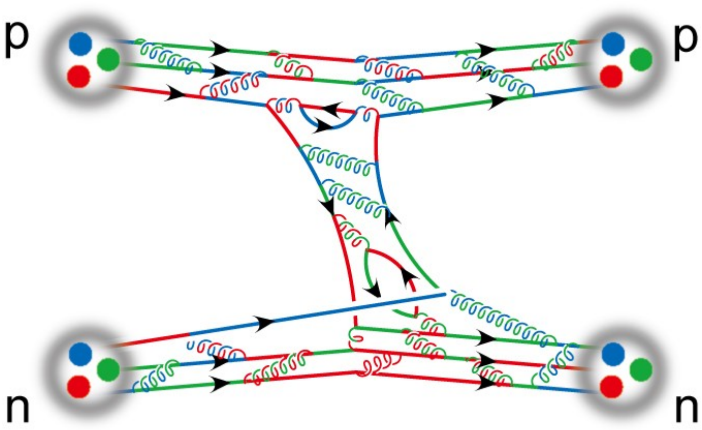
National Nuclear Physics Summer School 2014
William & Mary, VA

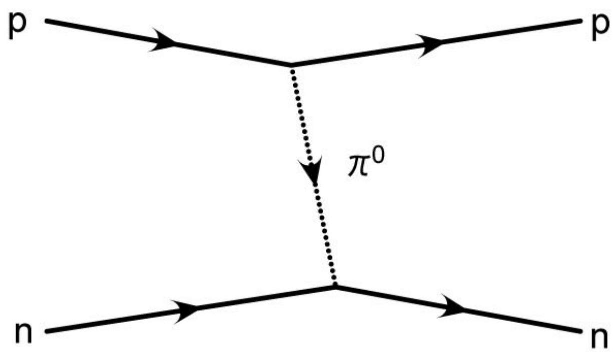
- Nuclear Force
- General principles
- Examples: quantitative nuclear theory; predictive capability
- Realities of high-performance



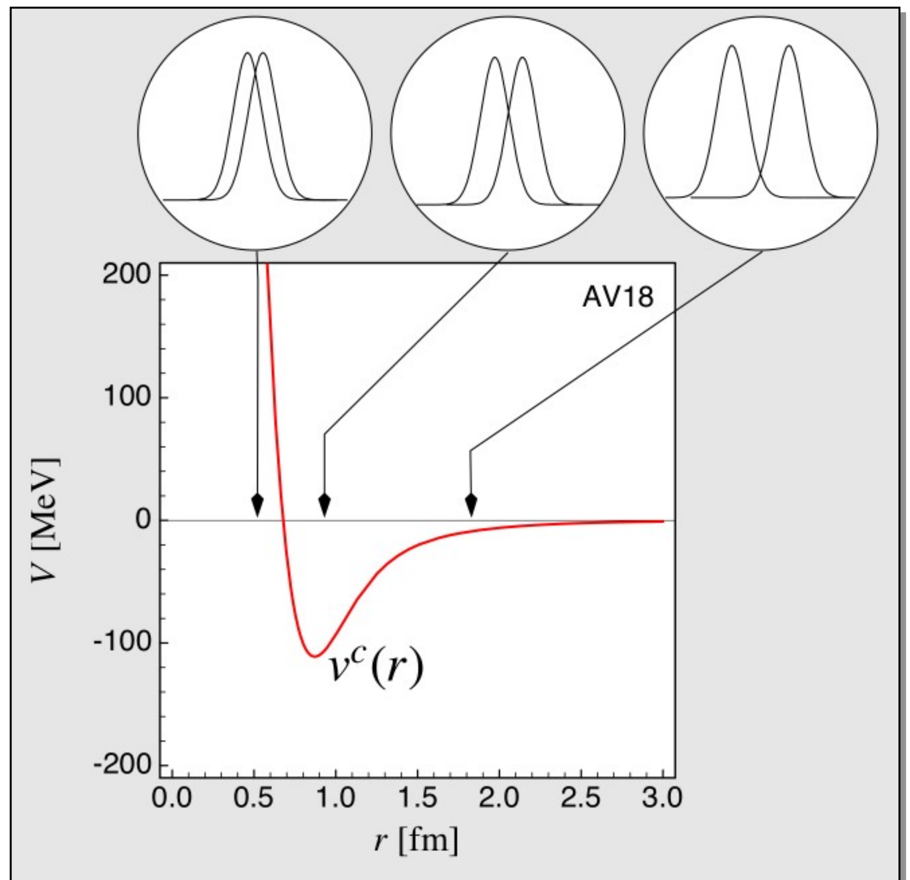
The Force

Nuclear force



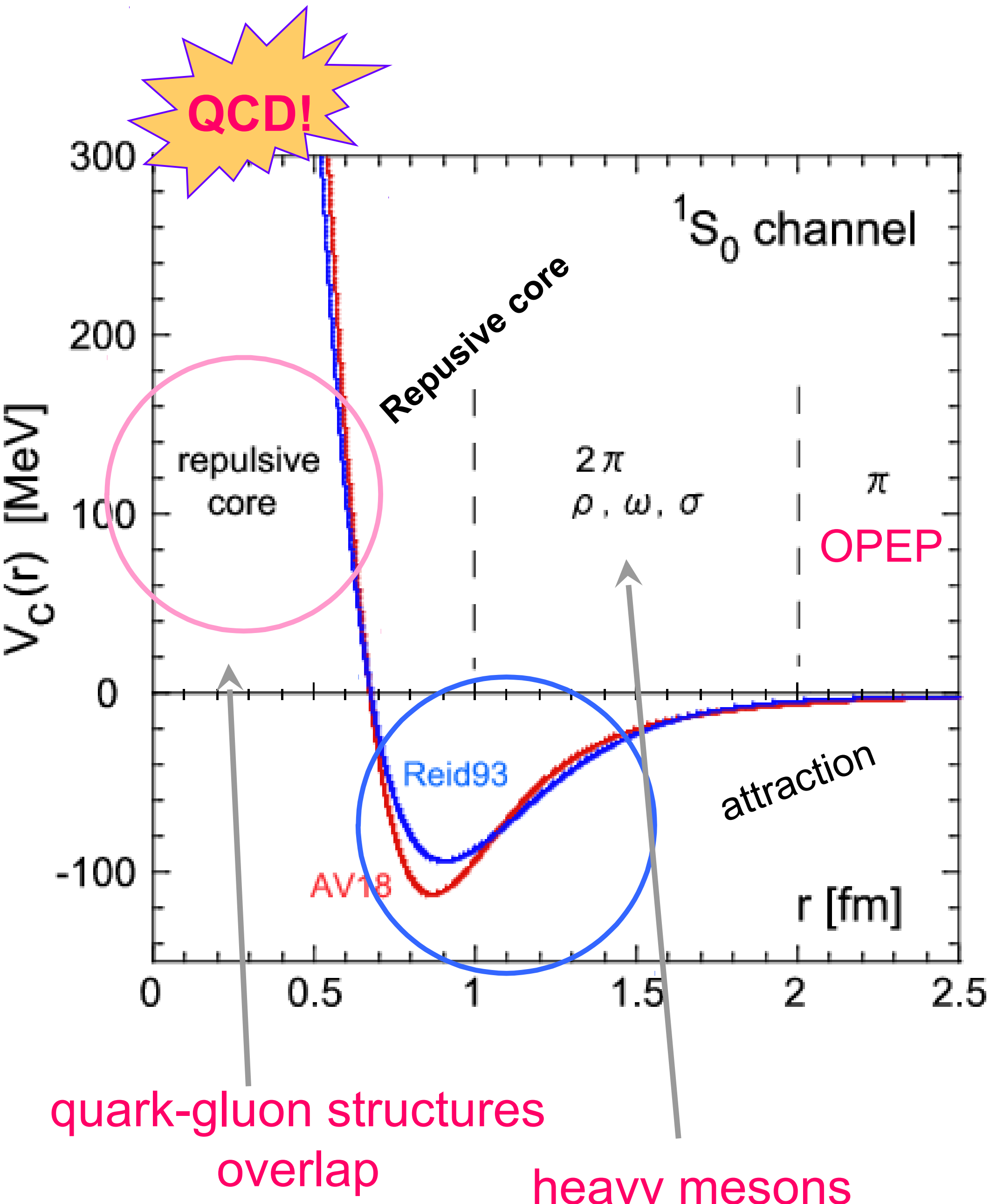


A realistic nuclear force force: schematic view



- Nucleon r.m.s. radius ~0.86 fm
- Comparable with interaction range
- Half-density overlap at max. attarction
- V_{NN} not fundamental (more like inter-molecular van der Waals interaction)
- Since nucleons are composite objects, three-and higher-body forces are expected.

Nucleon-Nucleon interaction (qualitative analysis)



There are infinitely many equivalent nuclear potentials!

$$\hat{H}\Psi = E\Psi$$

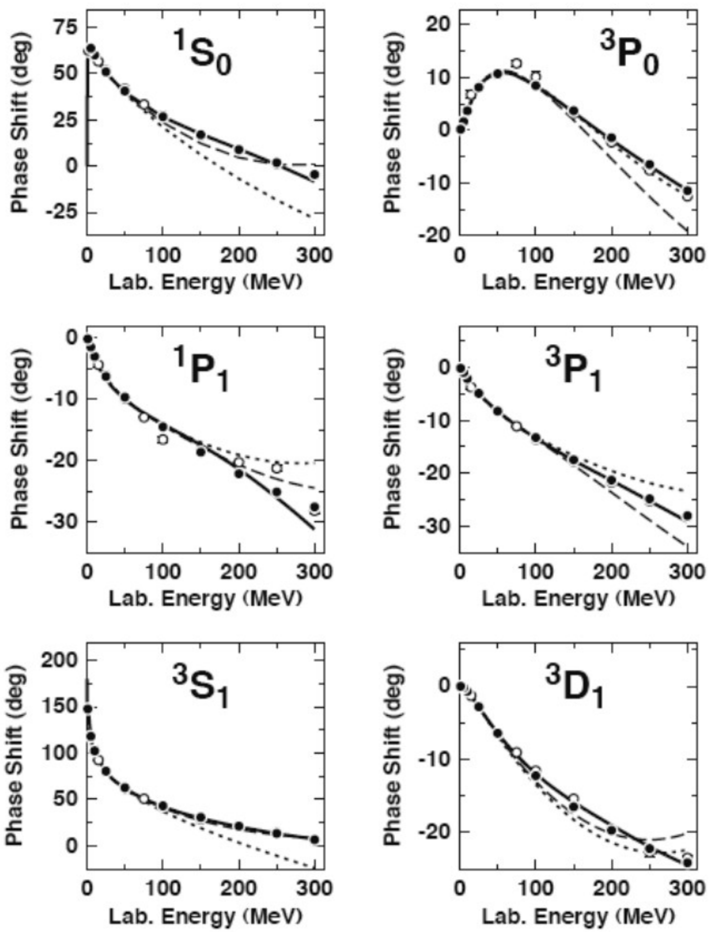
$$(\hat{U}\hat{H}\hat{U}^{-1})\hat{U}\Psi = E\hat{U}\Psi$$

Reid93 is from
V.G.J.Stoks et al., PRC**49**, 2950 (1994).

AV16 is from
R.B.Wiringa et al., PRC**51**, 38 (1995).

nucleon-nucleon interactions

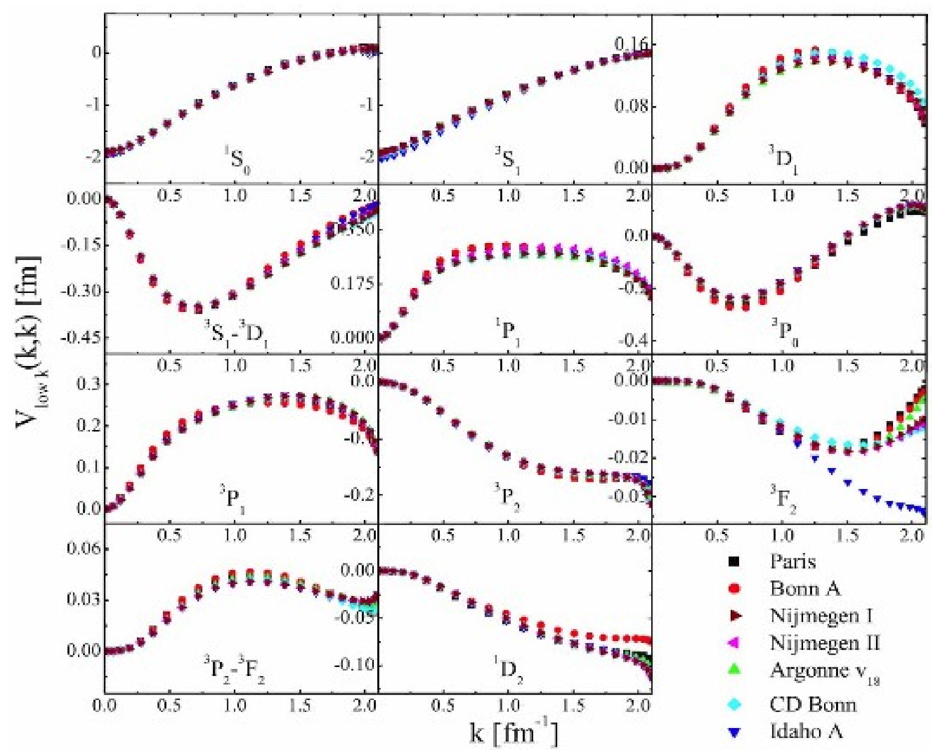
Effective-field theory potentials



N^3LO: Entem et al., PRC68, 041001 (2003)
Epelbaum, Meissner, et al.

