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

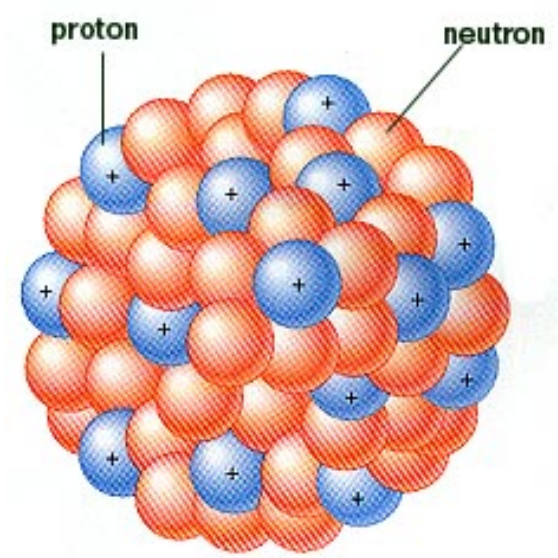
Virgil, Georgica

Theories
Models

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

Alexander I. Kitaigorodskii

Modeling the Atomic Nucleus



Theoretical bag of tricks…

The Nuclear Many-Body Problem

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

$$\hat{H} = \hat{T} + \hat{V}$$

$$\hat{T} = \sum_{i=1}^{A} \frac{\hat{p}_i^2}{2m_i},$$

one-body

Kinetic energy

$$\hat{V} = \sum_{i<i} \hat{V}_{2b}(i,j) + \sum_{i<i<k} \hat{V}_{3b}(i,j,k)$$

two-body three-body

Potential energy

$$\Psi = \Psi\left(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_A; s_1, s_2, \ldots, s_A; t_1, t_2, \ldots, t_A\right)$$

3A nucleon coordinates in r-space

nucleon spins: ±1/2

nucleon isospins (p or n): ±1/2

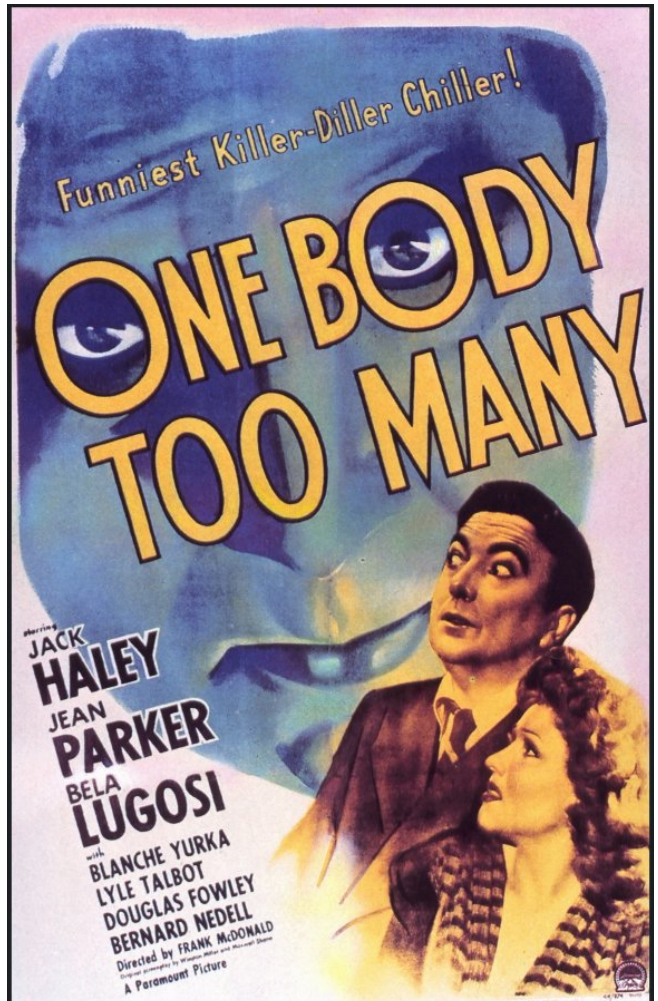
Eigenstate of angular momentum, parity, and ~isospin

Bottom line:

$$2^A \times \frac{A!}{N!Z!}$$

coupled integro-differential equations in 3A dimensions

The nuclear many-body problem



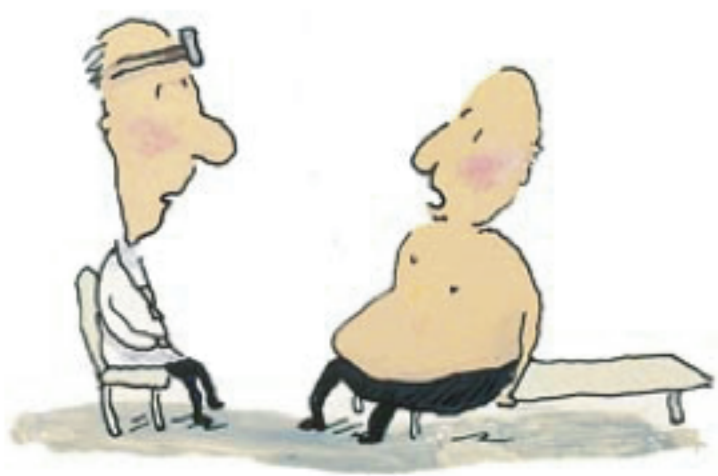
Weinberg's Laws of Progress in Theoretical Physics

