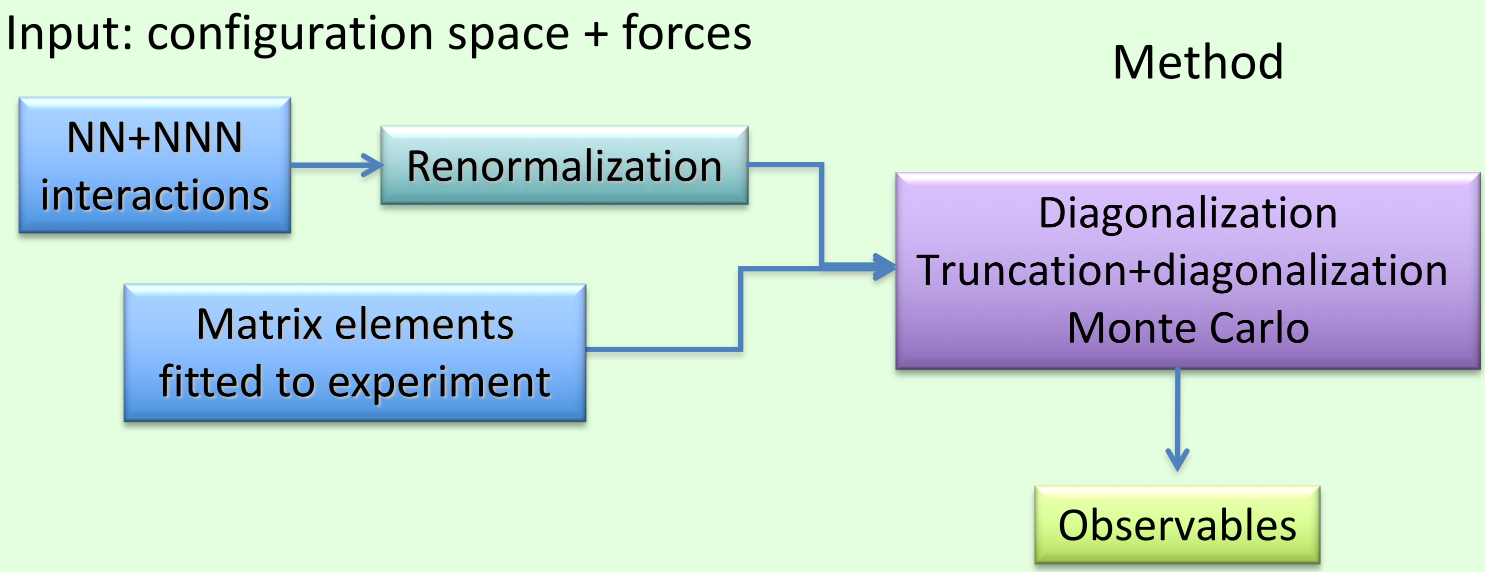
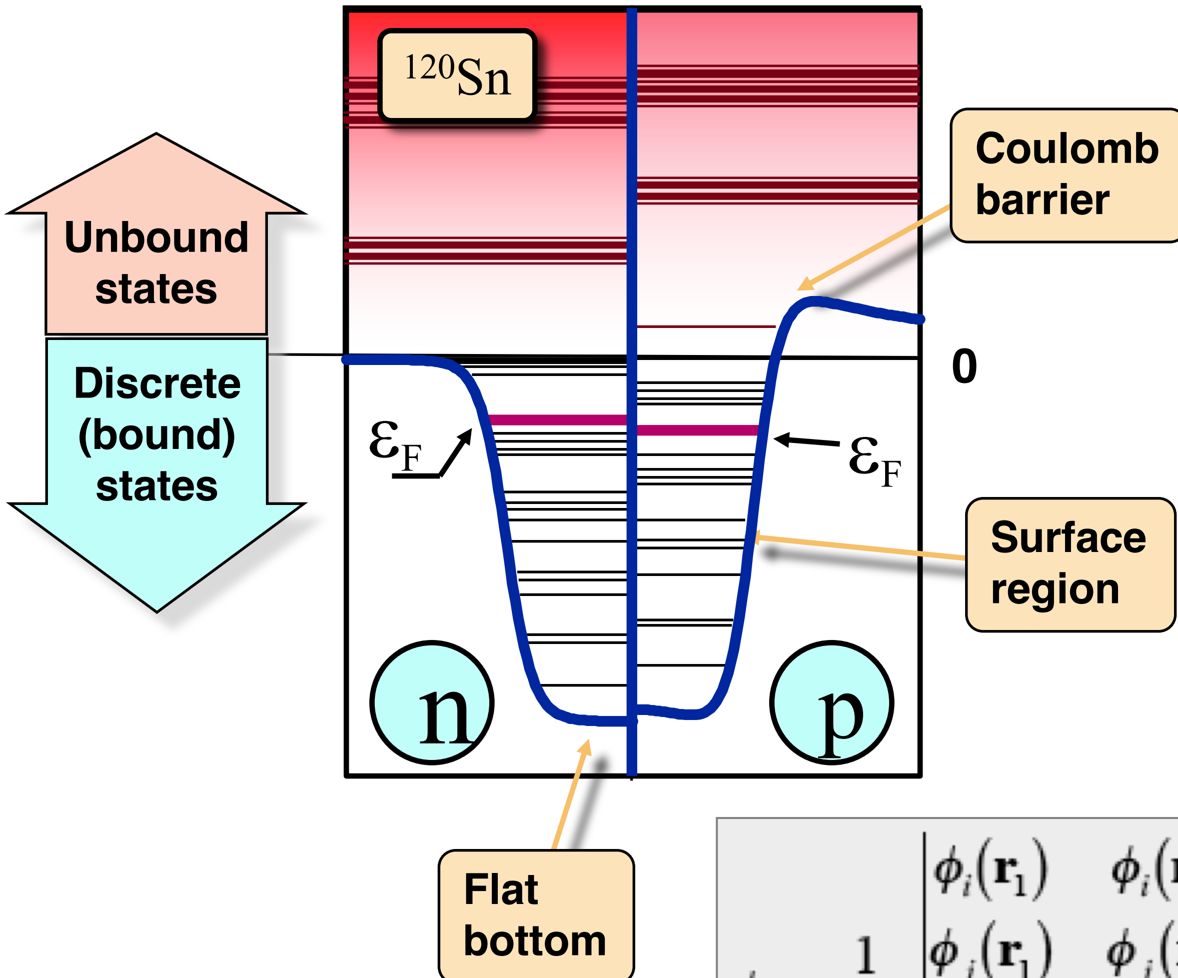
Configuration interaction techniques