Renormalization group (RG) evolved nuclear potentials

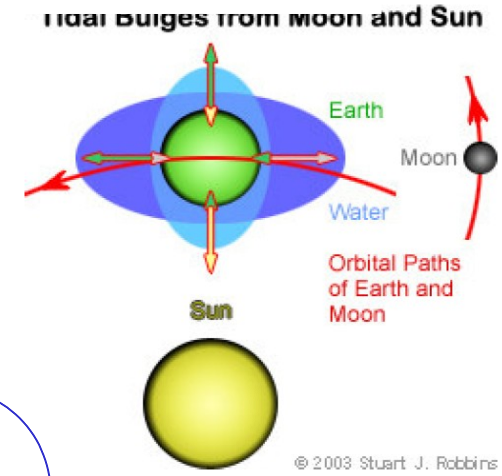
$V_{\text{low-k}}$ unifies NN interactions at low energy



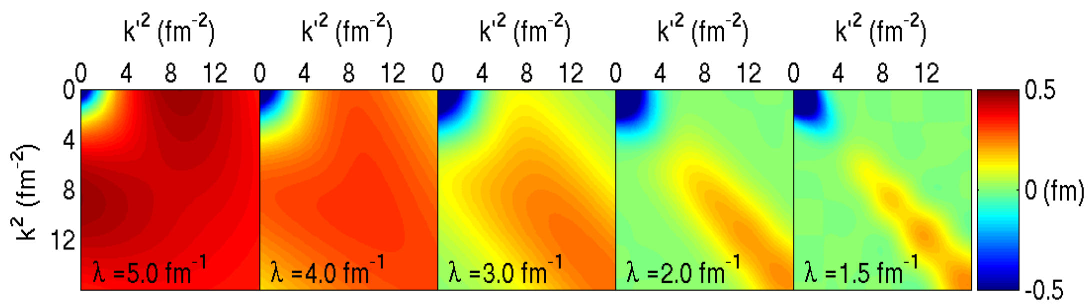
Bogner, Kuo, Schwenk, Phys. Rep. 386, 1 (2003)

three-nucleon interactions

Three-body forces between protons and neutrons are analogous to tidal forces: the gravitational force on the Earth is *not* just the sum of Earth-Moon and Earth-Sun forces (if one employs point masses for Earth, Moon, Sun)

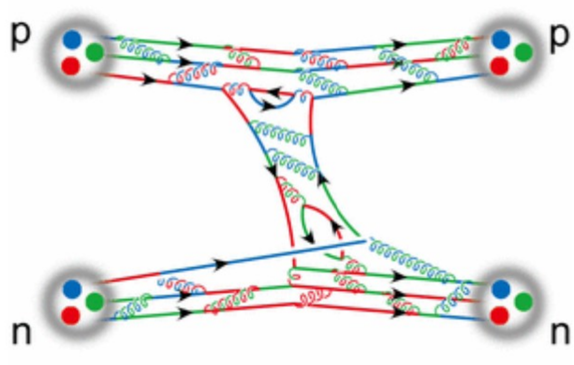


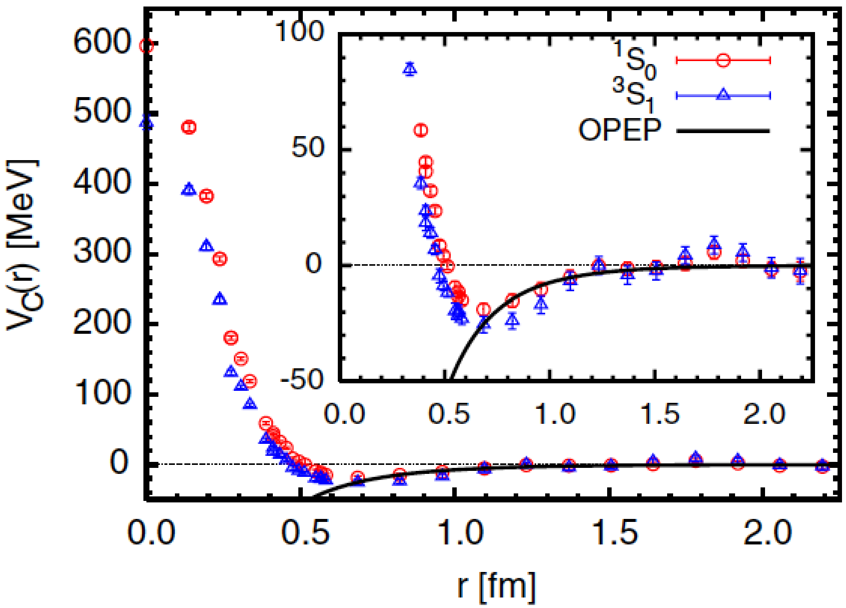
The computational cost of nuclear 3-body forces can be greatly reduced by decoupling low-energy parts from high-energy parts, which can then be discarded.



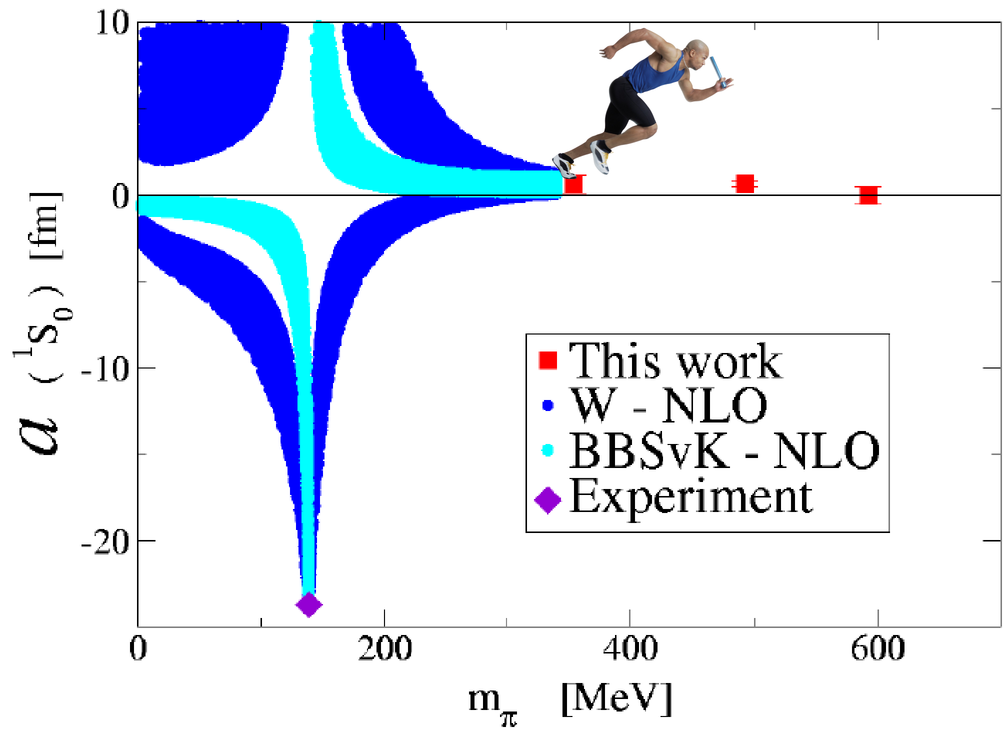
Recently the first consistent Similarity Renormalization Group softening of three-body forces was achieved, with rapid convergence in helium. With this faster convergence, calculations of larger nuclei are possible!

The challenge and the prospect: NN force





Ishii et al. PRL 99, 022001 (2007)



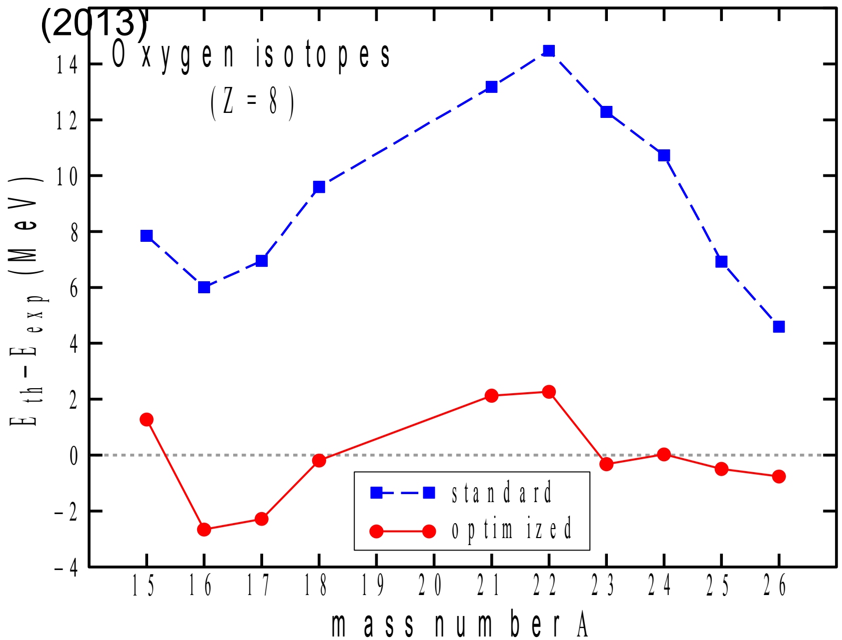
Beane et al. PRL 97, 012001 (2006)
and Phys. Rev. C 88, 024003 (2013)

Optimizing the nuclear force

input matters: garbage in, garbage out

- The derivative-free minimizer POUNDERS was used to systematically optimize NNLO chiral potentials
- The optimization of the new interaction $\mathrm{NNLO}_{\mathrm{opt}}$ yields a χ^2/datum ≈ 1 for laboratory NN 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
- Ongoing: Optimization of NN + 3NF

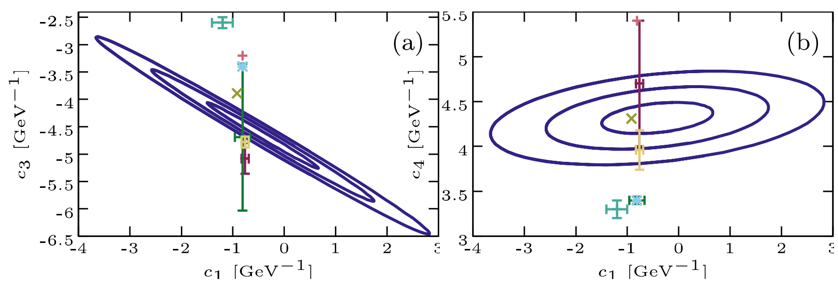
A. Ekström et al., Phys. Rev. Lett. 110, 192502 (2013)



http://science.energy.gov/np/highlights/2014/np-2014-05-e/

- Used a coarse-grained representation of the short-distance interactions with 30 parameters
- The optimization of a chiral interaction in NNLO yields a χ^2/datum ≈ 1 for a mutually consistent set of 6713 NN scattering data
- Covariance matrix yields correlation between LECCs and predictions with error bars.

Navarro Perez, Amaro, Arriola,
Phys. Rev. C 89, 024004 (2014) and
arXiv:1406.0625



	This work	Emp./Rec. [36–41]	δ she
E_d (MeV)	Input	2.224575(9)	In
η	0.02473(4)	0.0256(5)	0.02
A_S (fm$^{1/2}$)	0.8854(2)	0.8845(8)	0.88
r_m (fm)	1.9689(4)	1.971(6)	1.96
Q_D (fm^2)	0.2658(5)	0.2859(3)	0.26
P_D	5.30(3)	5.67(4)	5.62
$\langle r^{-1}\rangle$ (fm^{-1})	0.4542(2)		0.45

Deuteron, Light Nuclei

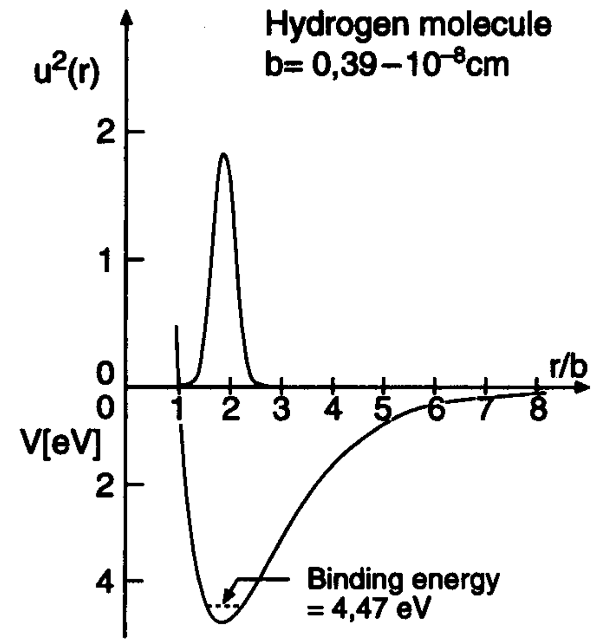
Deuteron

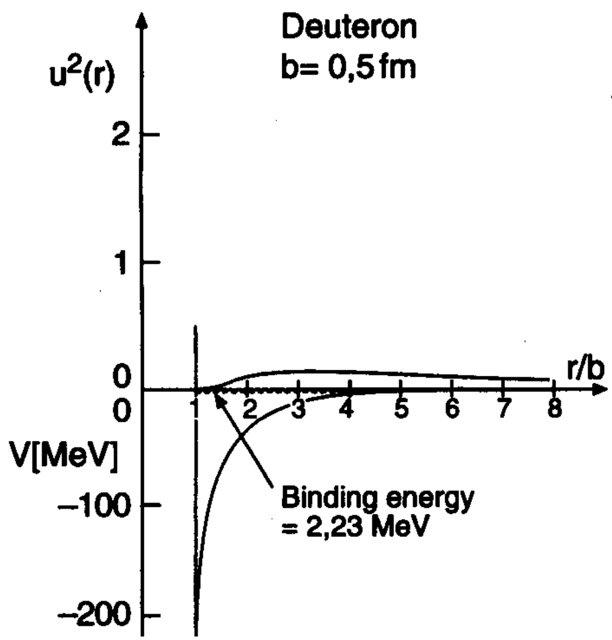
Binding energy	2.225 MeV
Spin, parity	1^+
Isospin	0
Magnetic moment	μ=0.857 μ_N
Electric quadrupole moment	Q=0.282 e fm^2

$$\mu_p + \mu_n = 2.792\mu_N - 1.913\mu_N = 0.879\mu_N$$

$$|\psi_d\rangle = 0.98\,|{}^3S_1\rangle + 0.20\,|{}^3D_1\rangle$$

produced by tensor force!





Nucleon-Nucleon Interaction

NN, NNN, NNNN,…, forces

GFMC calculations tell us that:

$$\langle V_\pi \rangle / \langle V \rangle \sim 70-80\%$$

$$\langle V_\pi \rangle \sim -15\,\mathrm{MeV/pair}$$

$$\langle V^R \rangle \sim -5\,\mathrm{MeV/pair}$$

ge

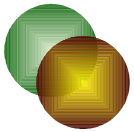
$$\langle V^3 \rangle \sim -1\,\mathrm{MeV/three}$$

dy

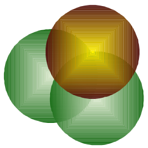
$$\langle T \rangle \sim 15\,\mathrm{MeV/nucleon}$$

$$\langle V_C \rangle \sim 0.66\,\mathrm{MeV/pair\ of\ protons}$$

Few-nucleon systems
(theoretical struggle)

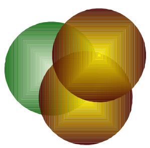


A=2: many years ago…

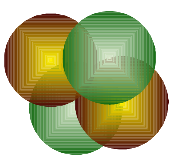


3H: 1984 (1% accuracy)

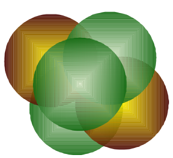
- **Faddeev**
- **Schroedinger**



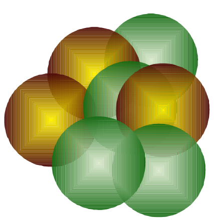
3He: 1987



4He: 1987



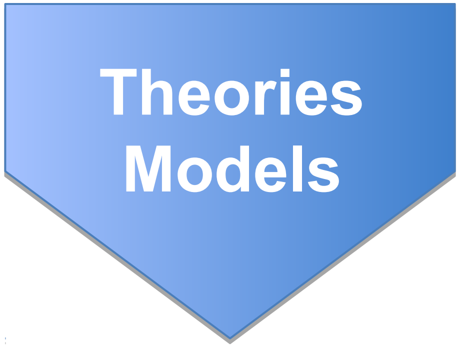
5He: 1994 (n-α resonance)