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

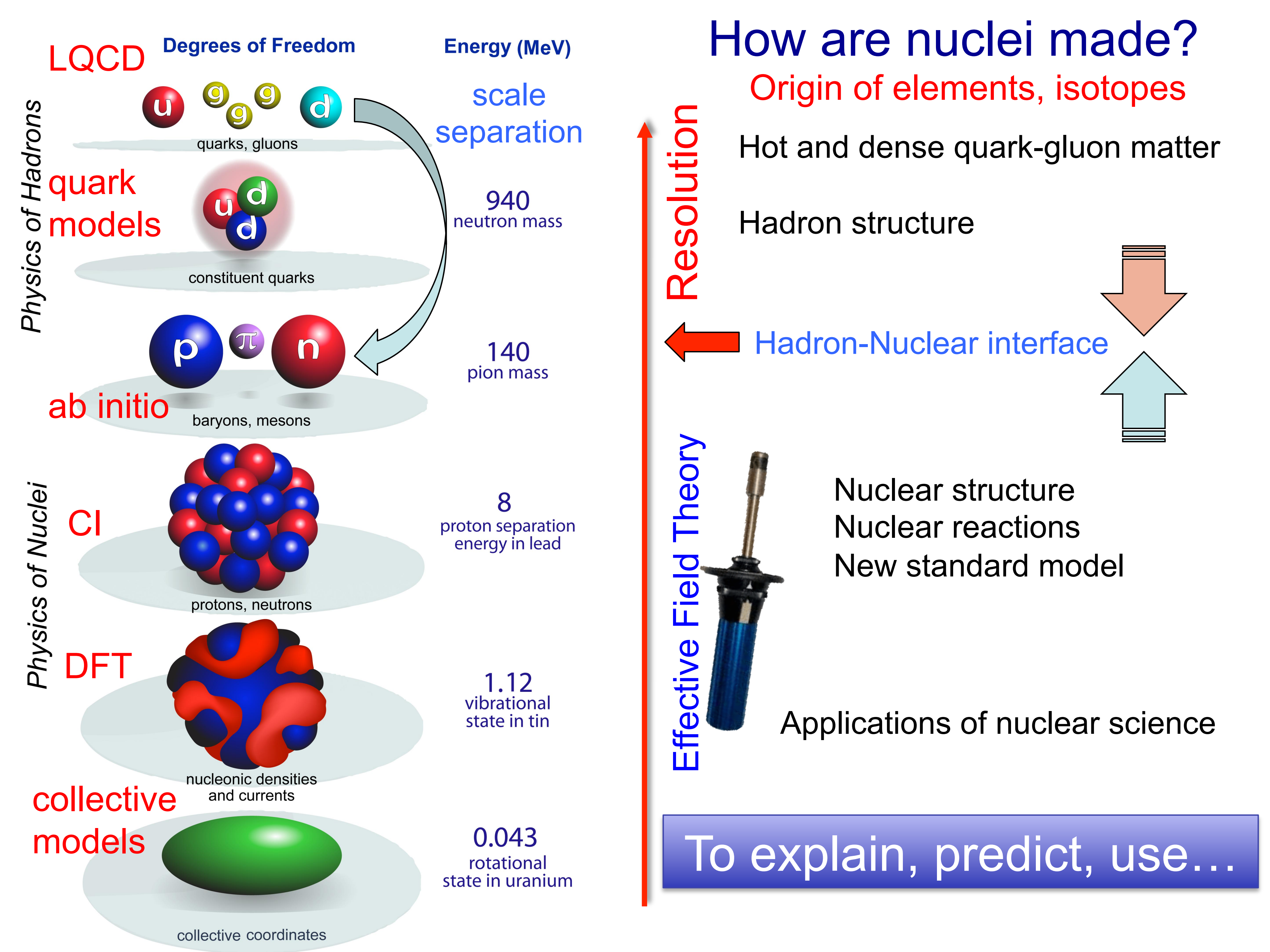
First Law: "The conservation of Information" (*You will get nowhere by churning equations*)