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



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

Average one-body Hamiltonian



$$\hat{H}_0 = \sum_{i=1}^{A} h_i, \quad h_i = -\frac{\hbar^2}{2M}\nabla_i^2 + V_i$$

$$h_i \phi_k(i) = \varepsilon_k \phi_k(i)$$

$$\phi = \frac{1}{\sqrt{A!}} \begin{vmatrix} \phi_i(\mathbf{r}_1) & \phi_i(\mathbf{r}_2) & \ldots & \phi_i(\mathbf{r}_A) \\ \phi_j(\mathbf{r}_1) & \phi_j(\mathbf{r}_2) & & \phi_j(\mathbf{r}_A) \\ & \vdots & \ddots & \vdots \\ \phi_l(\mathbf{r}_1) & \phi_l(\mathbf{r}_2) & \ldots & \phi_l(\mathbf{r}_A) \end{vmatrix}$$

$$= a_l^+ \ldots a_j^+ a_i^+ |0\rangle$$

Nuclear shell model

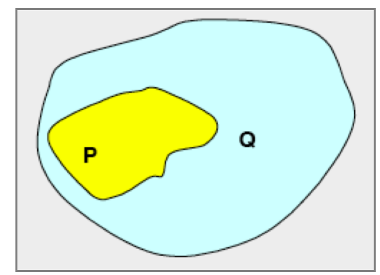
$$\hat{H} = \sum_i t_i + \frac{1}{2}\sum_{\substack{i,j \\ i\neq j}} v_{ij} = \sum_i (t_i + V_i) \quad + \quad \left[\frac{1}{2}\sum_{\substack{i,j \\ i\neq j}} v_{ij} - \sum_i V_i\right]$$

One-body Hamiltonian

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

$$P + Q = 1$$

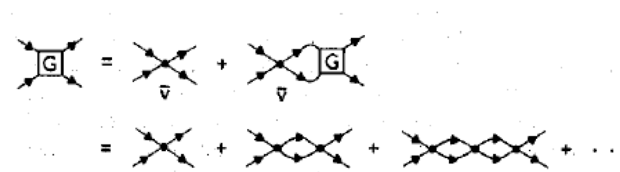


$$\text{Full } fp \text{ shell for } {}^{60}\text{Zn}: \quad \approx 2\times 10^9 \; J_z \text{ states}$$

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

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

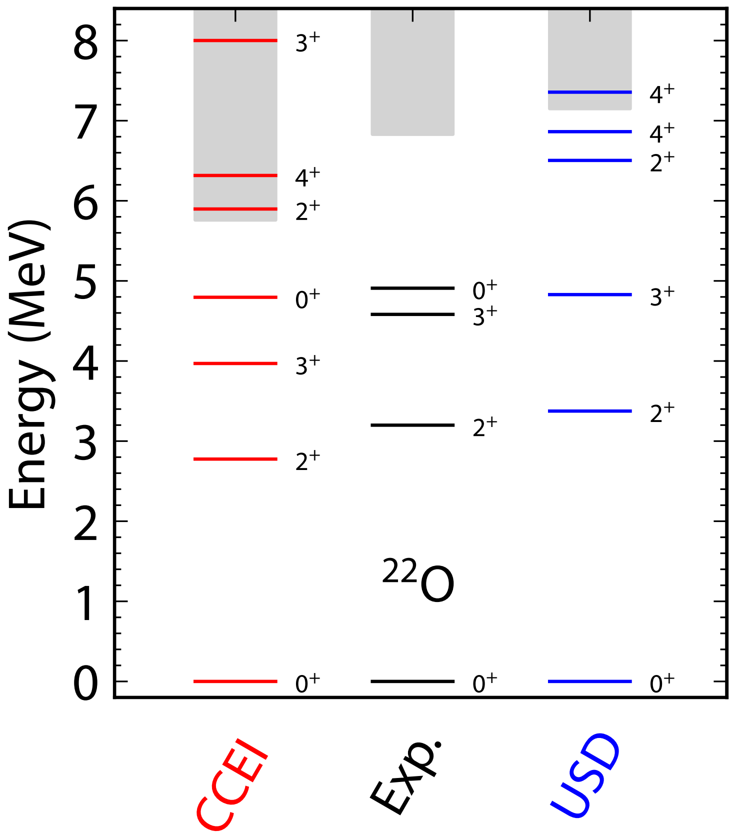
- Can we get around this problem? Effective interactions in truncated spaces (*P*-included, finite; *Q*-excluded, infinite)
- Residual interaction (*G*-matrix) depends on the configuration space. Effective charges
- Breaks down around particle drip lines



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

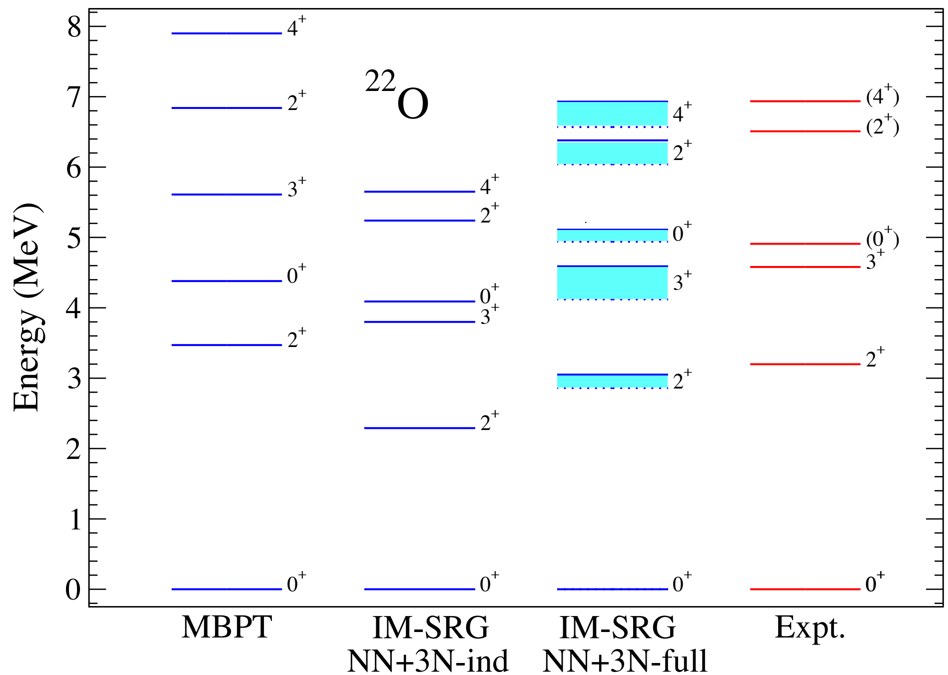
Microscopic valence-space Shell Model Hamiltonian