A=6,7,..12: 1995-2014

Happy the man who has been able to discern the cause of things

Virgil, Georgica



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

Alexander I. Kitaigorodskii

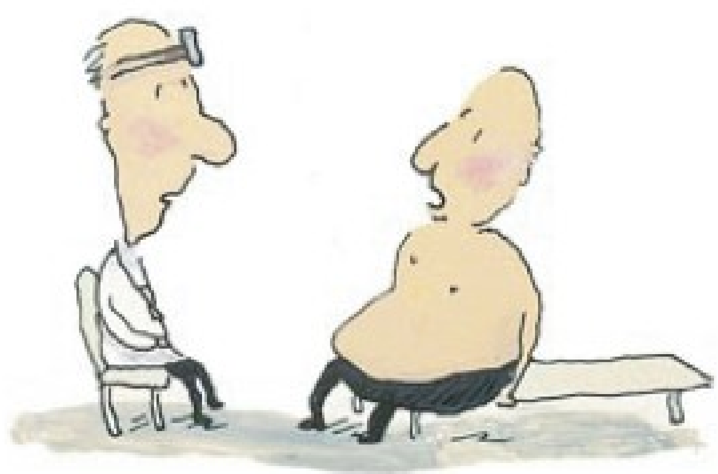
Weinberg's Laws of Progress in Theoretical Physics

From: "Asymptotic Realms of Physics" (ed. by Guth, Huang, Jaffe, MIT Press, 1983)

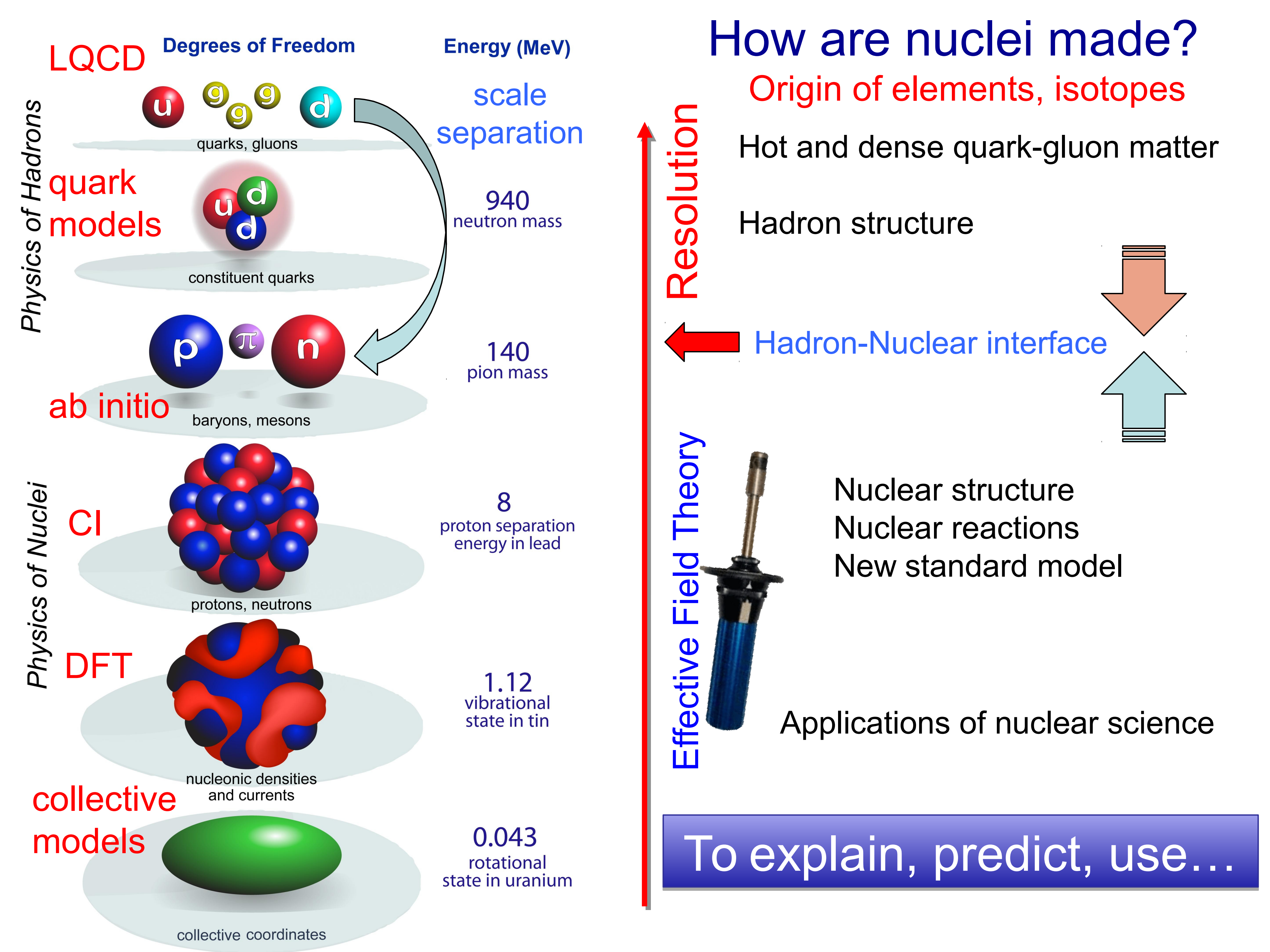
First Law: "The conservation of Information" (*You will get nowhere by churning equations*)

Second Law: "Do not trust arguments based on the lowest order of perturbation theory"

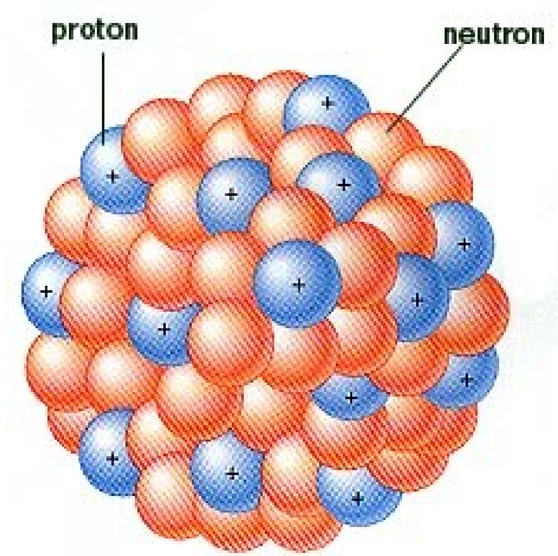
Third Law: "You may use any degrees of freedom you like to describe a physical system, but if you use the wrong ones, you'll be sorry!"



Patient: Doctor, doctor, it hurts when I do this!
Doctor: Then don't do that.


How are nuclei made?
Origin of elements, isotopes
LQCD
Degrees of Freedom
Energy (MeV)
quarks, gluons
scale separation
Physics of Hadrons
quark models
constituent quarks
940
neutron mass
ab initio
baryons, mesons
140
pion mass
Physics of Nuclei
CI
protons, neutrons
8
proton separation energy in lead
DFT
nucleonic densities and currents
1.12
vibrational state in tin
collective models
collective coordinates
0.043
rotational state in uranium
Resolution
Effective Field Theory
Hot and dense quark-gluon matter
Hadron structure
Hadron-Nuclear interface
Nuclear structure
Nuclear reactions
New standard model
Applications of nuclear science
To explain, predict, use…

Modeling the Atomic Nucleus

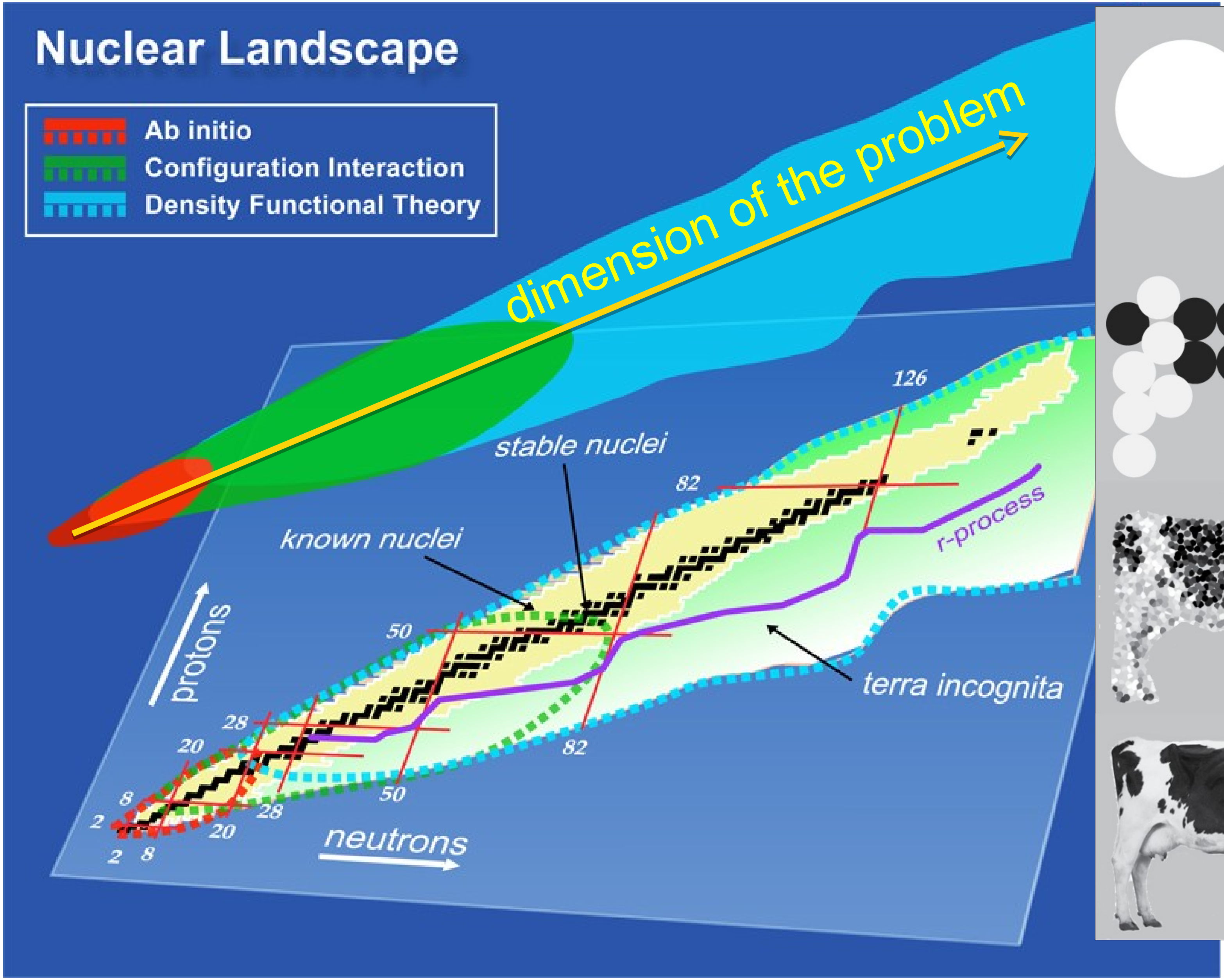


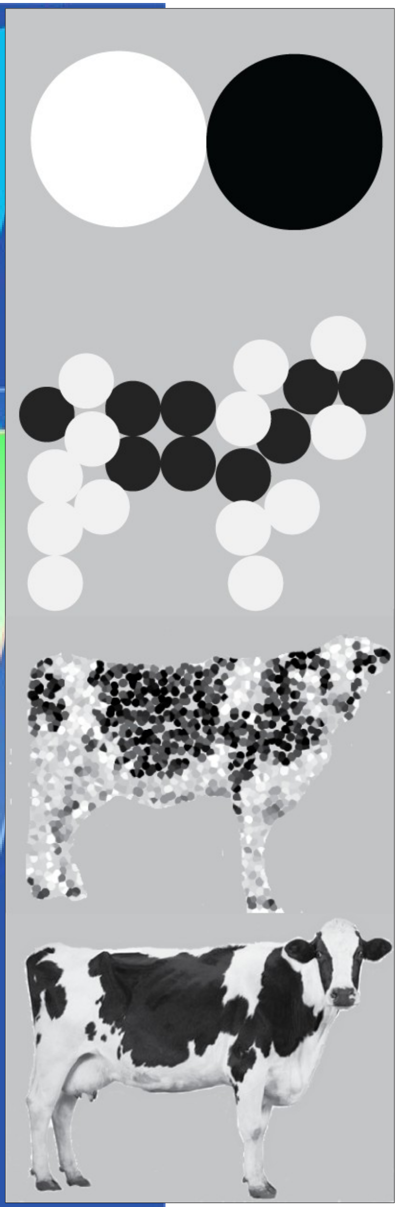
Theoretical bag of tricks…

The Nuclear Many-Body Problem

$$2^A \times \frac{A!}{N!Z!}$$ coupled integro-differential equations in 3A dimensions

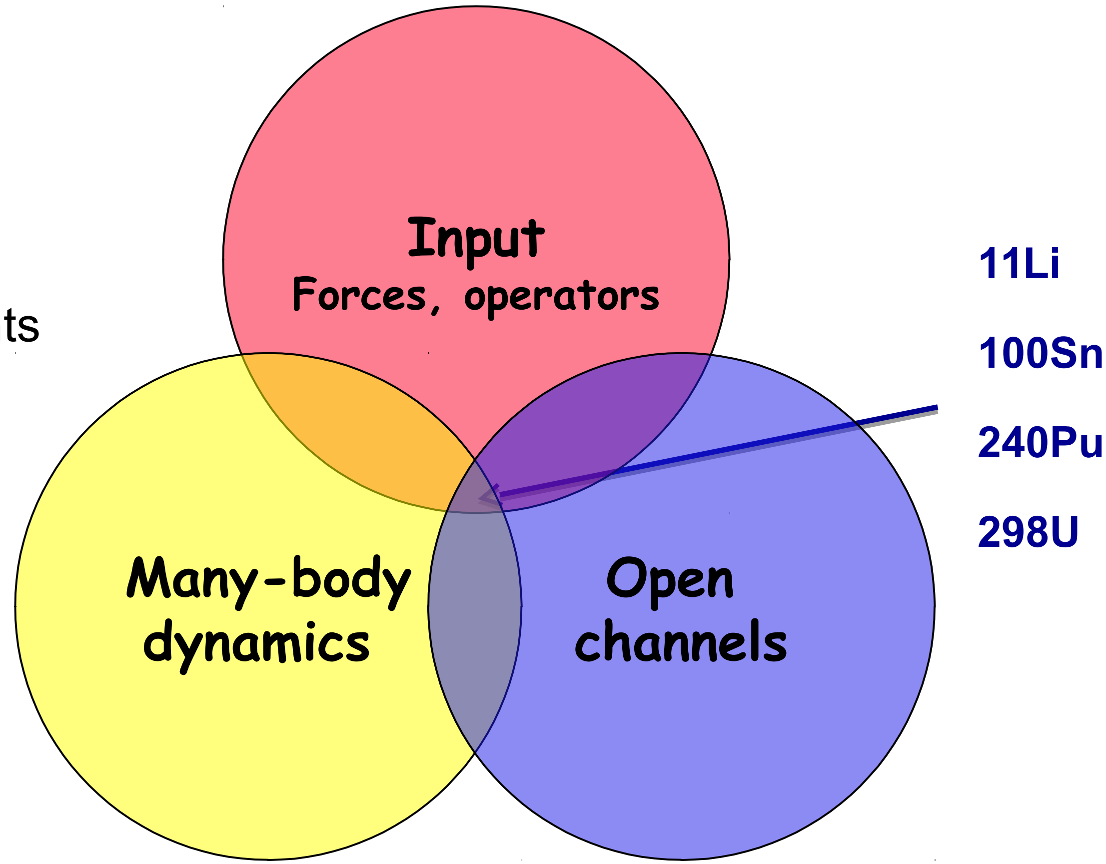
How to explain the nuclear landscape from the bottom up? **Theory roadmap**