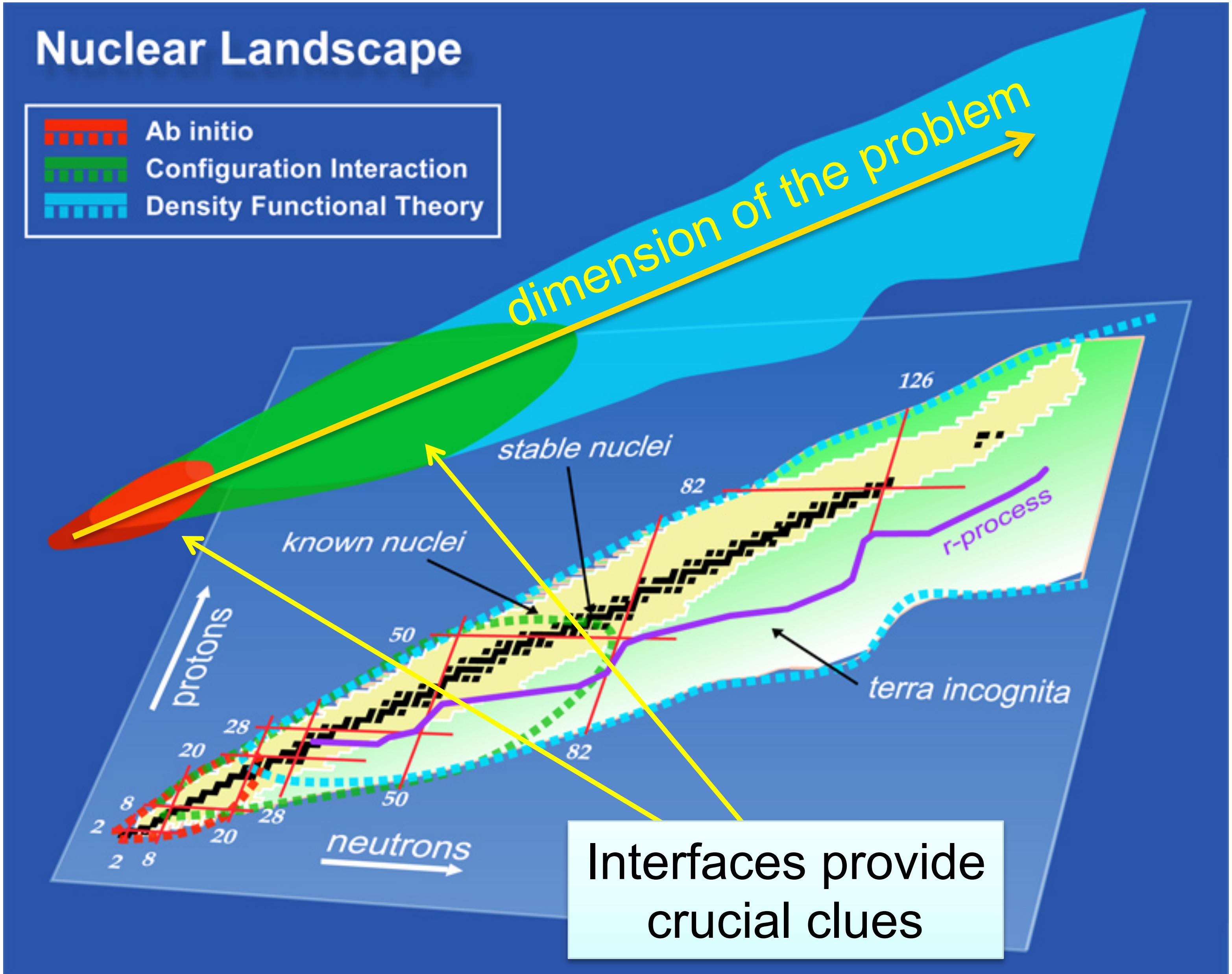
Second Law: "Do not trust arguments based on the lowest order of perturbation theory"

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.