Coupled Cluster Effective Interaction (valence cluster expansion)



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

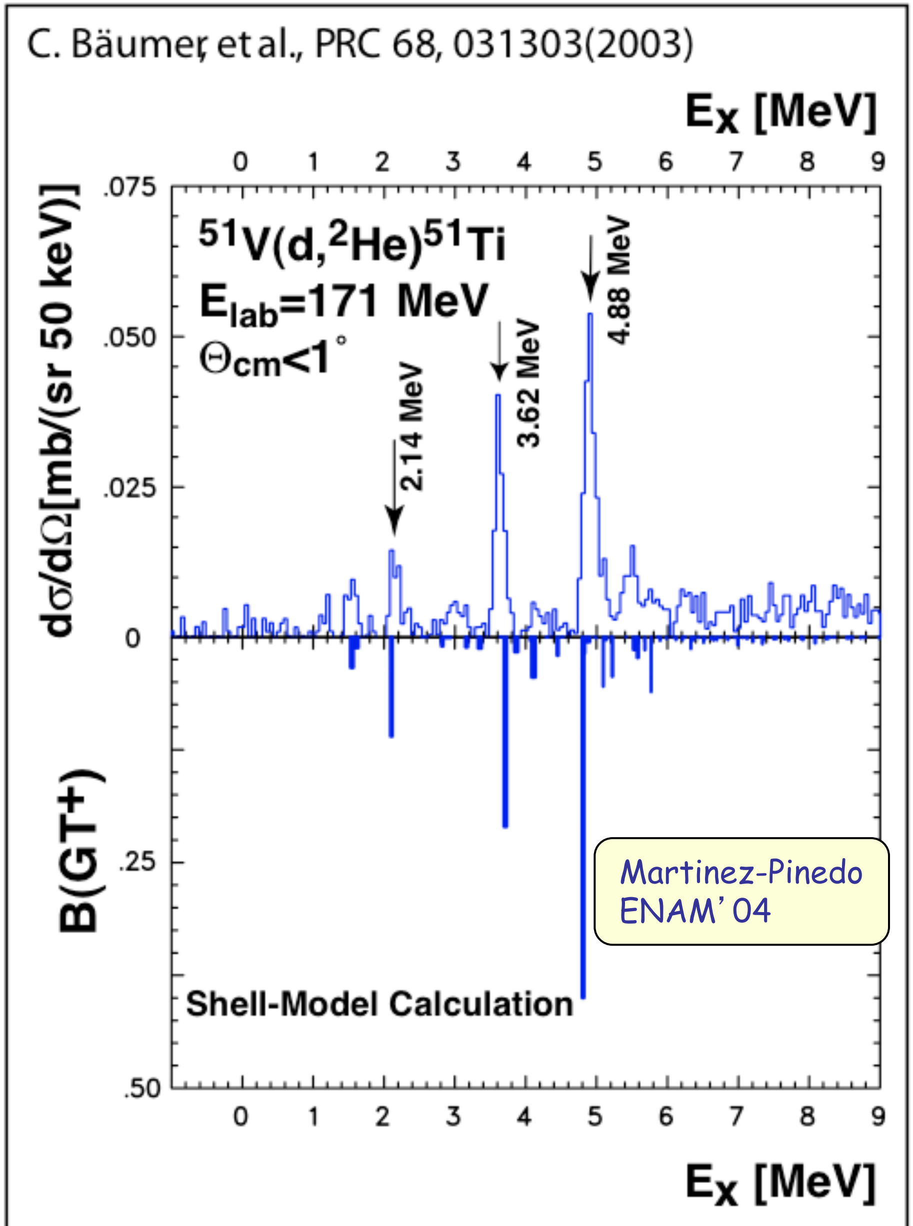
In-medium SRG Effective Interaction