Theory of nuclei is demanding

- rooted in QCD
- insights from EFT
- many-body interactions
- in-medium renormalization
- microscopic functionals
- low-energy coupling constants optimized to data
- crucial insights from exotic nuclei



- many-body techniques
  - direct *ab initio* schemes
  - symmetry breaking and restoration
- high-performance computing
- interdisciplinary connections

- nuclear structure impacted by couplings to reaction and decay channels
- clustering, alpha decay, and fission still remain major challenges for theory
- unified picture of structure and reactions

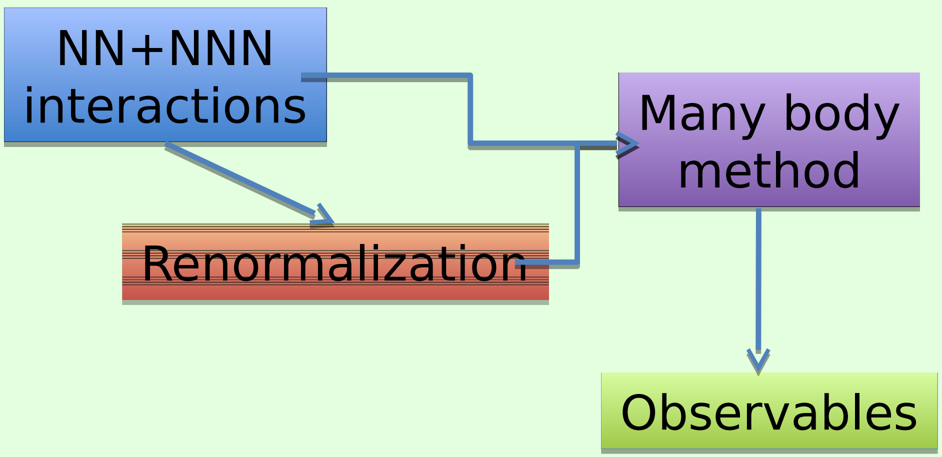
Illustrative physics examples

Ab initio theory for light nuclei and nuclear matter

Ab initio: QMC, NCSM, CCM,…

(nuclei, neutron droplets, nuclear matter)

Ab initio input



- Direct comparison with experiment
- Pseudo-data to inform theory

Input:

- Excellent forces based on the phase shift analysis and few-body data
- EFT based nonlocal chiral NN and NNN potentials
- SRG-softened potentials based on bare NN+NNN interactions

- Quantum Monte Carlo (GFMC) **12C**
- No-Core Shell Model **14F, 14C**
- Coupled-Cluster Techniques **17F, 56Ni, 61Ca**

Green's Function Monte Carlo (imaginary-time method)

$$|\psi_0\rangle = \lim_{\tau\to\infty} e^{-(\hat{H}-E_0)\tau}|\psi_V\rangle$$

Trial wave function

$$|\psi(\tau)\rangle = e^{-(\hat{H}-E_0)\tau}|\psi_V\rangle$$

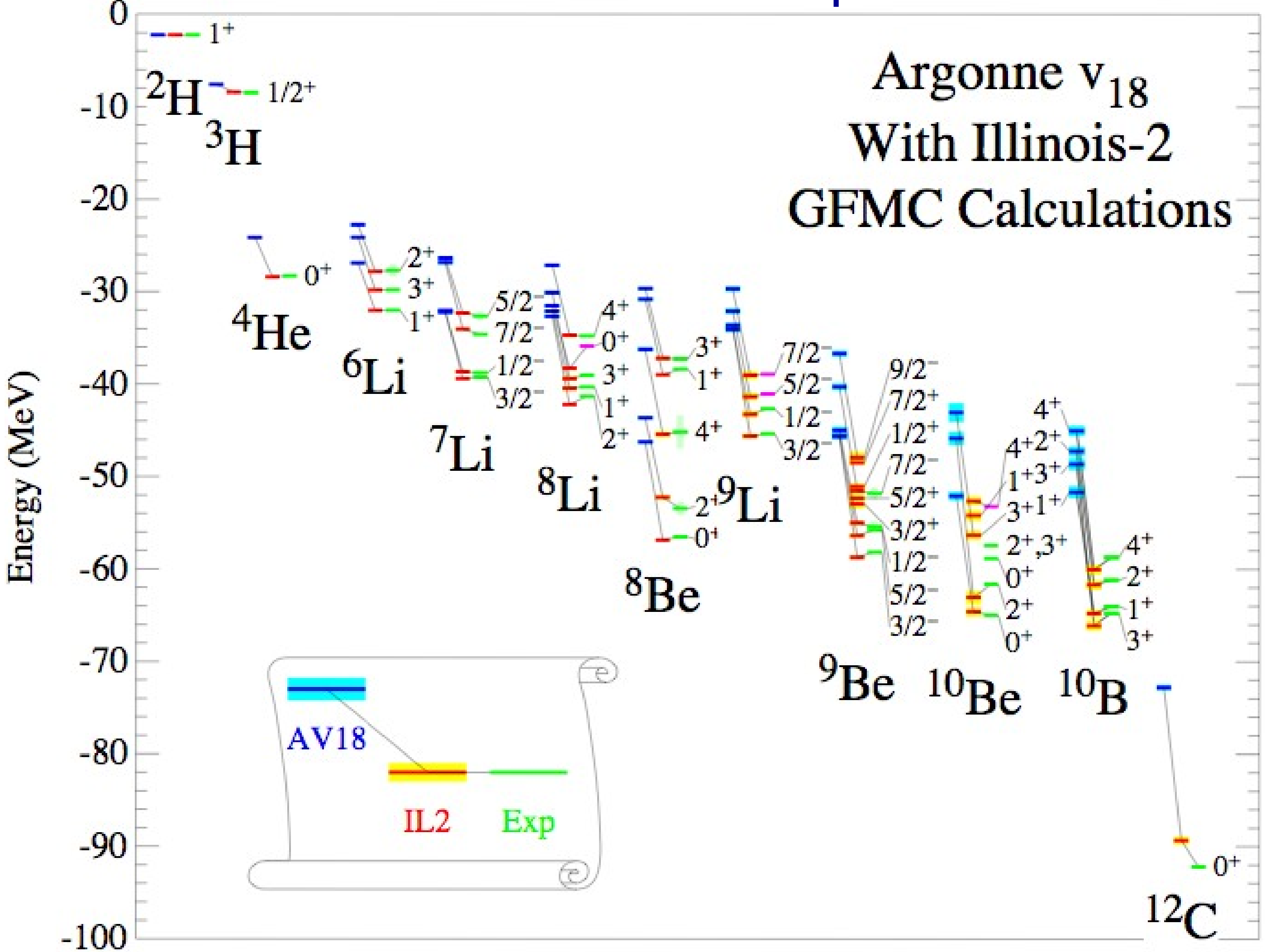
$$|\psi(0)\rangle = |\psi_V\rangle, \quad |\psi(\infty)\rangle = |\psi_0\rangle$$

$$\tau = n\Delta\tau \quad \Rightarrow \quad |\psi(\tau)\rangle = \left[e^{-(\hat{H}-E_0)\Delta\tau}\right]^n|\psi_V\rangle$$

Other methods:

- Faddeev-Yakubovsky method
- Hyperspherical harmonics method
- Coupled-cluster expansion method, exp(S)
- Cluster approaches (resonating group method)
- No-core shell model
- Lattice methods

Ab initio: Examples

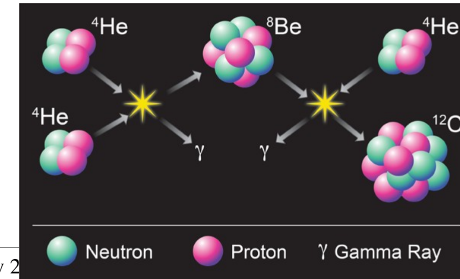


GFMC: S. Pieper, ANL

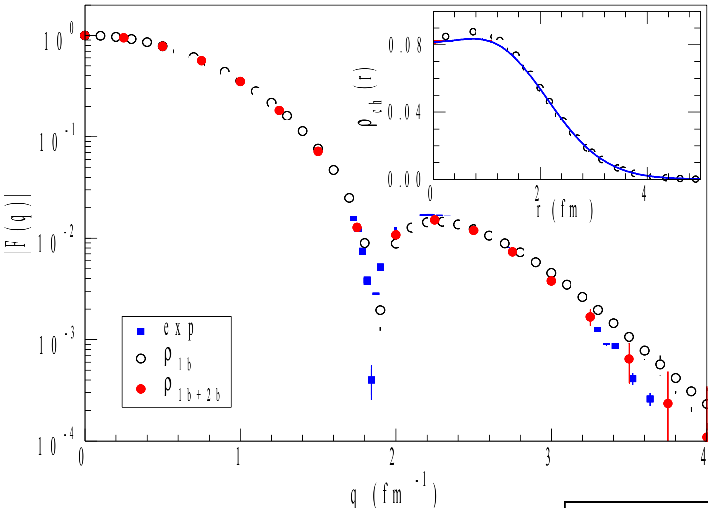
1-2% calculations of A = 6 – 12 nuclear energies are possible
excited states with the same quantum numbers computed

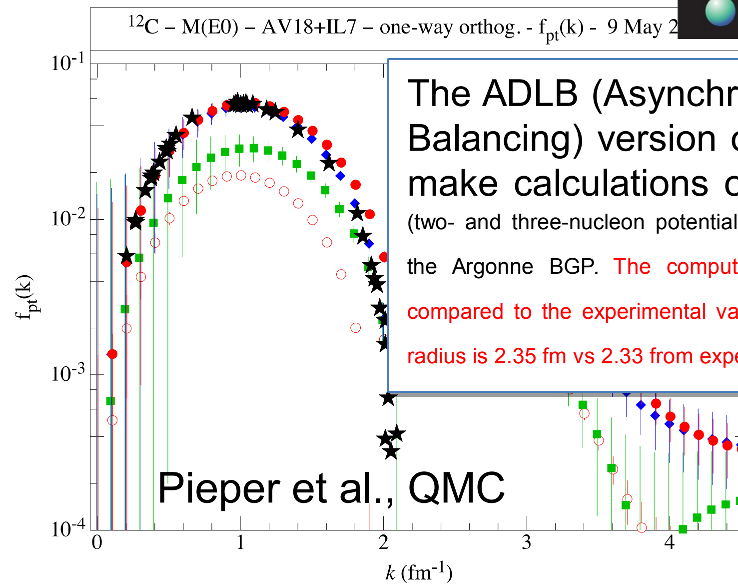
12C: ground state and Hoyle state

state-of-the-art computing

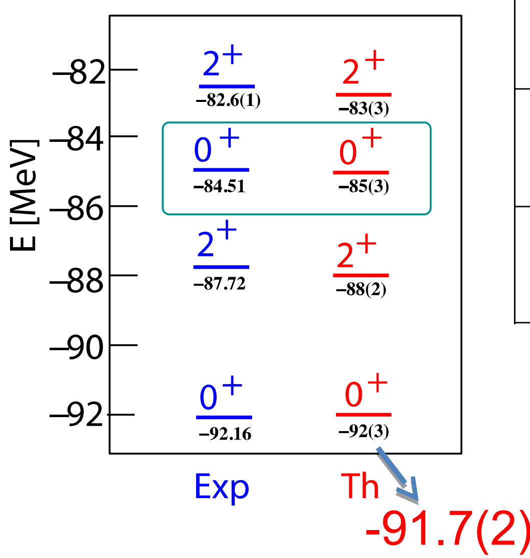


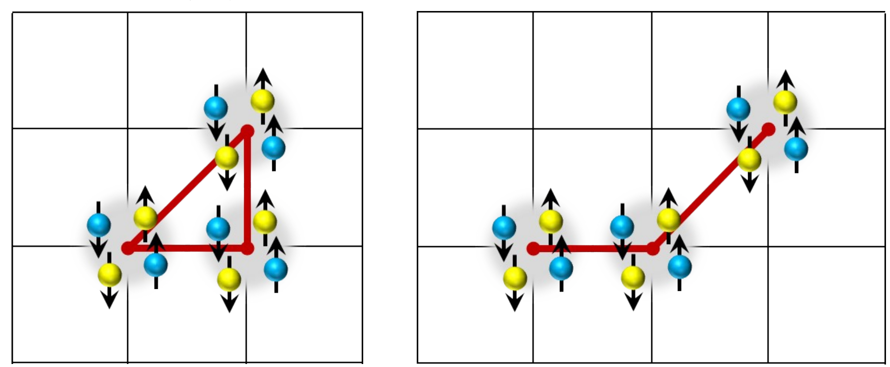
Wiringa et al. Phys. Rev. C 89, 024305 (2014); A. Lovato et al., Phys. Rev. Lett. 112, 182502 (2014)





The ADLB (Asynchronous Dynamic Load-Balancing) version of GFMC was used to make calculations of 12C with a complete Hamiltonian (two- and three-nucleon potential AV18+IL7) on 32,000 processors of the Argonne BGP. The computed binding energy is 93.5(6) MeV compared to the experimental value of 92.16 MeV and the point rms radius is 2.35 fm vs 2.33 from experiment.