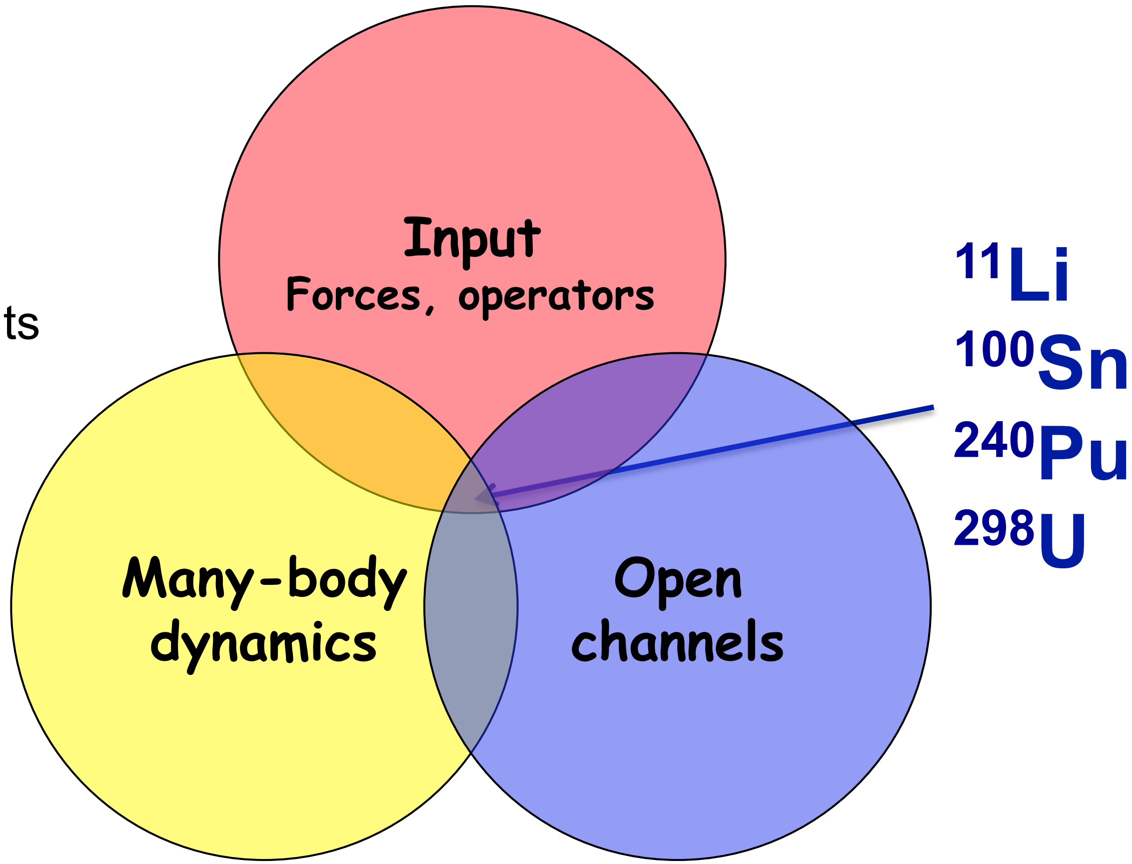

How are nuclei made?
Origin of elements, isotopes
LQCD
Degrees of Freedom
Energy (MeV)
quarks, gluons
scale separation
Physics of Hadrons
quark models
constituent quarks
940
neutron mass
ab initio
baryons, mesons
140
pion mass
Physics of Nuclei
CI
protons, neutrons
8
proton separation energy in lead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



number of nuclei < number of processors!

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

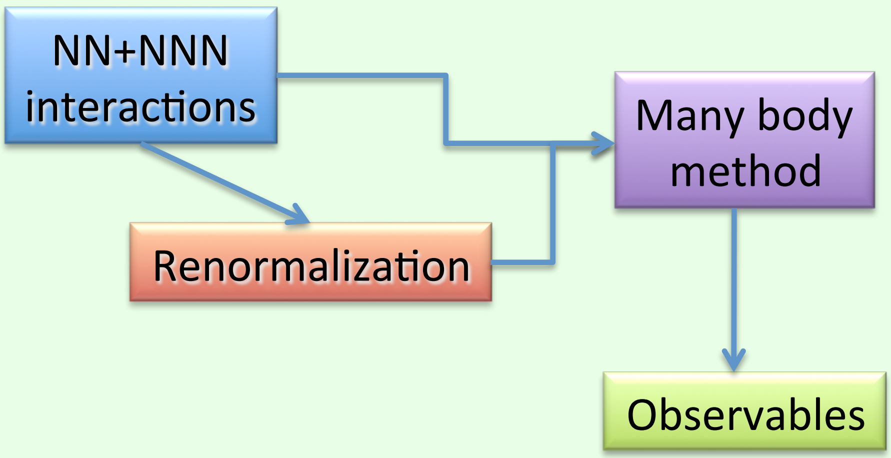
- nuclear structure impacted by couplings to reaction and decay channels
- clustering, alpha decay, and fission still remain major challenges for theory
- unified picture of structure and reactions

Ab initio theory for light nuclei and nuclear matter

Ab initio: QMC, NCSM, CCM,…

(nuclei, neutron droplets, nuclear matter)

Ab initio input

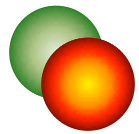


- Direct comparison with experiment
- Pseudo-data to inform theory

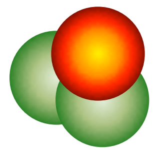
Input:

- 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

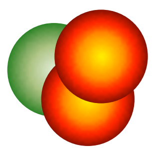
Few-nucleon systems



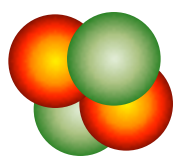
A=2: many years ago…



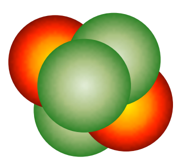
^{3}H: 1984 (1% accuracy)