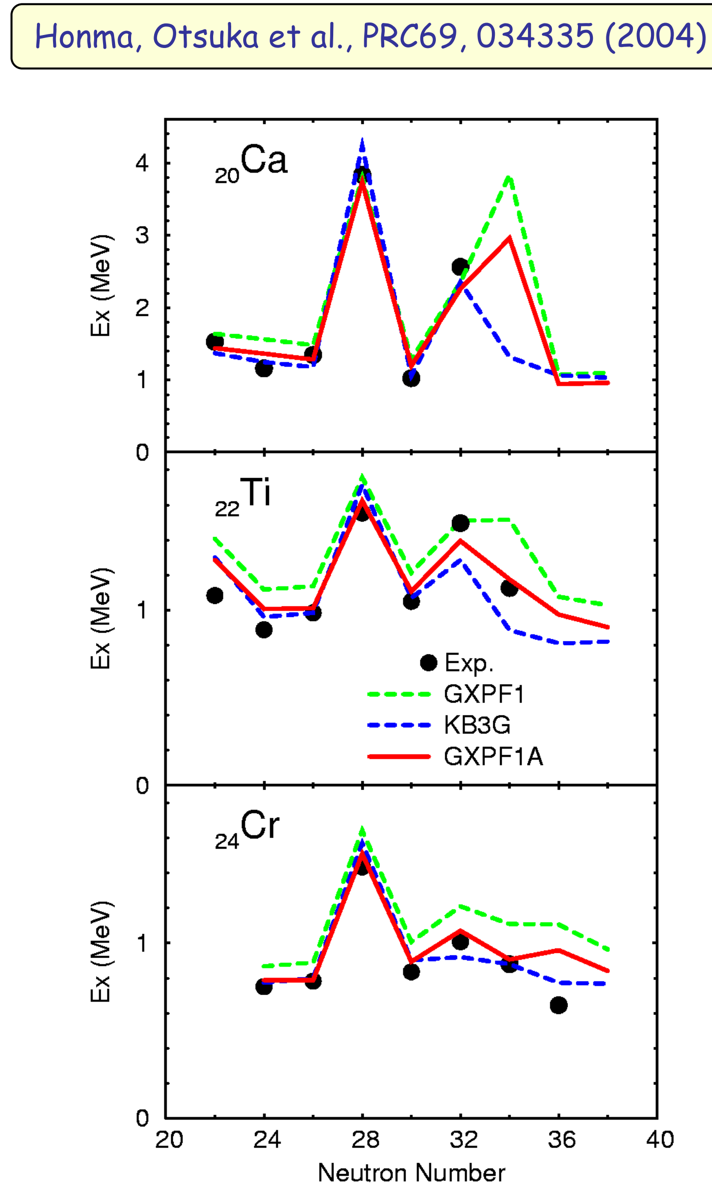


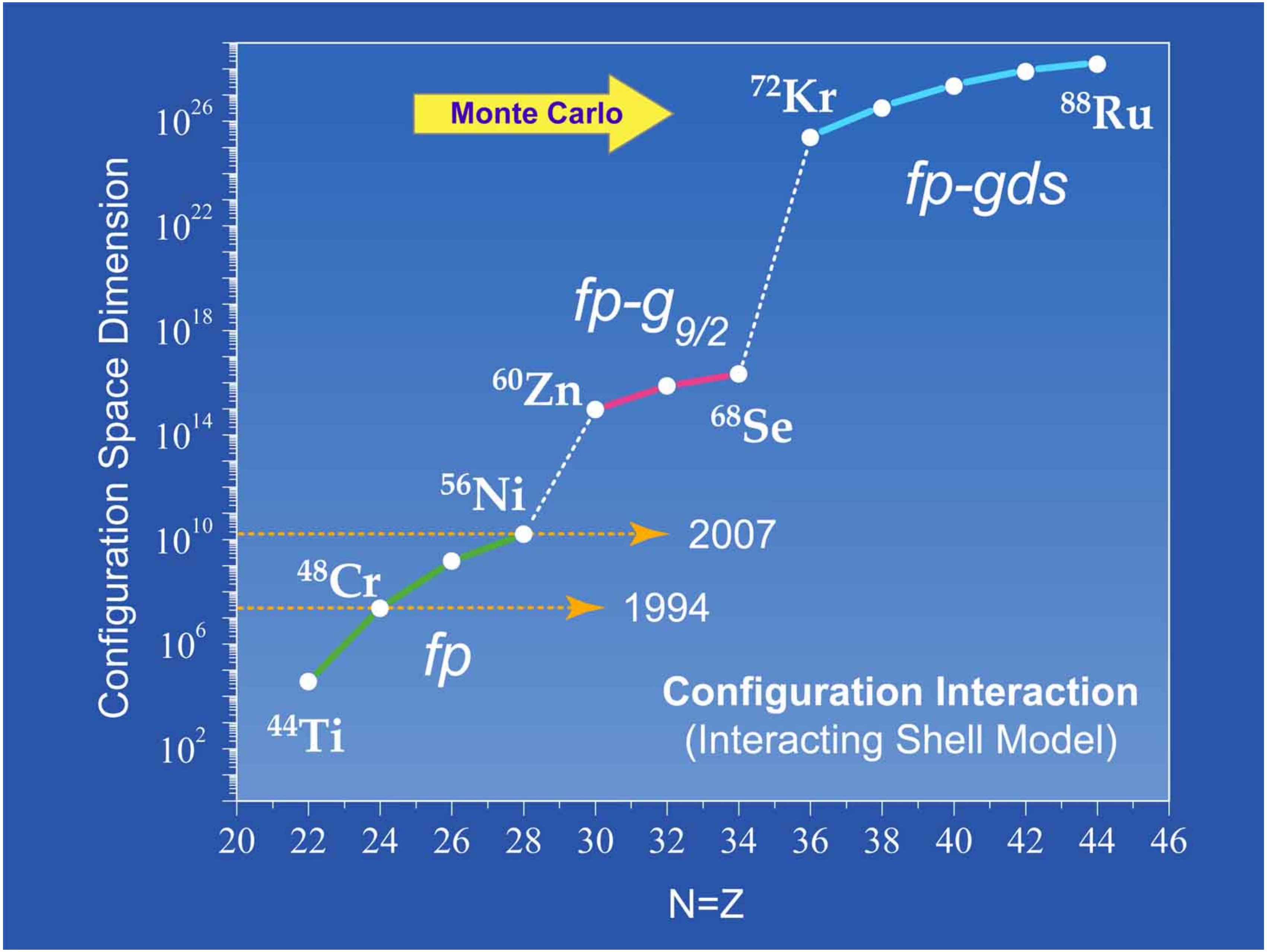
S.K. Bogner et al., Phys. Rev. Lett. **113**, 142501 (2014)

Diagonalization Shell Model

(medium-mass nuclei reached;dimensions 10^9!)