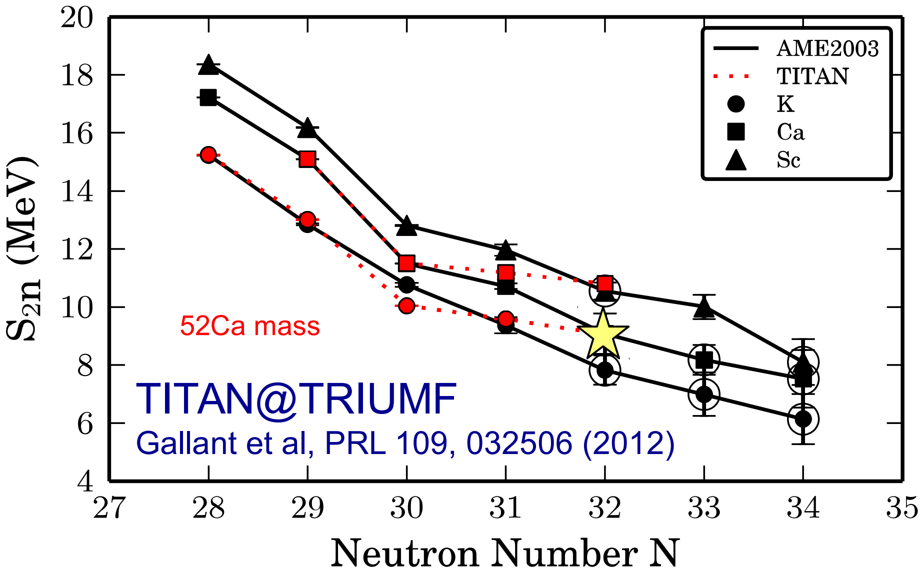




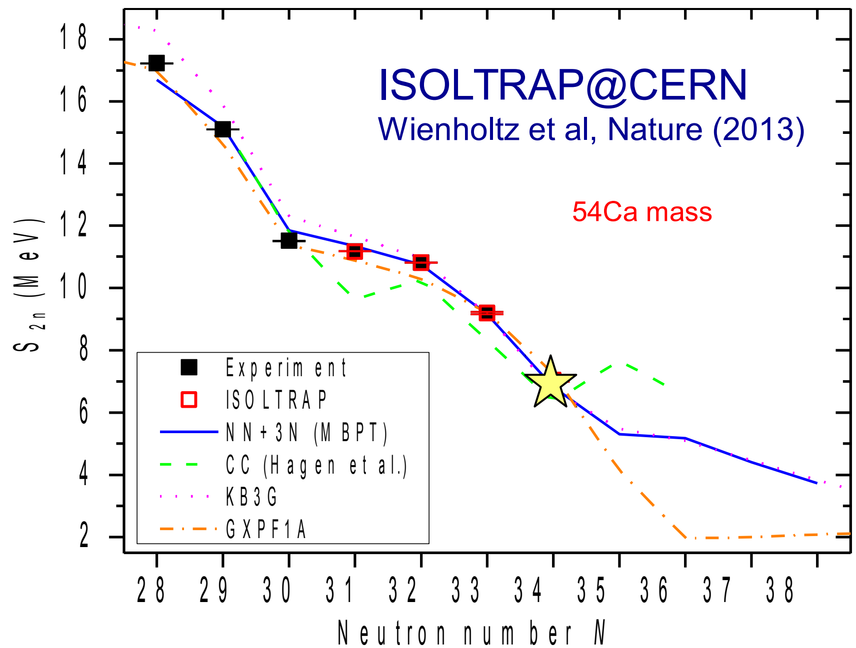
Epelbaum et al., Phys. Rev. Lett. 109, 252501 (2012). Lattice EFT
Lahde et al., Phys. Lett. B 732, 110 (2014).

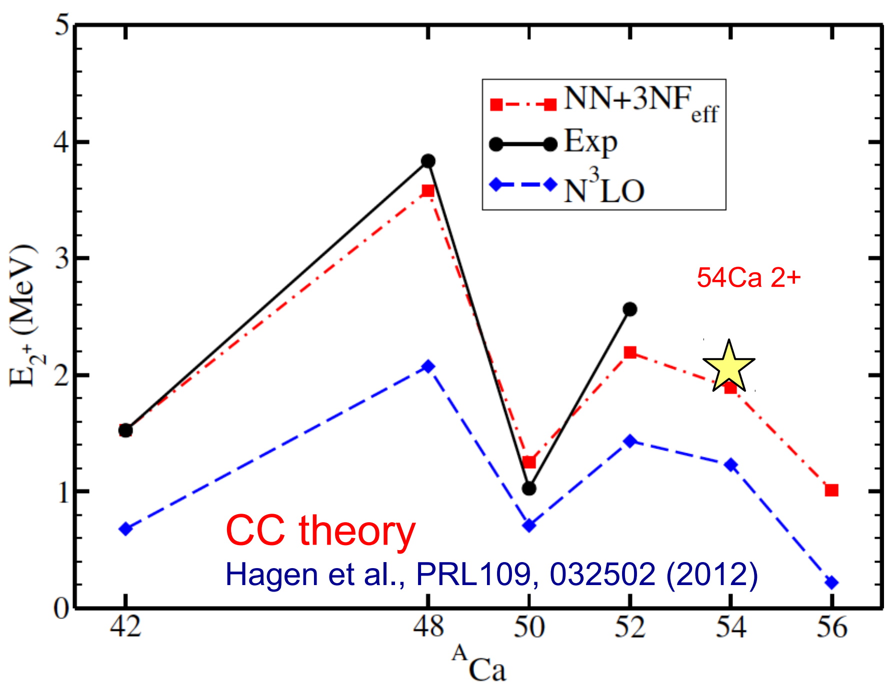
The frontier: neutron-rich calcium isotopes

probing nuclear forces and shell structure in a neutron-rich medium



54Ca: 20 protons, 34 neutrons

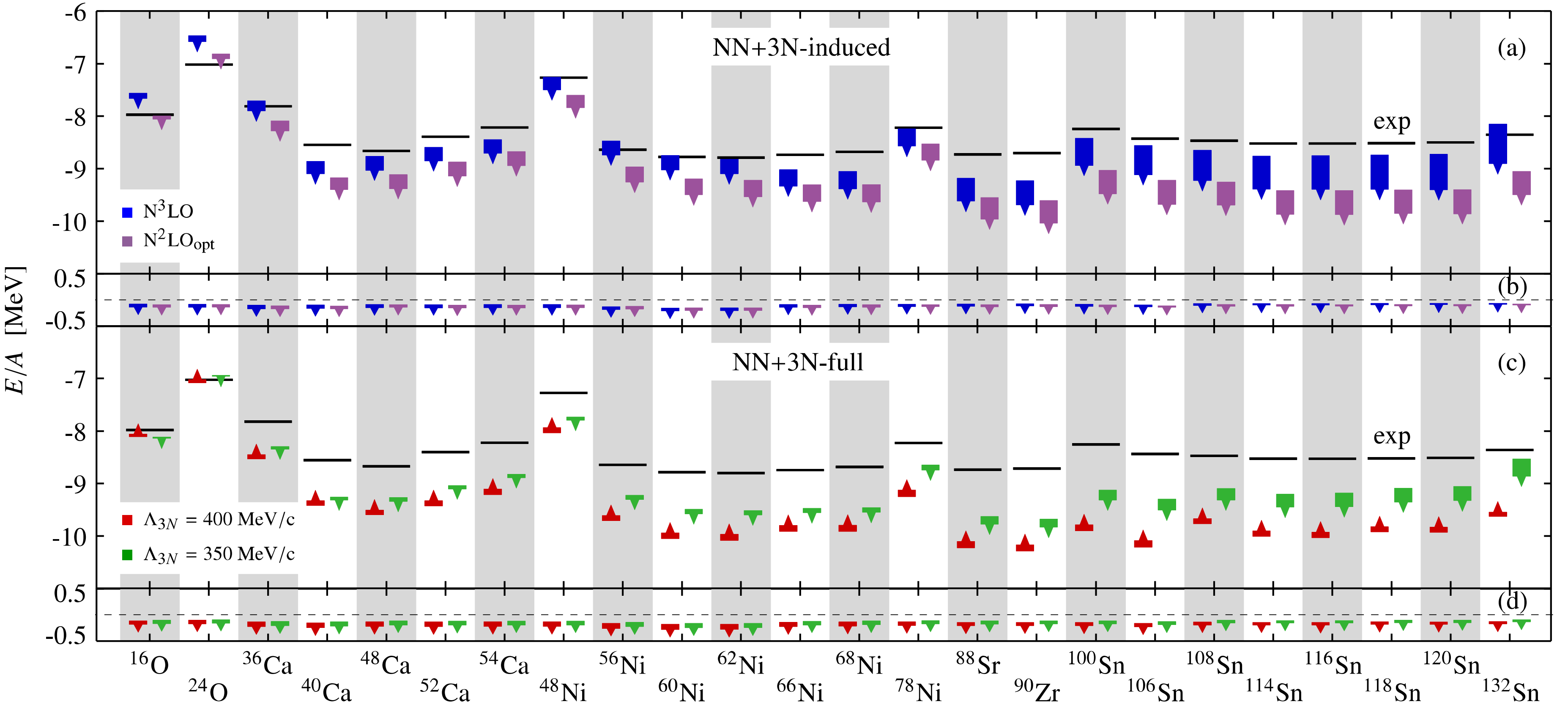




RIBF@RIKEN
Steppenbeck et al
Nature (2013)

Ab Initio Path to Heavy Nuclei

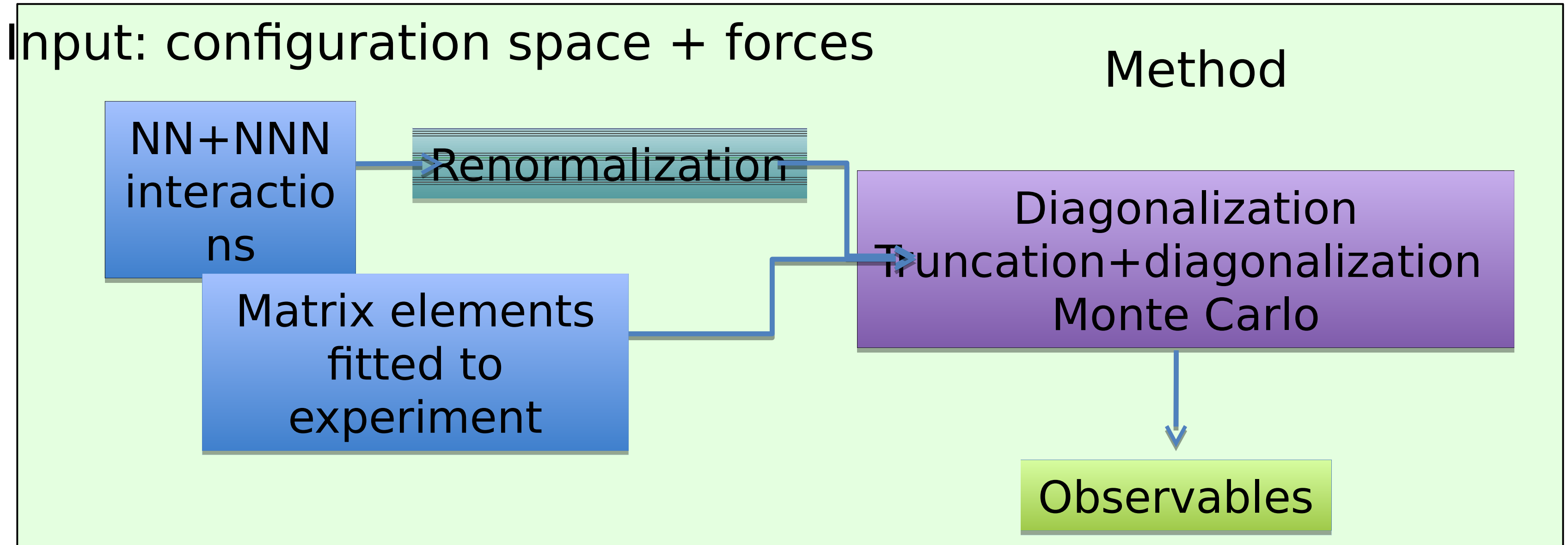
Binder et al., arXiv:1312.5685



- The first accurate ab initio cupled cluster calculations for heavy nuclei using *SRG-evolved chiral interactions*. A number of technical hurdles eliminated
- Many-body calculations up to 132Sn are now possible with controlled uncertainties on the order of 2%
- A first direct validation of chiral Hamiltonians in the regime of heavy nuclei using ab initio techniques.
- Future studies will have to involve consistent chiral Hamiltonians at N3LO considering initial and SRG-induced 4N interactions and provide an exploration of other observables.

Configuration interaction techniques

- light and heavy nuclei
- detailed spectroscopy
- quantum correlations (lab-system description)



- Direct comparison with experiment
- Pseudo-data to inform reaction theory and DFT

Nuclear shell model

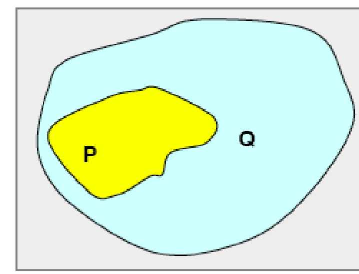
$$\hat{H} = \sum_i t_i + \tfrac{1}{2}\sum_{\substack{i,j \\ i\neq j}} v_{ij} = \sum_i (t_i + V_i) \quad + \quad \left[\tfrac{1}{2}\sum_{\substack{i,j \\ i\neq j}} v_{ij} - \sum_i V_i \right]$$

One-body Hamiltonia n

Residual interactioni

- Construct basis states with good (J_{z}, T_{z}) or (J,T)
- Compute the Hamiltonian matrix
- Diagonalize Hamiltonian matrix for lowest eigenstates
- Number of states increases dramatically with particle number

$$P + Q = 1$$

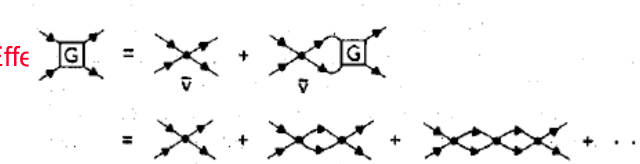


$$\text{Full } fp \text{ shell for } {}^{60}\text{Zn}: \quad \approx 2\times 10^{9}\ J_z \text{ states}$$

$$5,053,594 \qquad J = 0, T = 0 \text{ states}$$

$$81,804,784 \quad J = 6, T = 1 \text{ states}$$

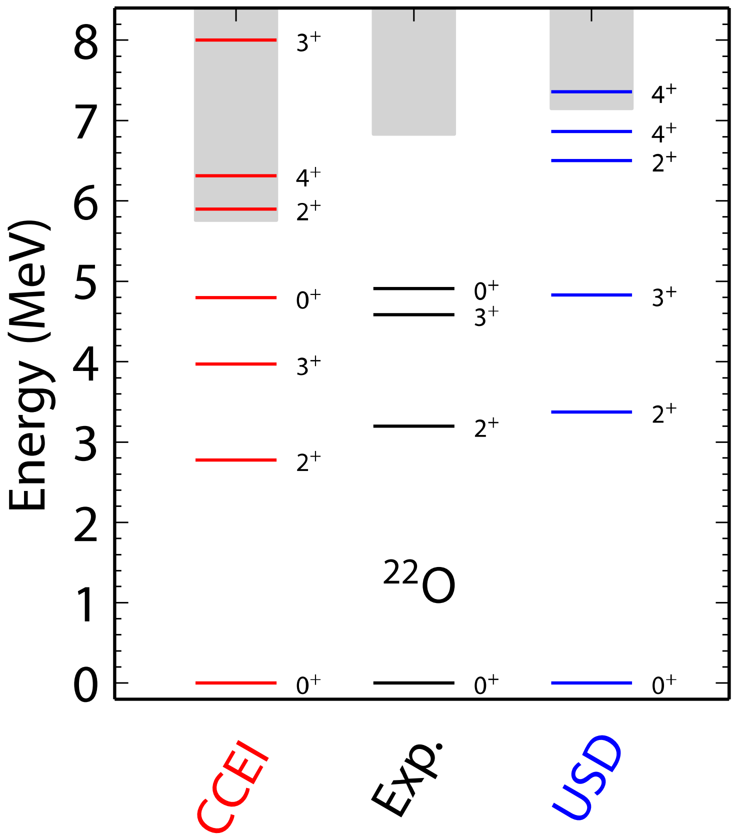
- Can we get around this problem? Effective interactions in truncated spaces (P-included, finite; Q-excluded, infinite)
- Residual interaction (G-matrix) depends on the configuration space. Effe
- Breaks down around particle drip lines



G-matrix, obtained from the Bethe-Goldstone equation (scattering within a nuclear medium)