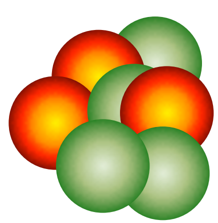
^{3}He: 1987



^{4}He: 1987



^{5}He: 1994 (n-α resonance)



A=6,7,..12: 1995-2011

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

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

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

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

- Quantum Monte Carlo (GFMC) **^{12}C**
- No-Core Shell Model **^{14}F, ^{14}C**
- Faddeev-Yakubovsky
- Lattice EFT **^{12}C (Hoyle)**
- Coupled-Cluster Techniques **^{17}F, ^{56}Ni**
- Fermionic Molecular Dynamics
- …

Nucleon-Nucleon Interaction

NN, NNN, NNNN,..., forces

GFMC calculations tell us that:

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

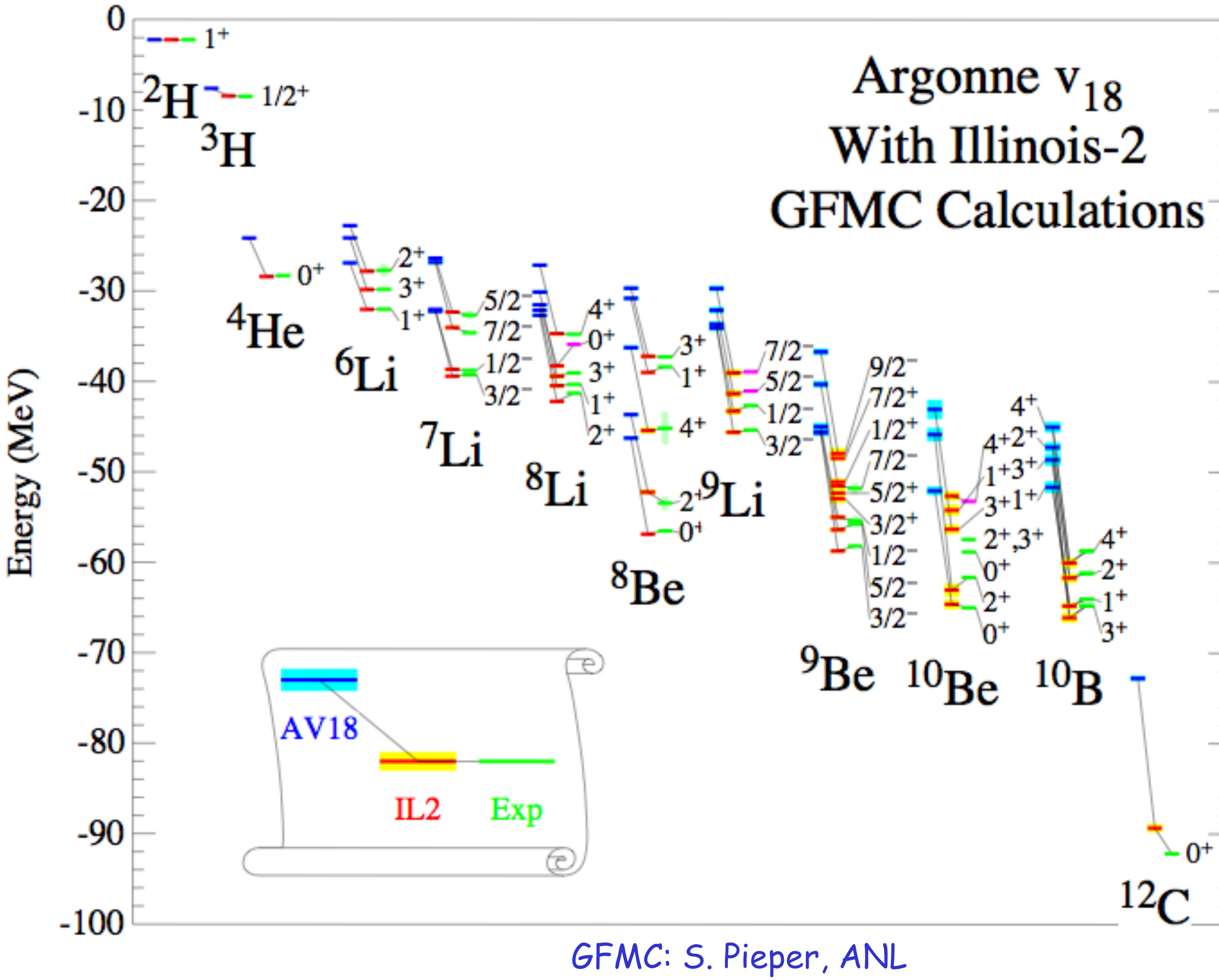
$$\langle V_\pi \rangle \sim -15\,\text{MeV/pair}$$

$$\langle V^R \rangle \sim -5\,\text{MeV/pair}$$ **short-range**

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

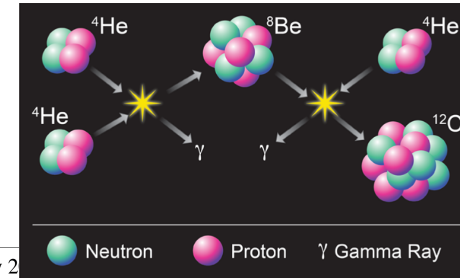
$$\langle T \rangle \sim 15\,\text{MeV/nucleon}$$