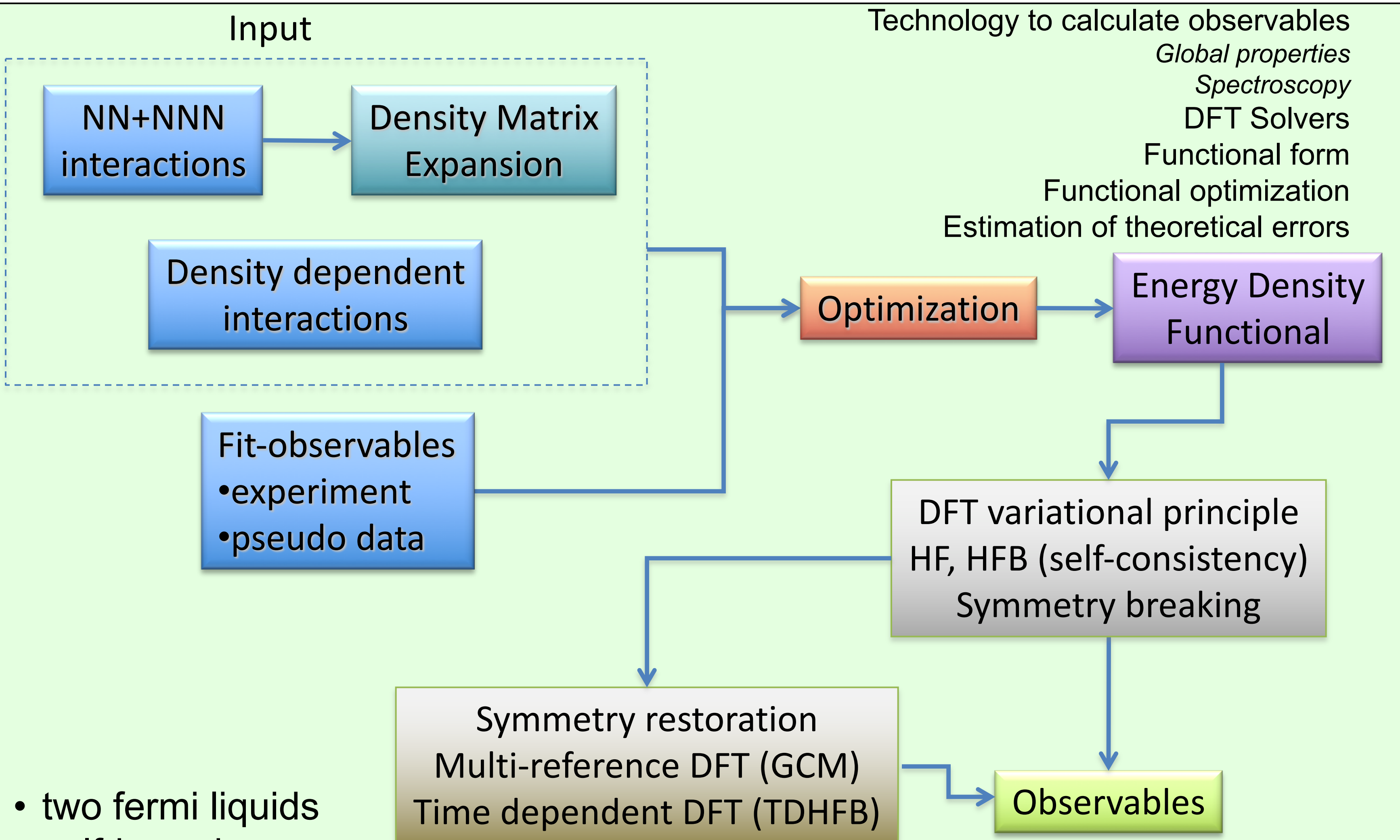






Monte Carlo
72Kr
88Ru
fp-gds
fp-g9/2
60Zn
68Se
56Ni
2007
48Cr
1994
fp
44Ti
Configuration Interaction
(Interacting Shell Model)
Configuration Space Dimension
10^26
10^22
10^18
10^14
10^10
10^6
10^2
20
22
24
26
28
30
32
34
36
38
40
42
44
46
N=Z

Nuclear Density Functional Theory and Extensions

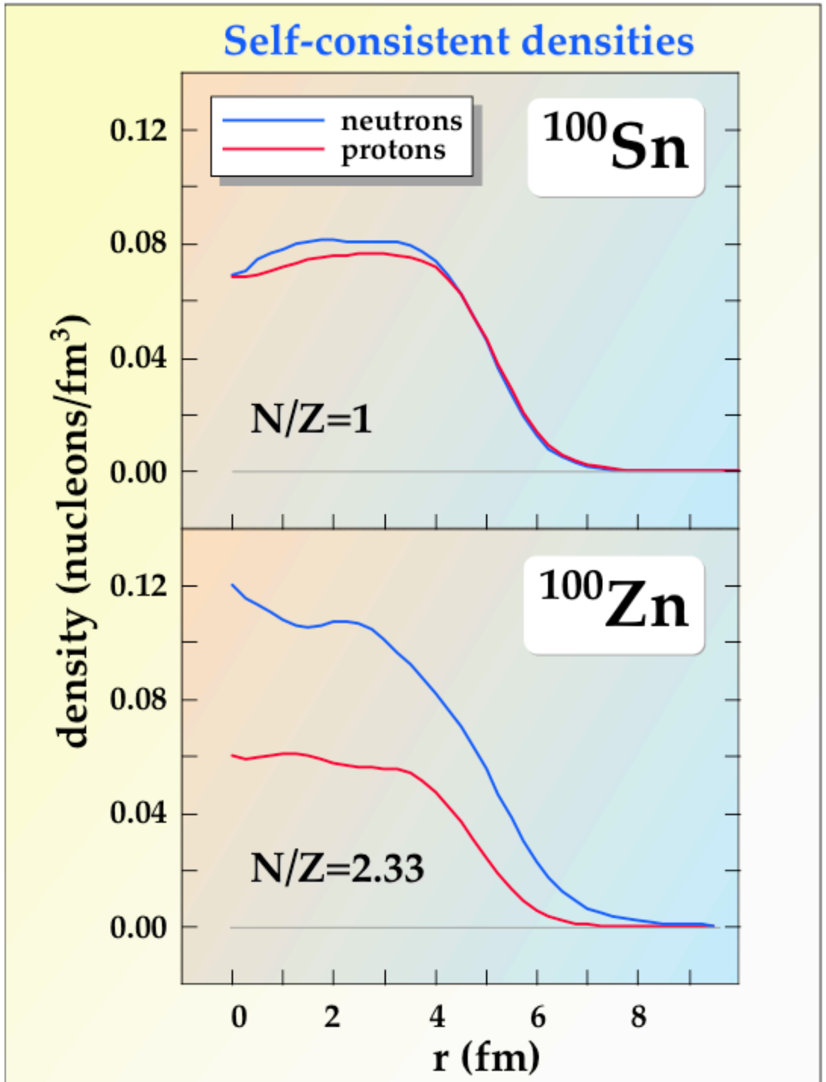


- two fermi liquids
- self-bound
- superfluid (ph and pp channels)
- self-consistent mean-fields
- broken-symmetry generalized product states

- Direct comparison with experiment
- Pseudo-data for reactions and astrophysics

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.

Nuclear Energy Density Functional

isoscalar (T=0) density $\left(\rho_0 = \rho_n + \rho_p\right)$

isovector (T=1) density $\left(\rho_1 = \rho_n - \rho_p\right)$

+isoscalar and isovector densities:
spin, current, spin-current tensor, kinetic, and kinetic-spin
+ pairing densities

$$E = \int \mathcal{H}(r) d^3 r$$

p-h density **p-p density (pairing functional)**

$$\mathcal{H}(r) = \frac{\hbar^2}{2m}\tau_0(r) + \sum_{t=0,1} \left(\chi_t(r) + \breve{\chi}_t(r)\right)$$