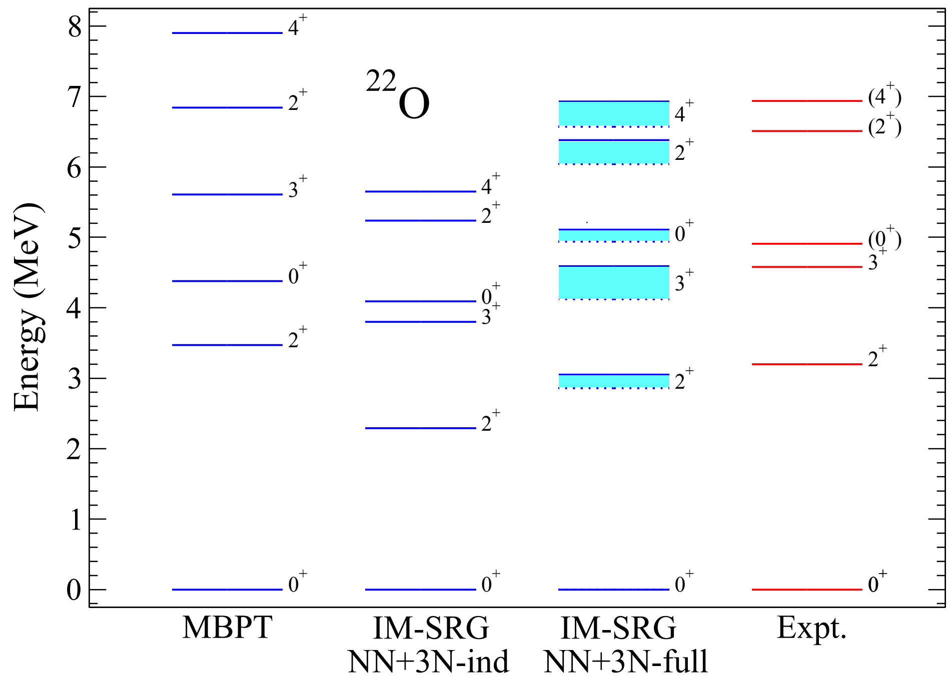
Microscopic valence-space Shell Model Hamiltonian

Coupled Cluster Effective Interaction (valence cluster expansion)



G.R. Jansen et al., arXiv:1402.2563

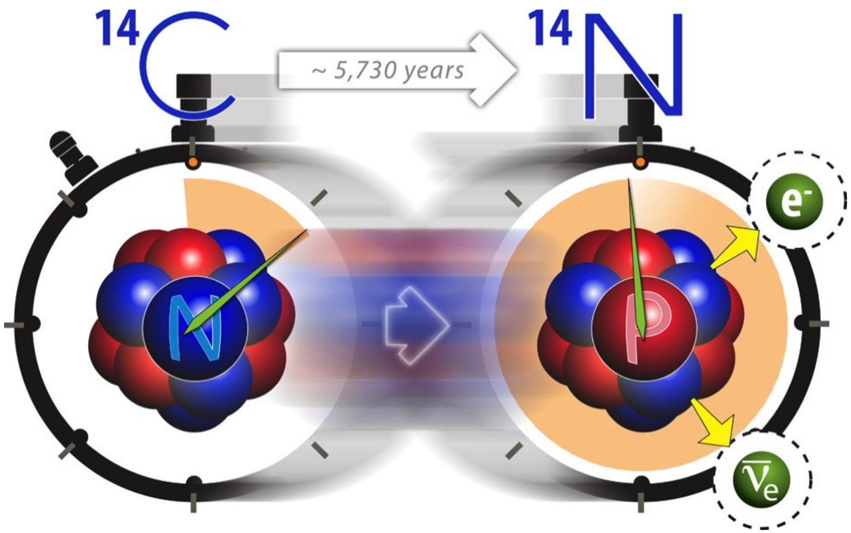
In-medium SRG Effective Interaction

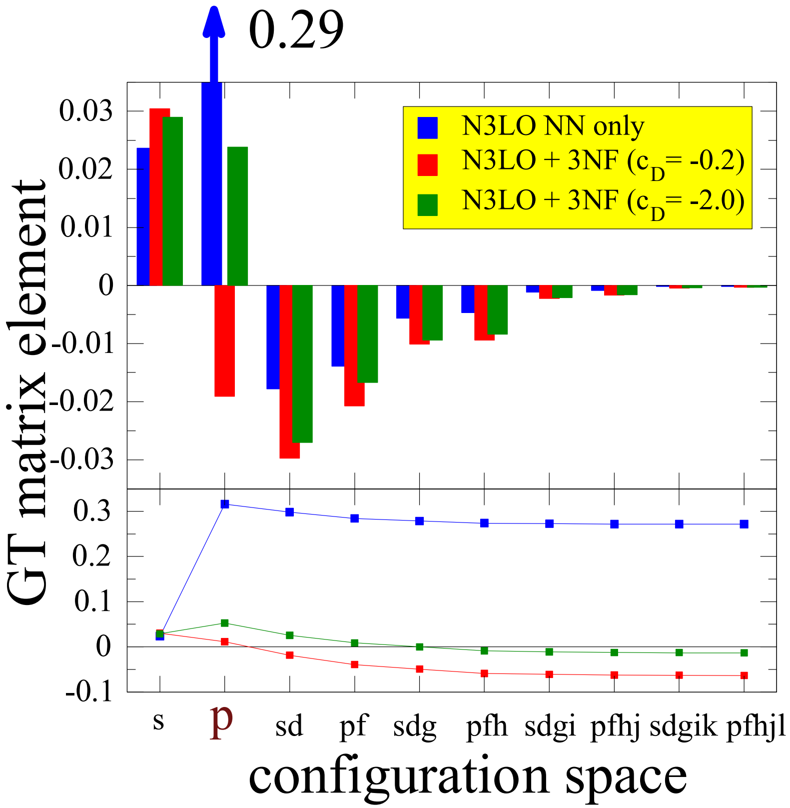


S.K. Bogner et al., arXiv:1402.1407

Anomalous Long Lifetime of ^{14}C

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





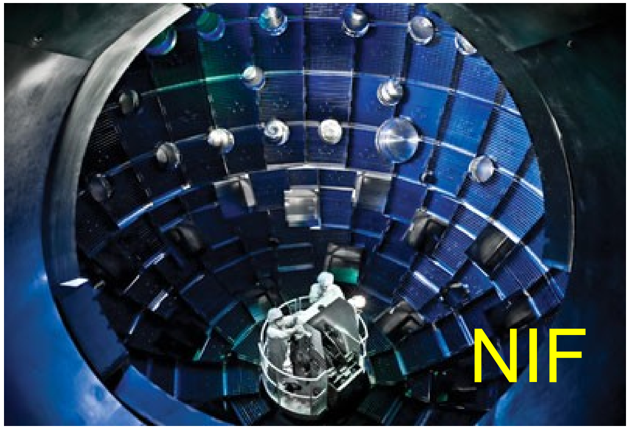
Maris et al., PRL 106, 202502 (2011)

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

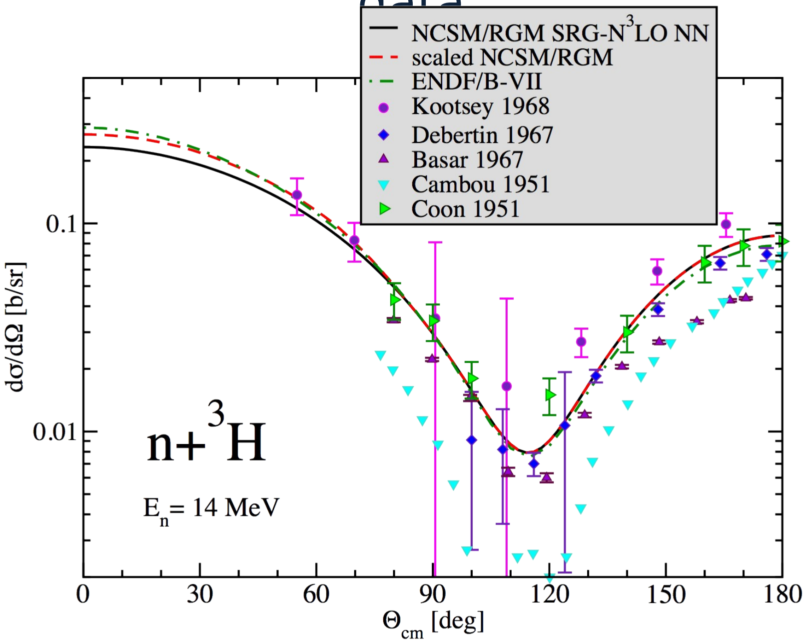
Solution took ~ 6 hours on 215,000 cores on Cray XT5 Jaguar at ORNL

Fusion of Light Nuclei

Computational nuclear physics enables us to reach into regimes where <u>experiments and analytic theory are not possible</u>, such as the cores of fission reactors or hot and dense evolving environments such as those found in inertial confinement fusion environment.

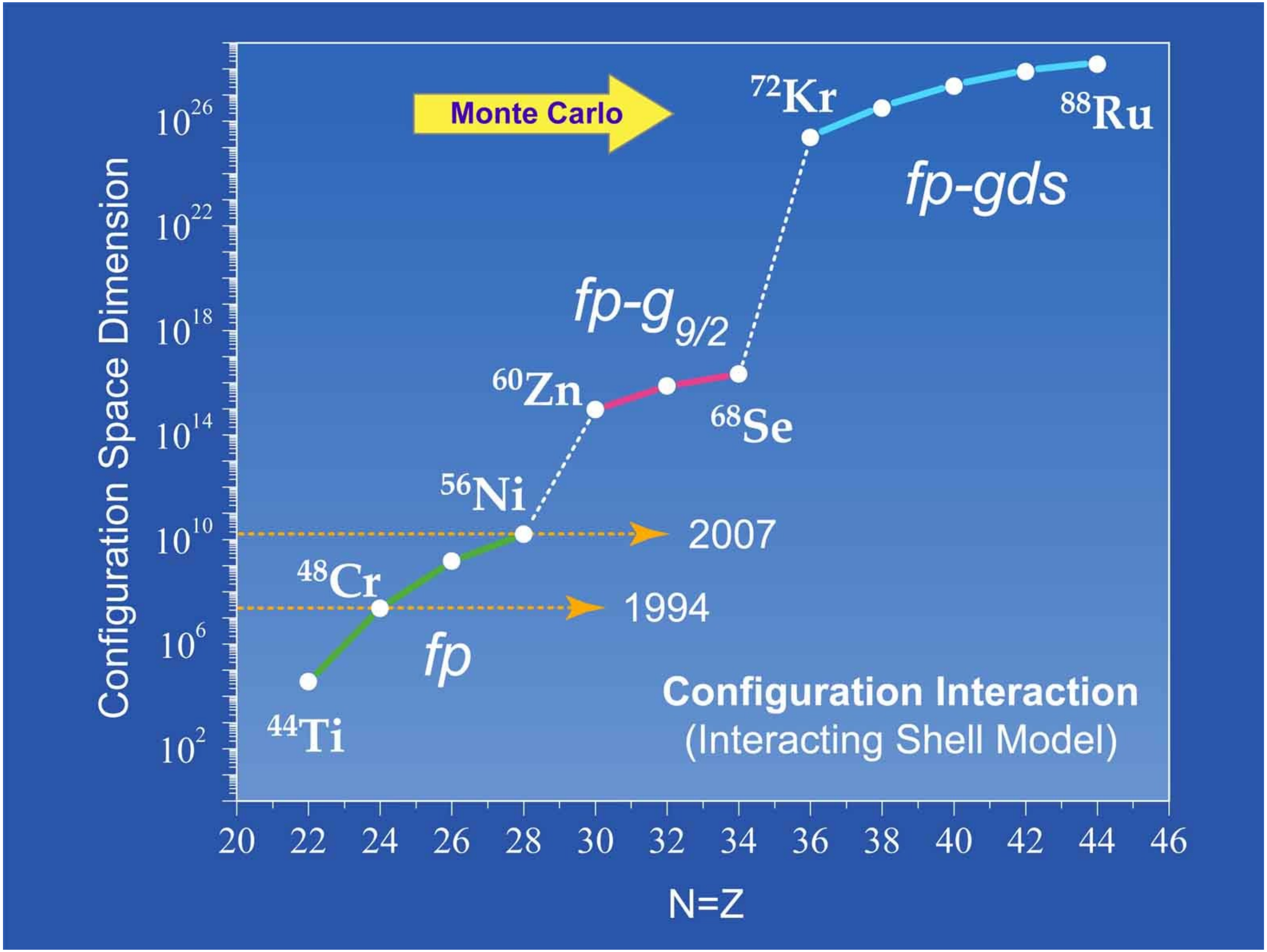


Ab initio theory reduces uncertainty due to conflicting data



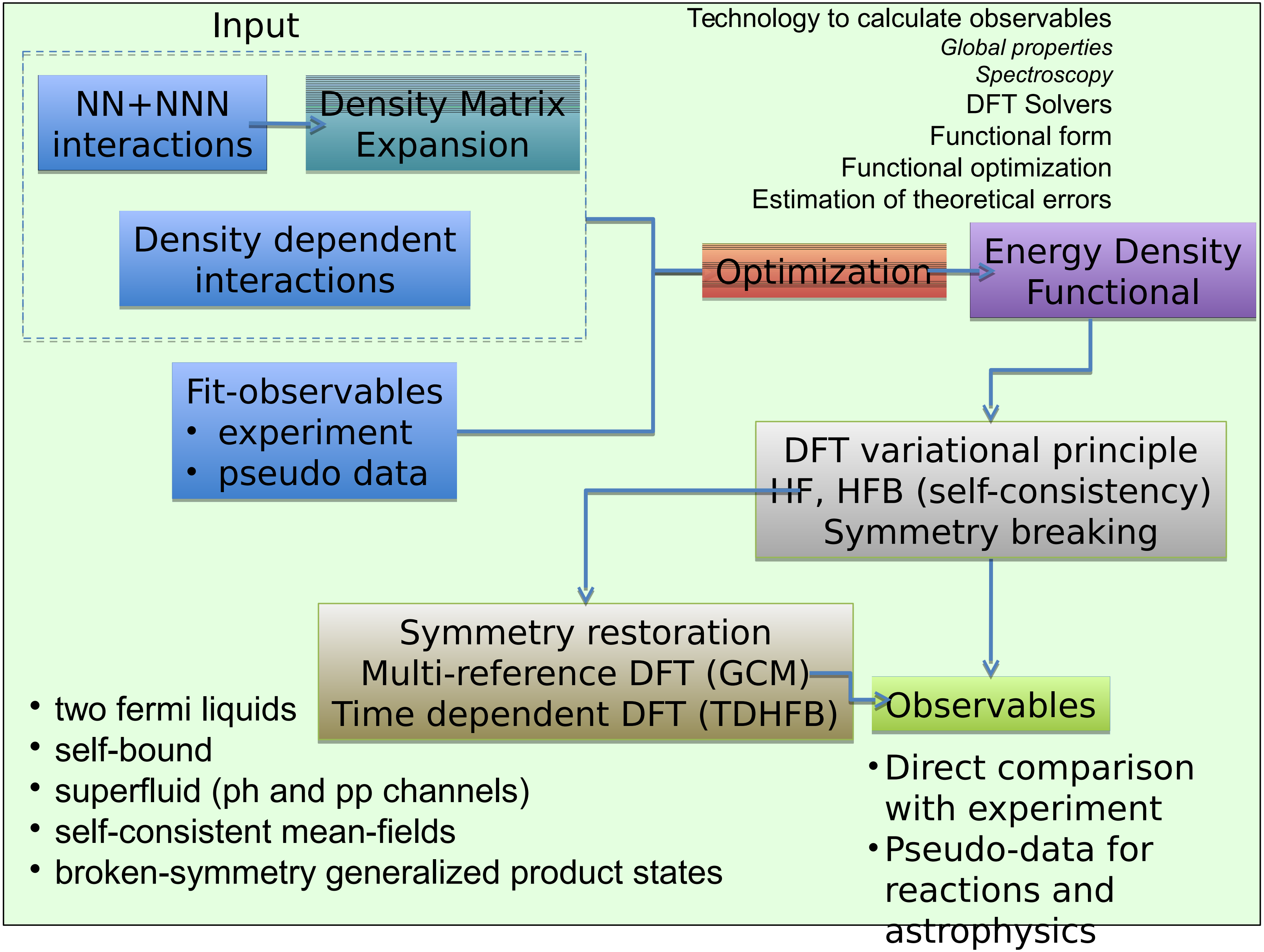
- The *n*-3H elastic cross section for 14 MeV neutrons, important for NIF, was not known precisely enough.
- Delivered evaluated data with required 5% uncertainty and successfully compared to measurements using an Inertial Confinement Facility
- "First measurements of the differential cross sections for the elastic n-2H and n-3H scattering at 14.1 MeV using an Inertial Confinement Facility", by J.A. Frenje *et al.,* Phys. Rev. Lett. **107,** 122502 (2011)