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

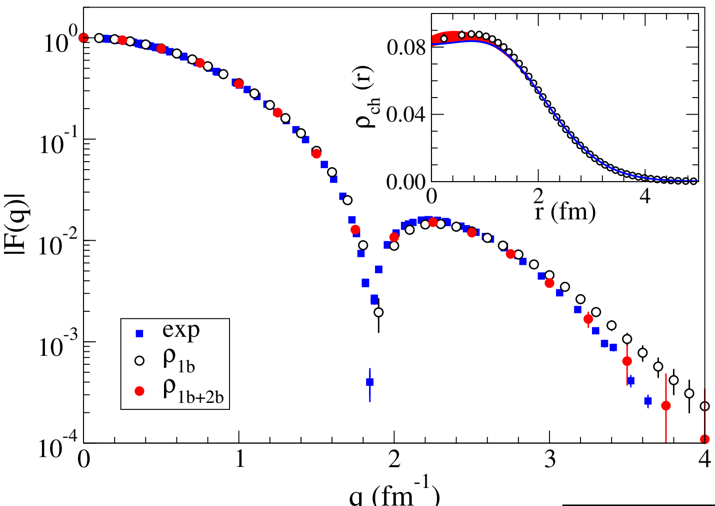


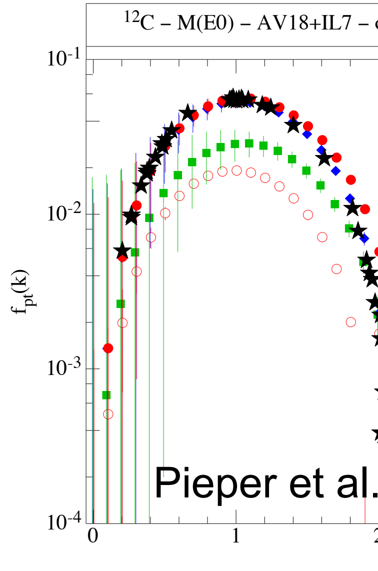
1-2% calculations of A = 6 – 12 nuclear energies are possible
excited states with the same quantum numbers computed

^{12}C: ground state and Hoyle state
state-of-the-art computing

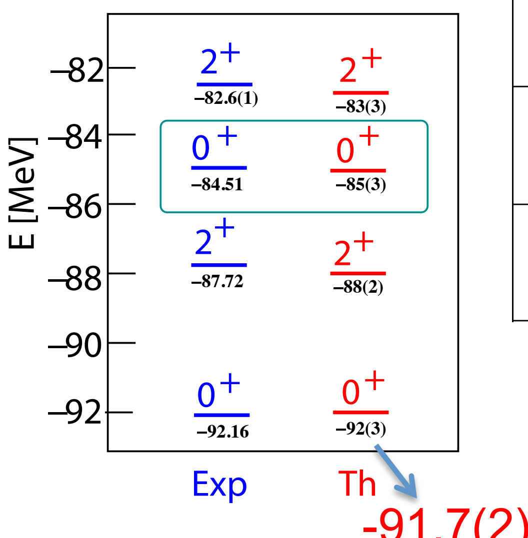


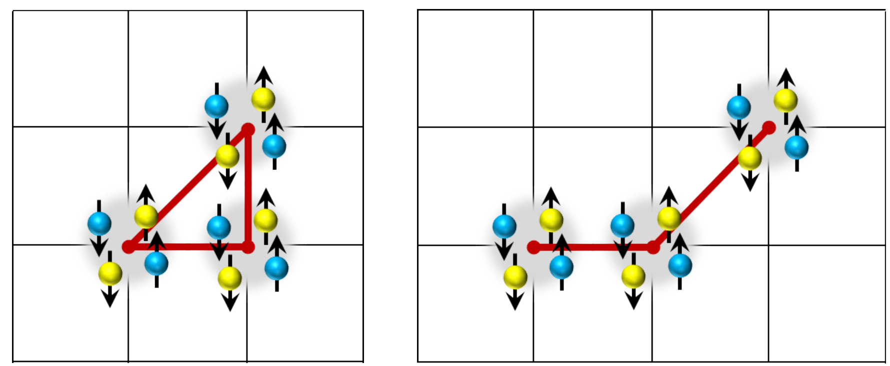
Wiringa et al. Phys. Rev. C 89, 024305 (2014); A. Lovato et al., Phys. Rev. Lett. 112, 182502 (2014)





The ADLB (Asynchronous Dynamic Load-Balancing) version of GFMC was used to make calculations of ^{12}C 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.