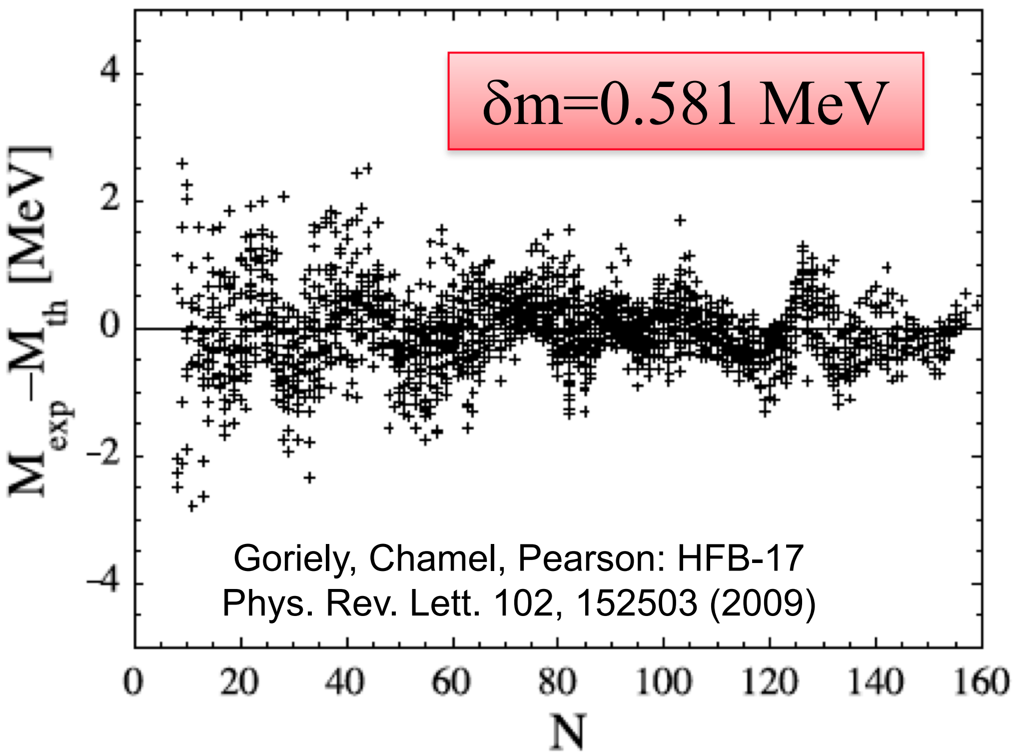
Expansion in densities and their derivatives

- Constrained by microscopic theory: ab-initio functionals provide quasi-data!
- Not all terms are equally important. Usually ~12 terms considered
- Some terms probe specific experimental data
- Pairing functional poorly determined. Usually 1-2 terms active.
- Becomes very simple in limiting cases (e.g., unitary limit)
- Can be extended into multi-reference DFT (GCM) and projected DFT

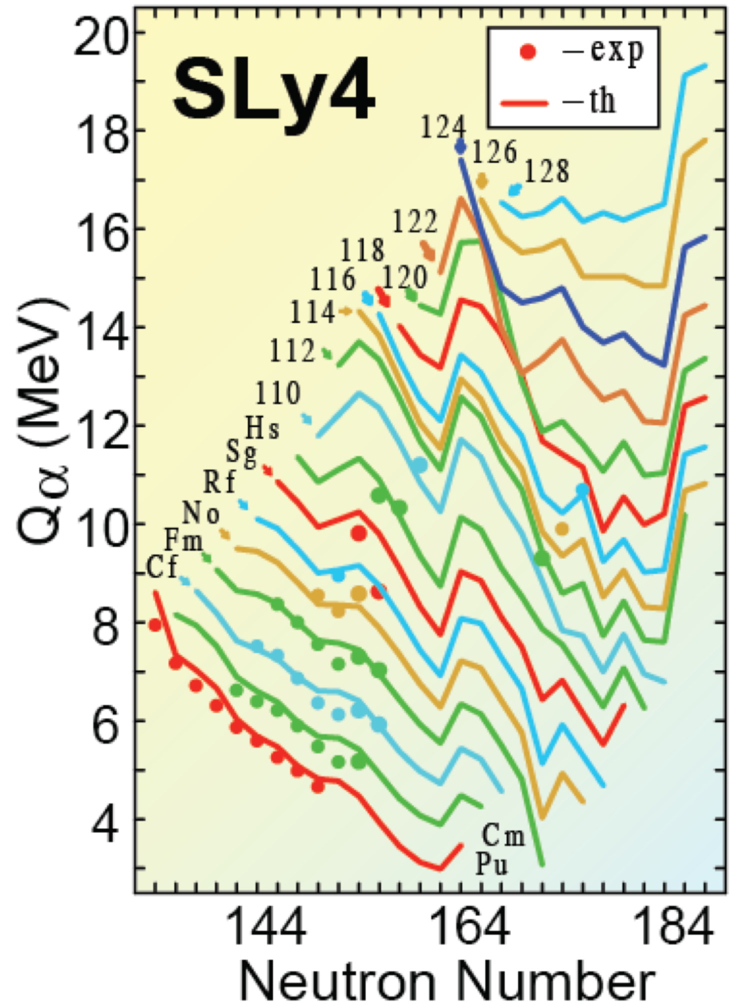
Examples: Nuclear Density Functional Theory