http://physics.aps.org/synopsis-for/10.1103/PhysRevLett.107.122502



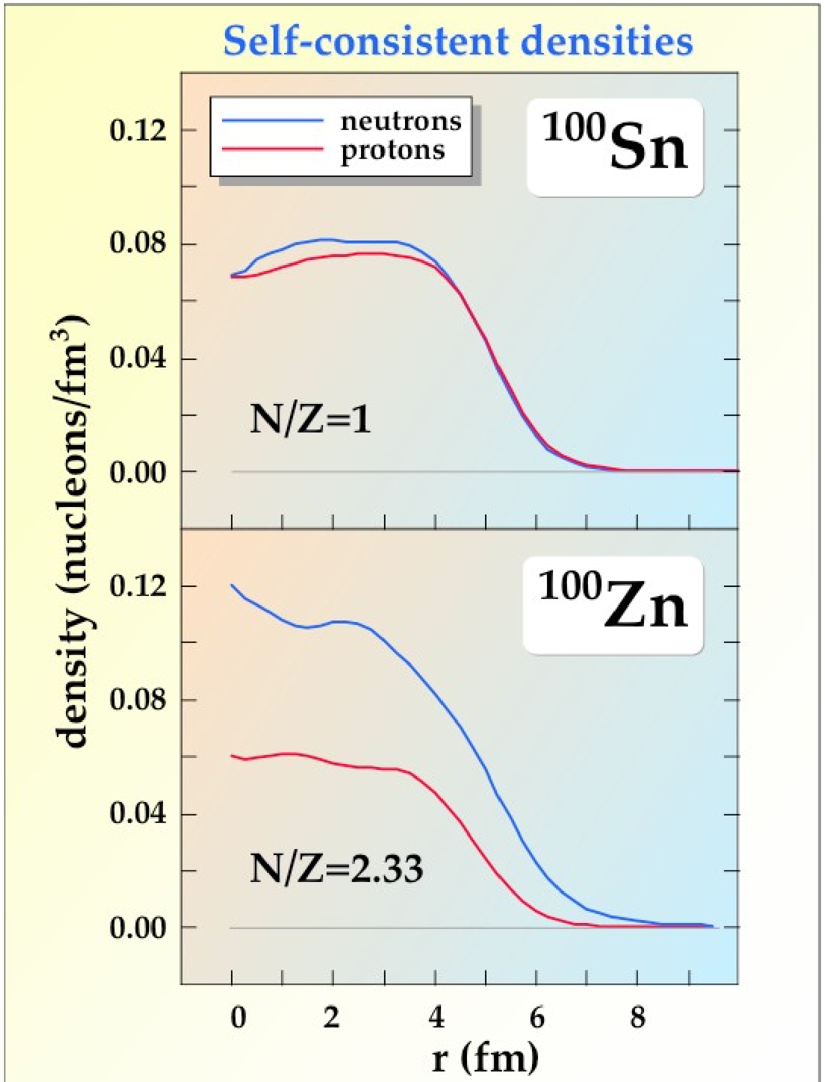
Configuration Space Dimension
10^{2}
10^{6}
10^{10}
10^{14}
10^{18}
10^{22}
10^{26}
20
22
24
26
28
30
32
34
36
38
40
42
44
46
N=Z
Monte Carlo
^{72}Kr
^{88}Ru
fp-gds
fp-$g_{9/2}$
^{60}Zn
^{68}Se
^{56}Ni
2007
^{48}Cr
1994
fp
^{44}Ti
Configuration Interaction
(Interacting Shell Model)

Nuclear Density Functional Theory and Extensions



Mean-Field Theory ⇒ Density Functional Theory

Degrees of freedom: nucleonic densities



Nuclear DFT

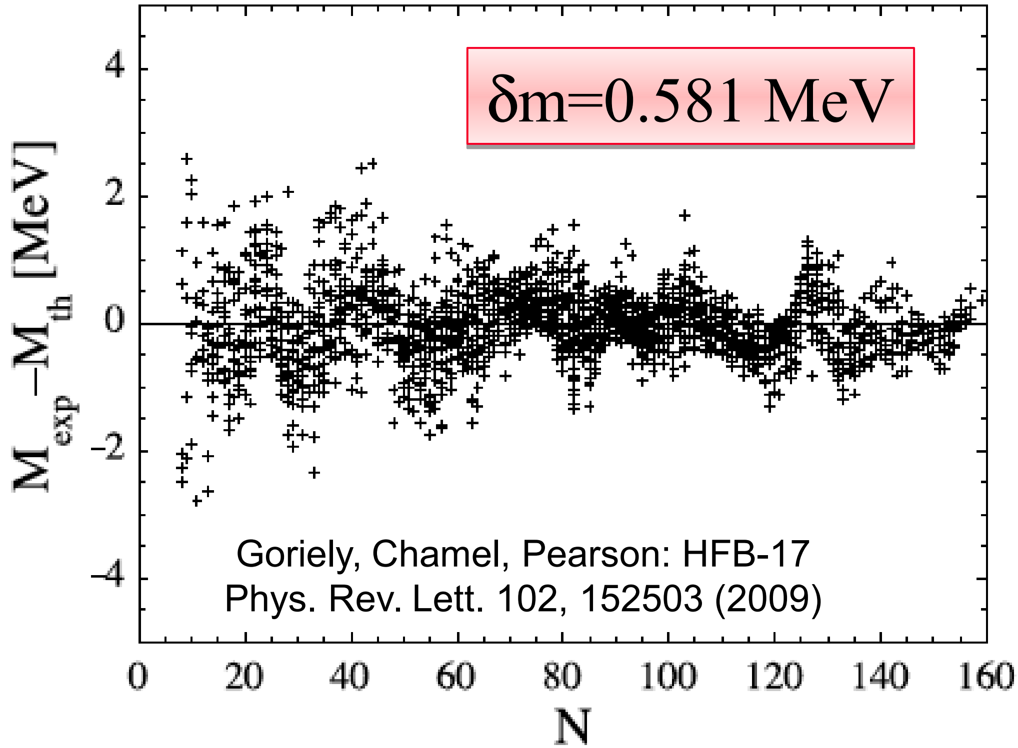
- two fermi liquids
- self-bound
- superfluid

- mean-field ⇒ one-body densities
- zero-range ⇒ local densities
- finite-range ⇒ gradient terms
- particle-hole and pairing channels
- Has been extremely successful. A broken-symmetry generalized product state does surprisingly good job for nuclei.

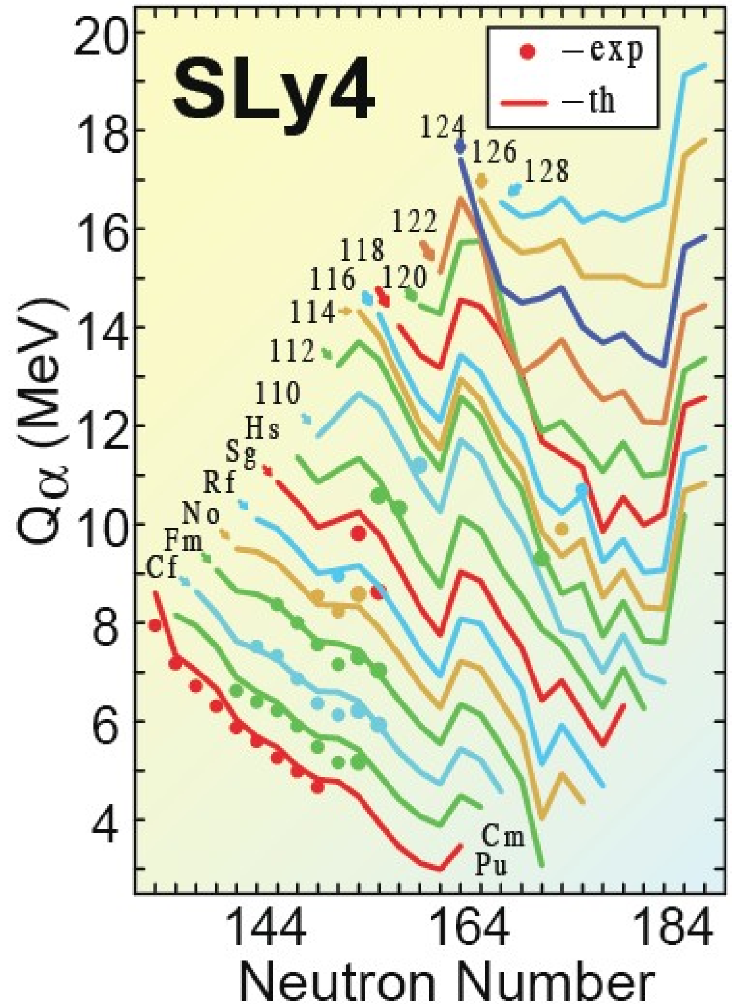
Examples: Nuclear Density Functional Theory

Traditional (limited) functionals
provide quantitative description

Mass table



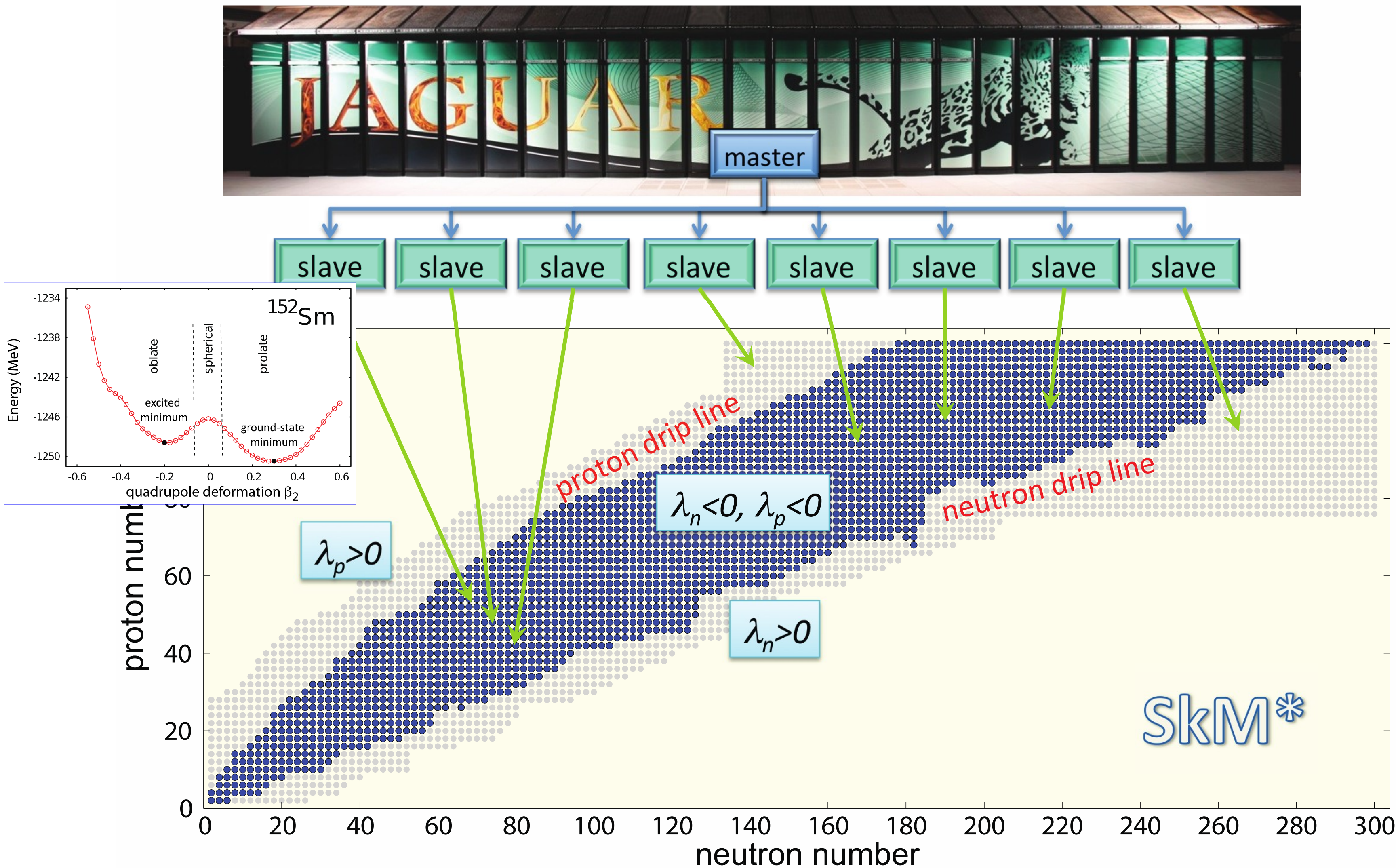
BE differences



Cwiok et al., Nature, 433, 705 (2005)