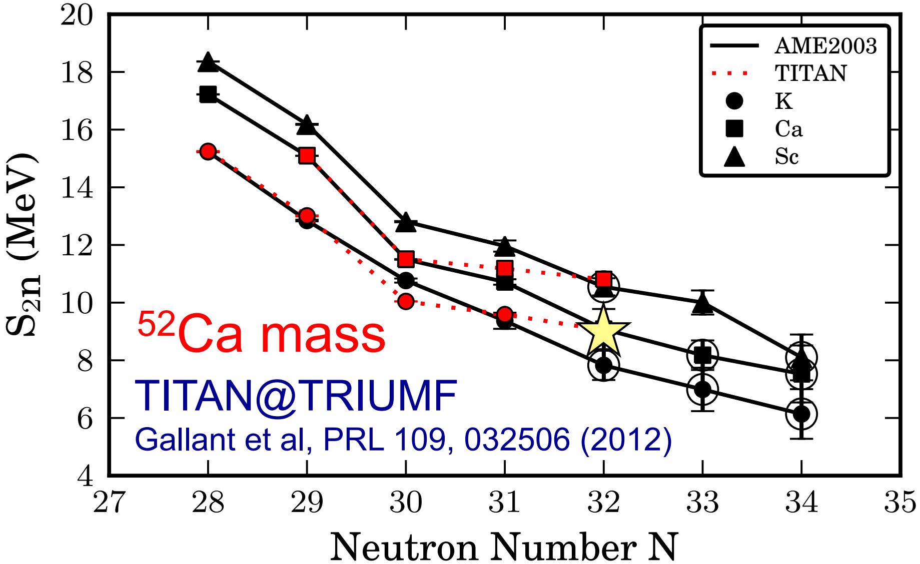




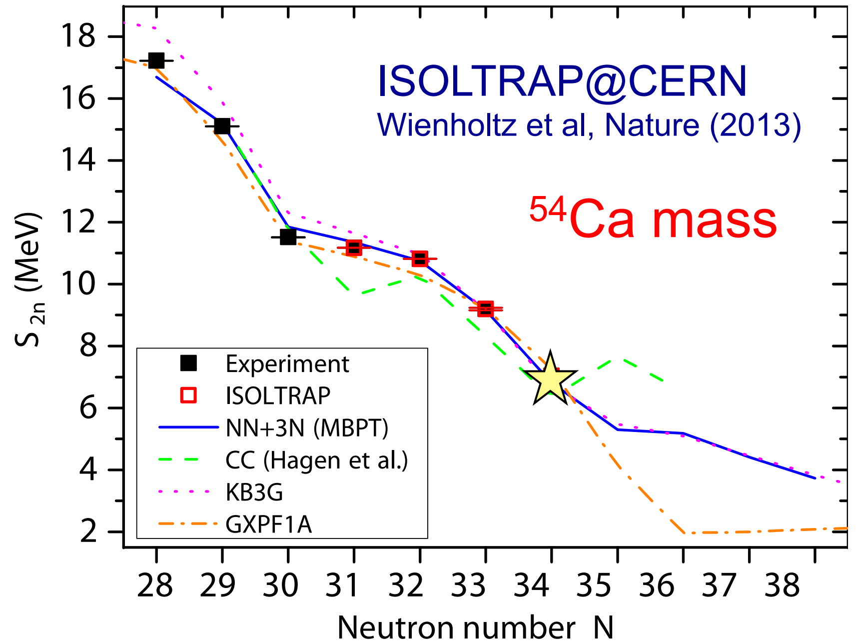
Epelbaum et al., Phys. Rev. Lett. 109, 252501 (2012). Lattice EFT
Lahde et al., Phys. Lett. B 732, 110 (2014).