Traditional (limited) functionals provide quantitative description

Mass table

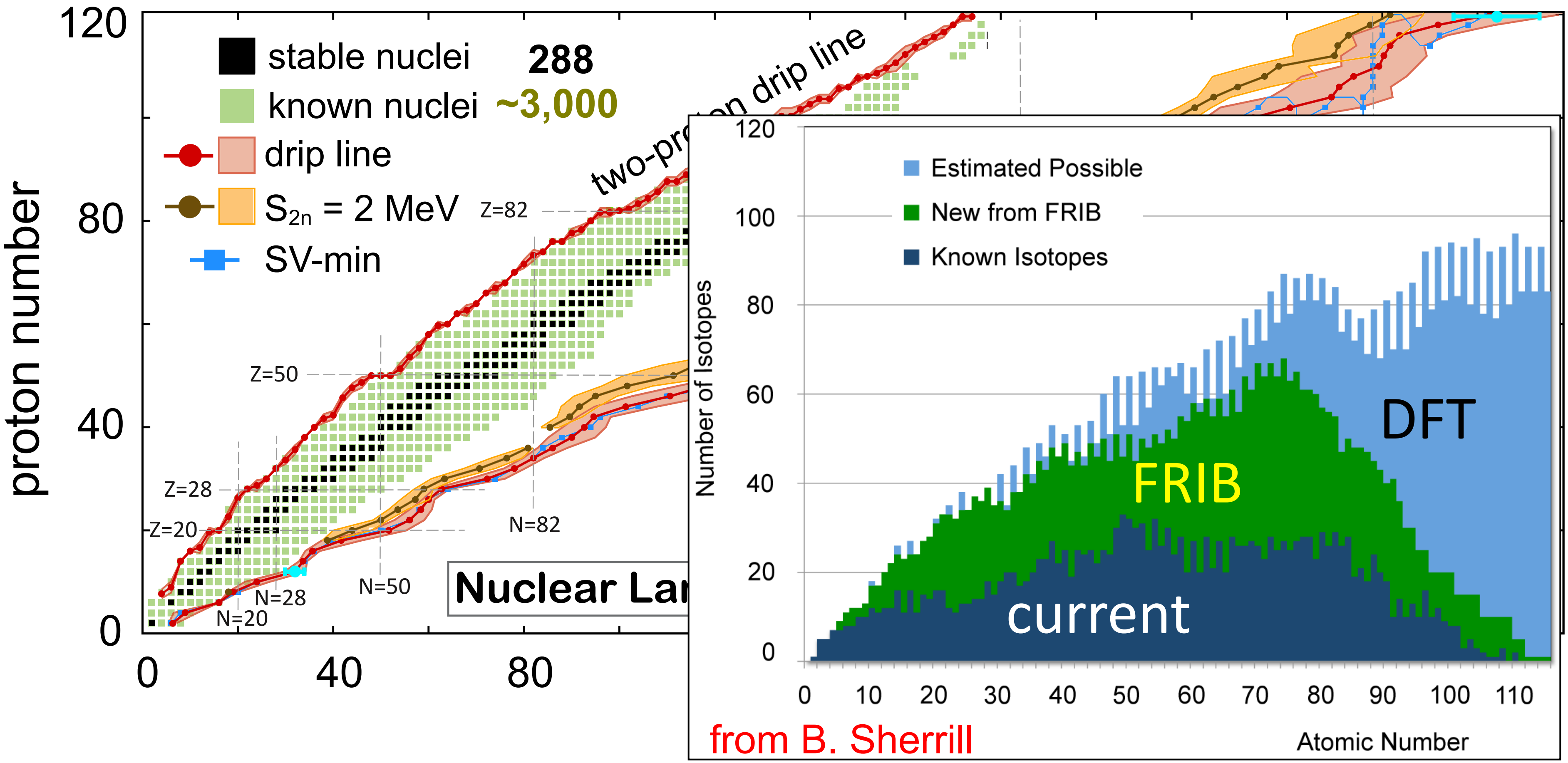


BE differences



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

Quantified Nuclear Landscape



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

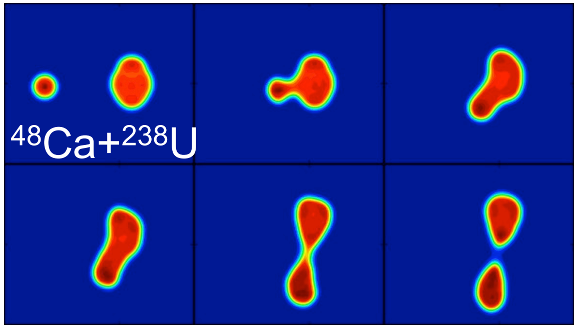
Erler et al.
Nature 486, 509 (2012)

Literature: 5,000-12,000

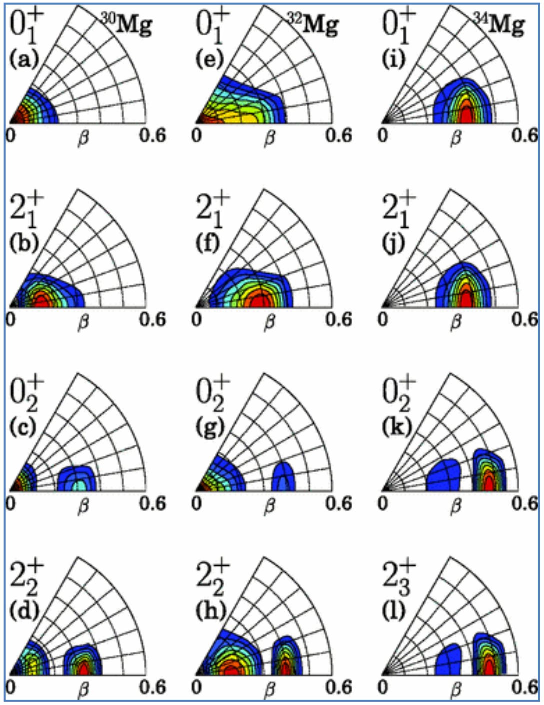
Skyrme-DFT: $6{,}900 \pm 500_{syst}$

Small and Large-Amplitude Collective Motion

- New-generation computational frameworks developed
  - Time-dependent DFT and its extensions
  - Collective Schrödinger Equation
  - Quasi-particle RPA
  - Projection techniques
- Applied to HI fusion, fission, coexistence phenomena



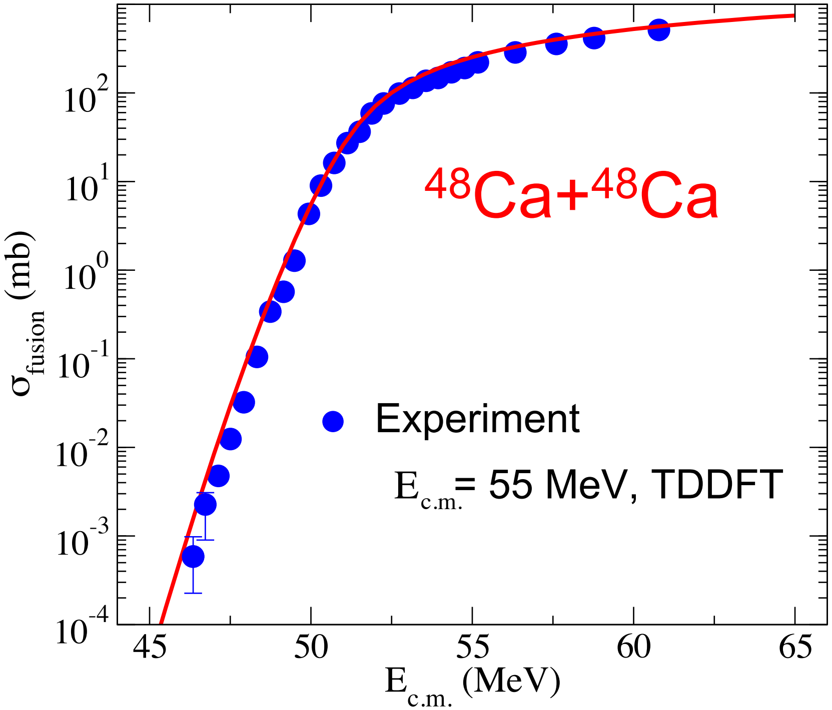
Shape coexistence



Hinohara et al. PRC 84, 061302(R) (2011)