Example: Large Scale Mass Table Calculations

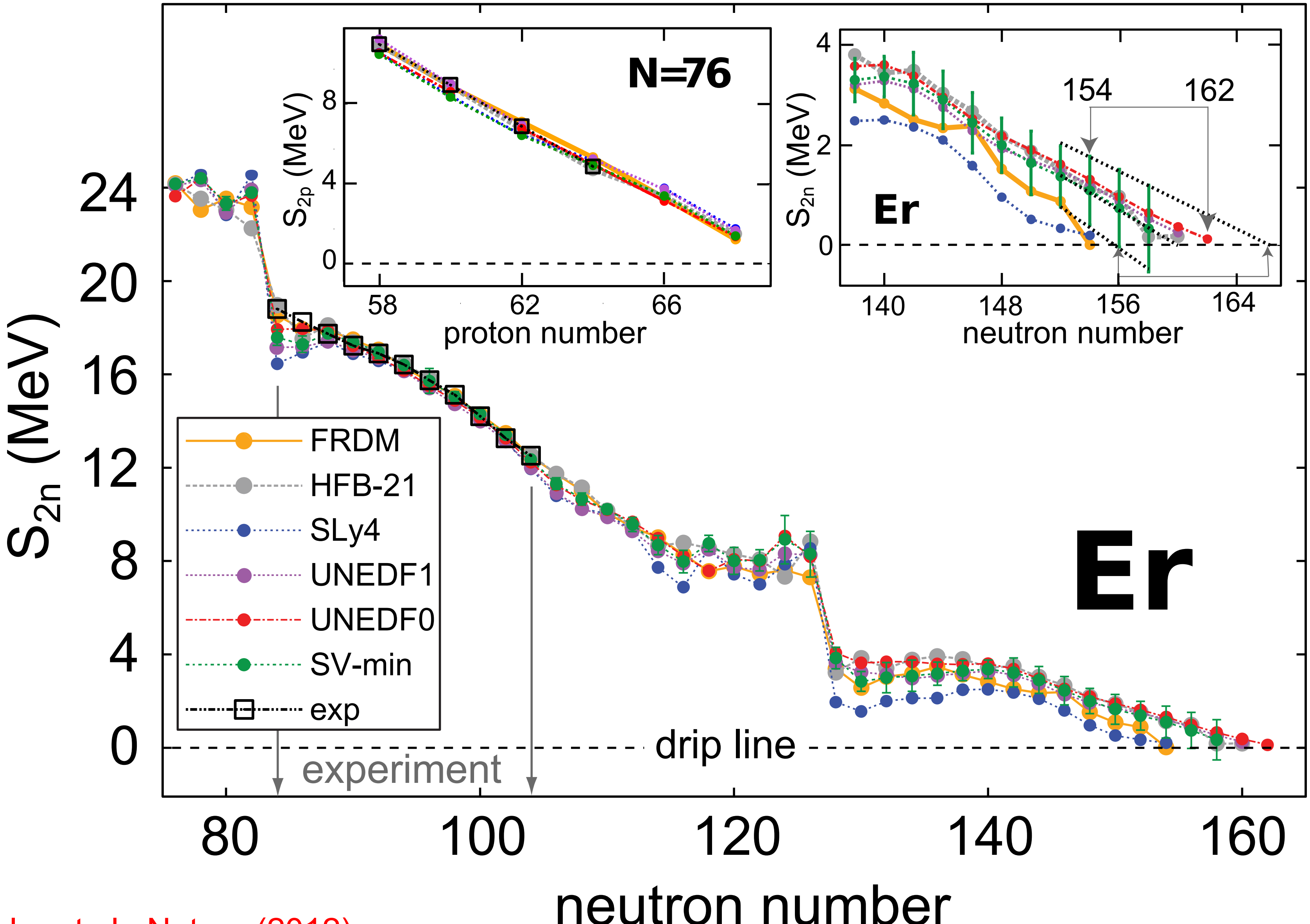
HFB+LN mass table, HFBTHO



- 5,000 even-even nuclei, 250,000 HFB runs, 9,060 processors – about 2 CPU hours
- Full mass table: 20,000 nuclei, 12M configurations — full JAGUAR

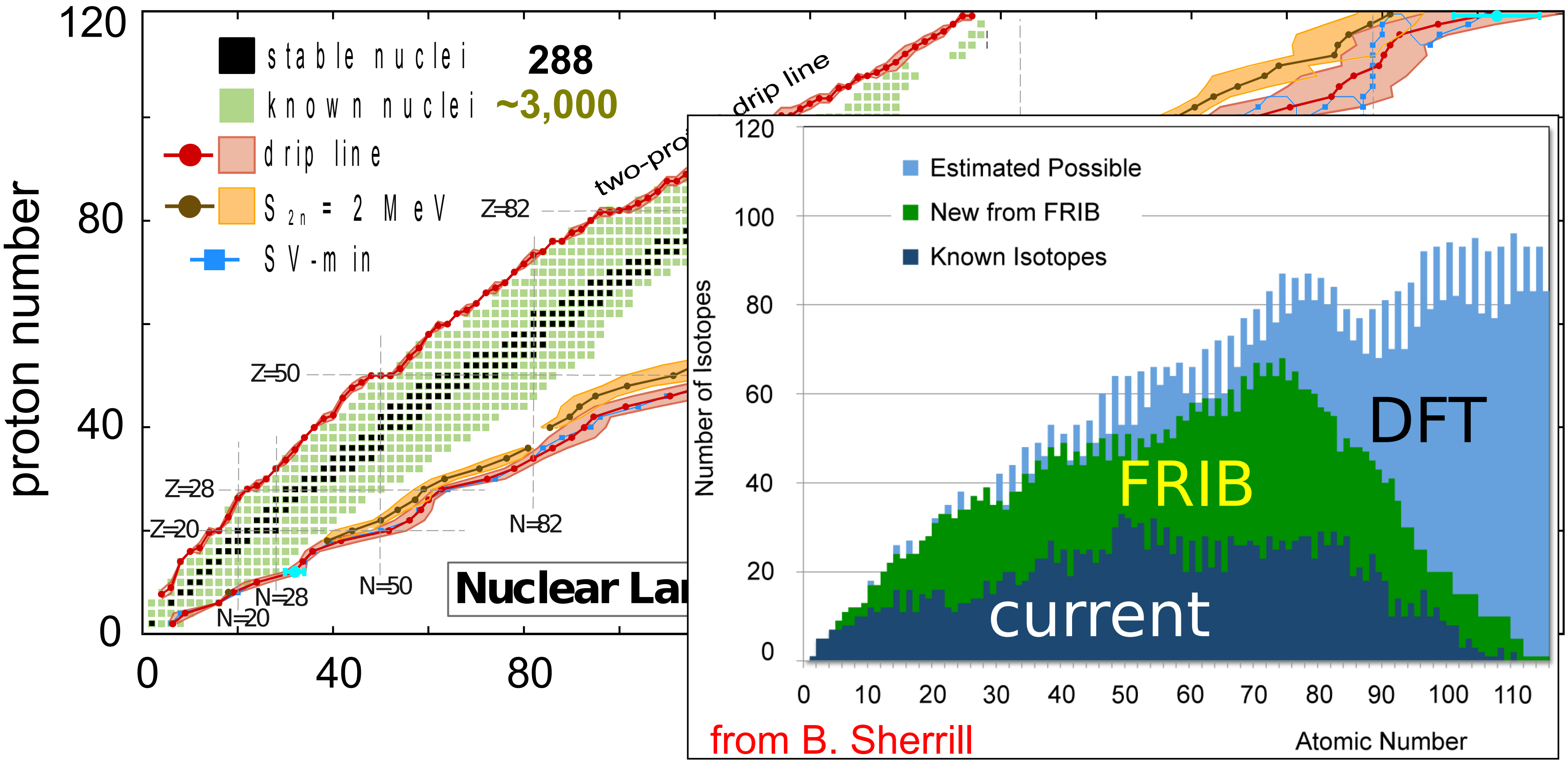
Description of observables and model-based extrapolation

- Systematic errors (due to incorrect assumptions/poor modeling)
- Statistical errors (optimization and numerical errors)



Erler et al., Nature (2012)

Quantified Nuclear Landscape



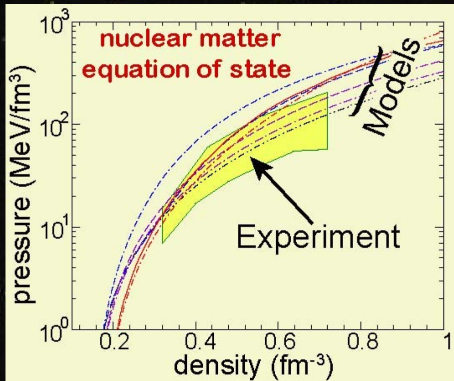
How many protons and neutrons can be bound in a nucleus?

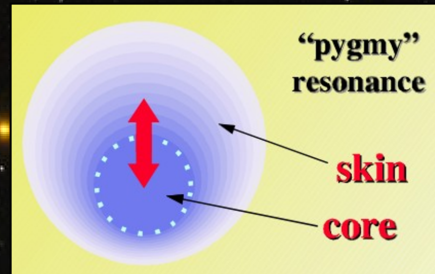
Erler et al.
Nature 486, 509 (2012)

Literature: 5,000-12,000

Skyrme-DFT: 6,900±500$_{syst}$

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





RNB facilities

Nuclear matter equation of state

Neutron star crust

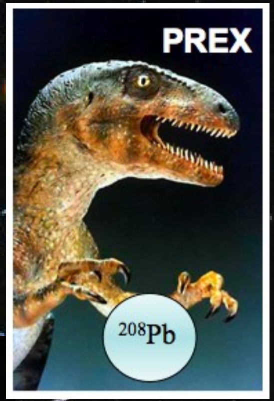
Microphysics (transport,...)

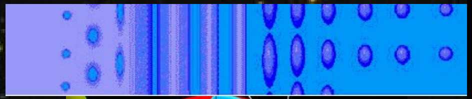
Nuclear interactions

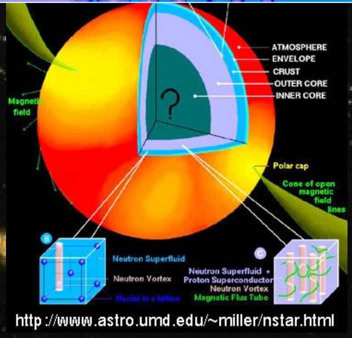
Many-body theory

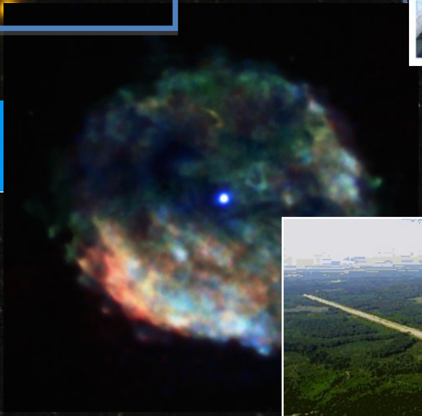
Nuclear observables

Astronomical observables



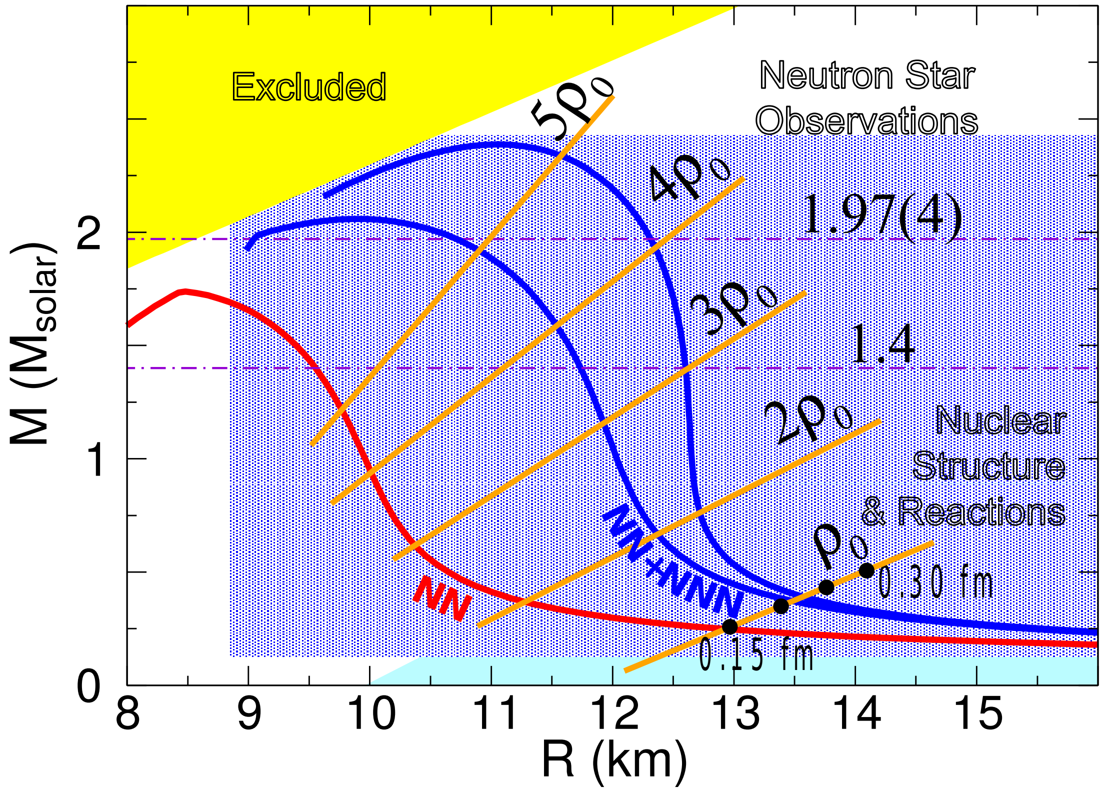




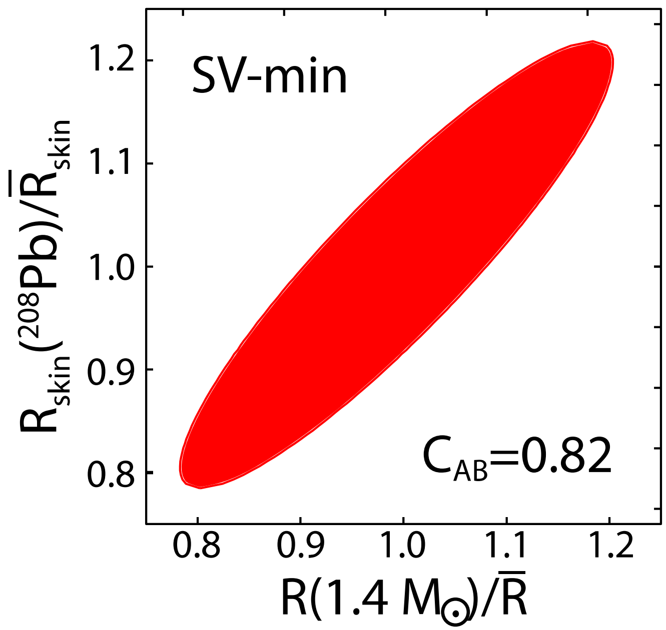


From nuclei to neutron stars (a multiscale problem)

Gandolfi et al. PRC85, 032801 (2012)

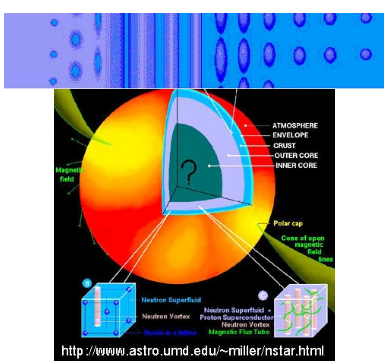


J. Erler et al., PRC 87, 044320 (2013)



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 Rskin= 0.17 fm.



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