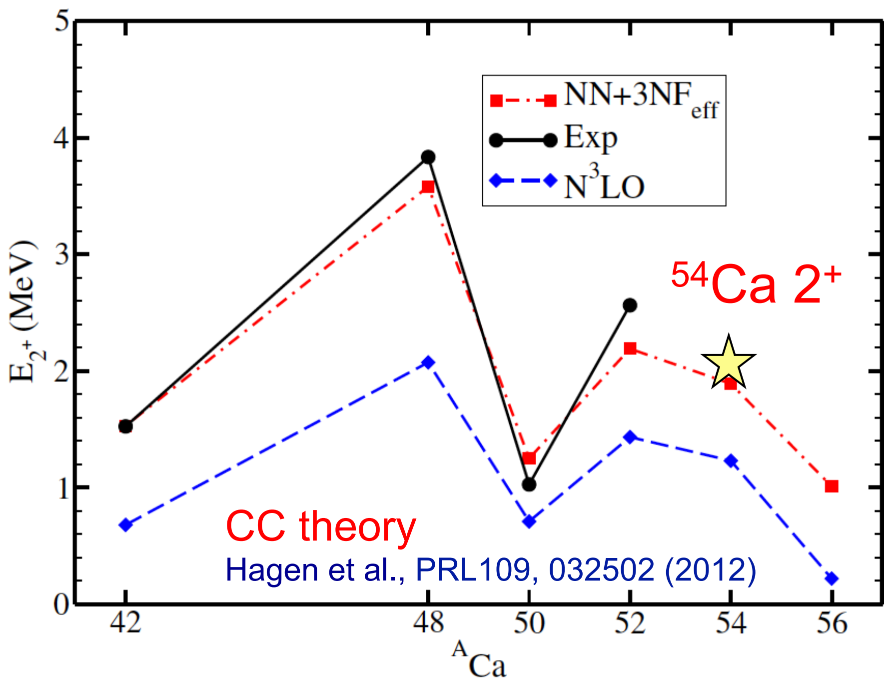
The frontier: neutron-rich calcium isotopes

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



^{54}Ca: 20 protons, 34 neutrons





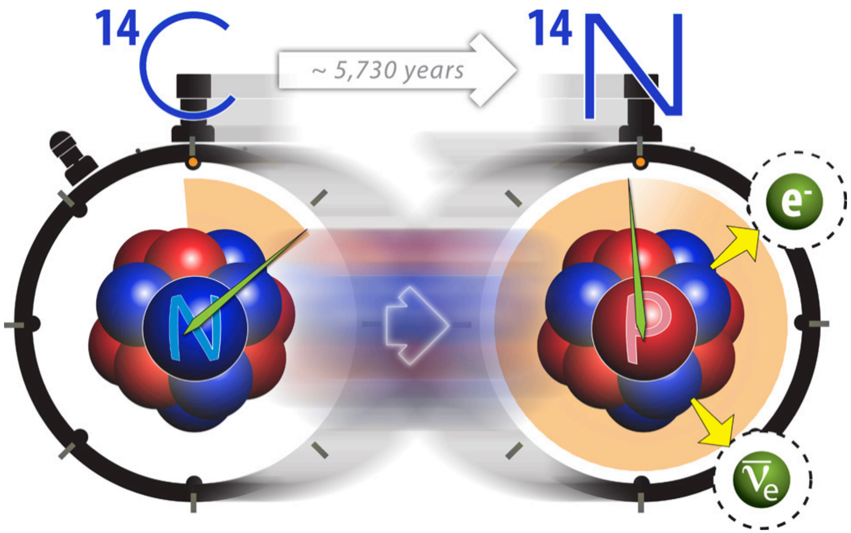
RIBF@RIKEN

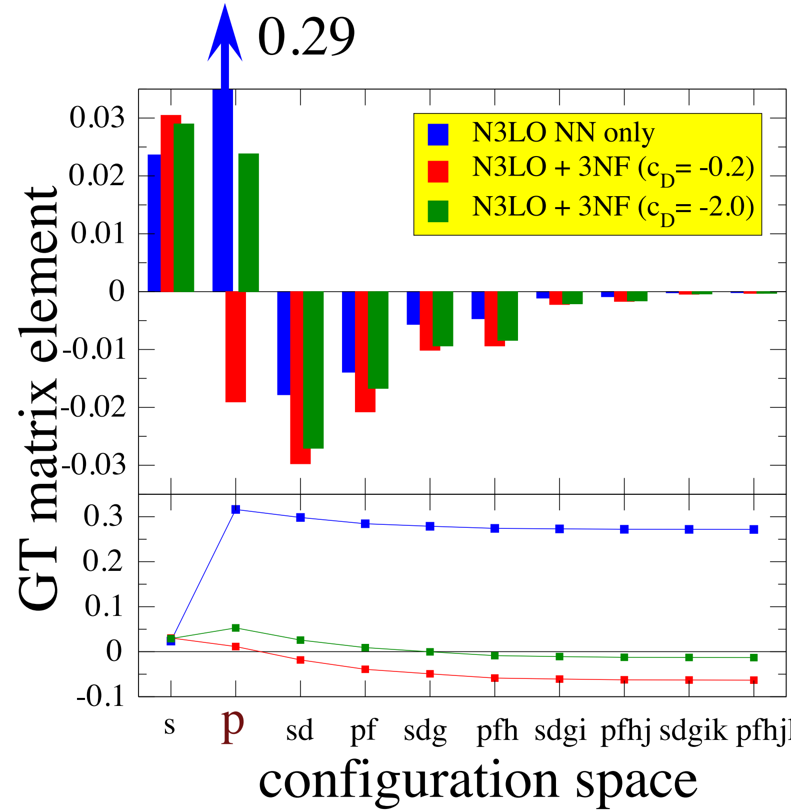
Steppenbeck et al

Nature (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