also: Tsunoda et al. Phys. Rev. C 89, 031301(R) (2014); HPCI

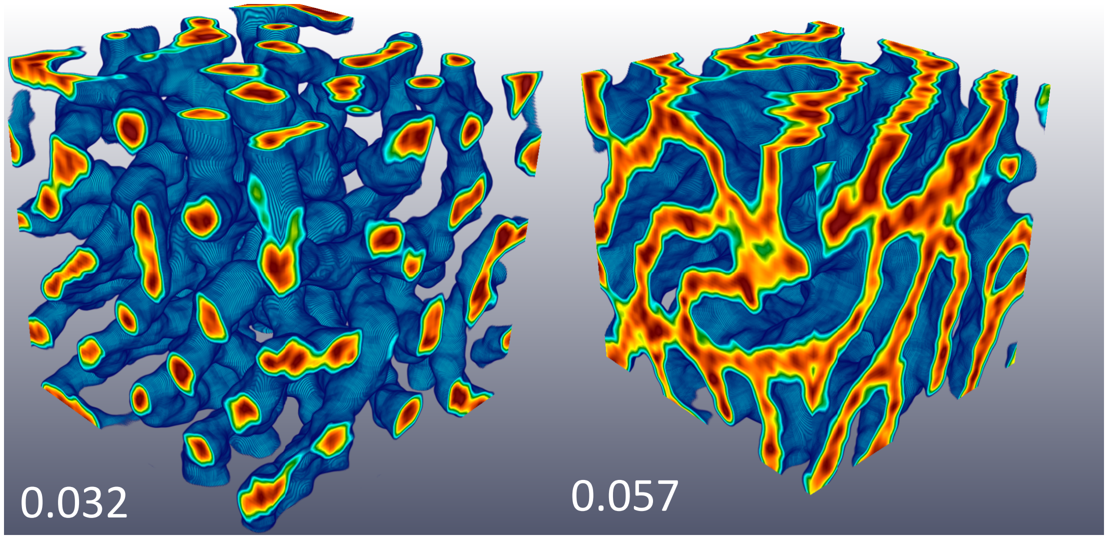
Fusion cross section

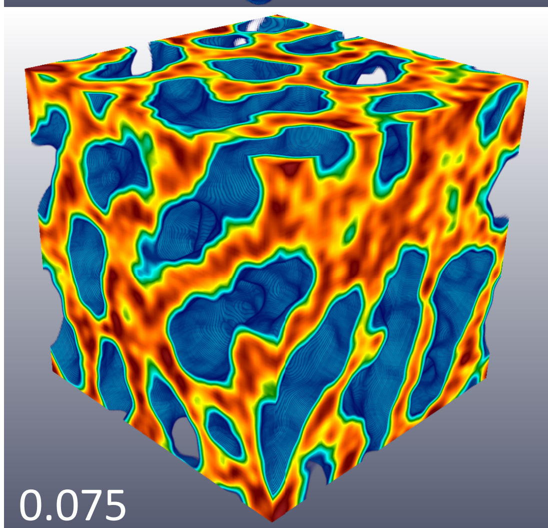


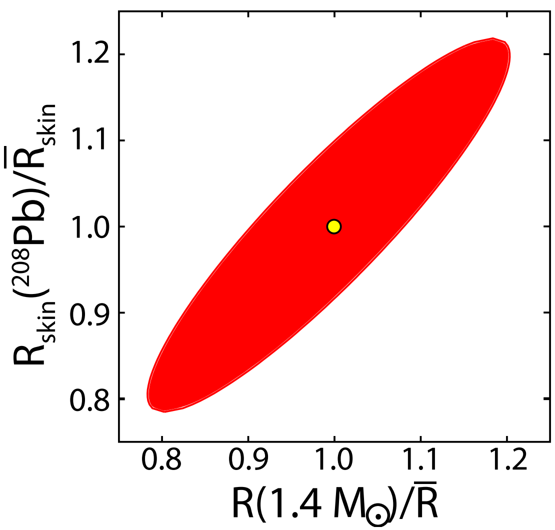
R. Keser et al., PRC 85, 044606 (2012)

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

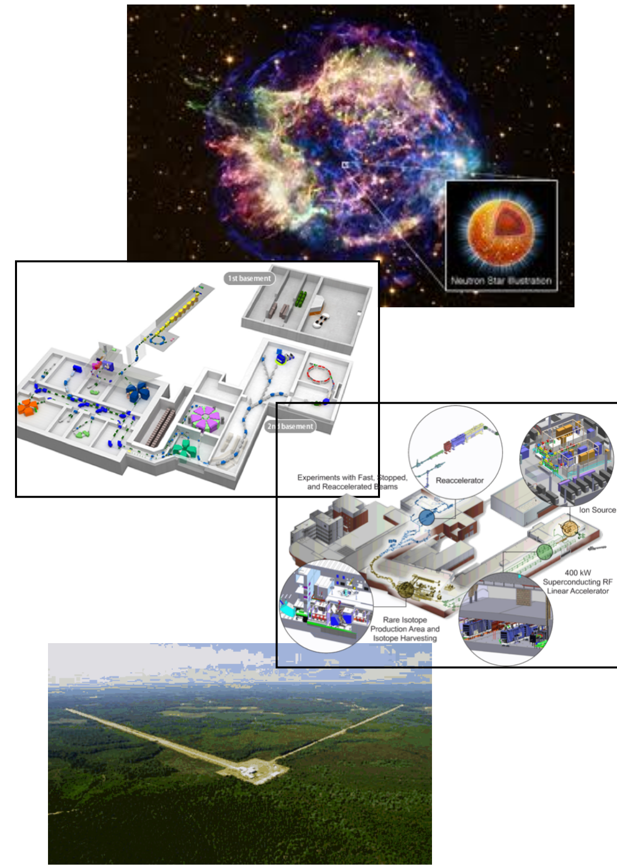
Crustal structures in neutron stars





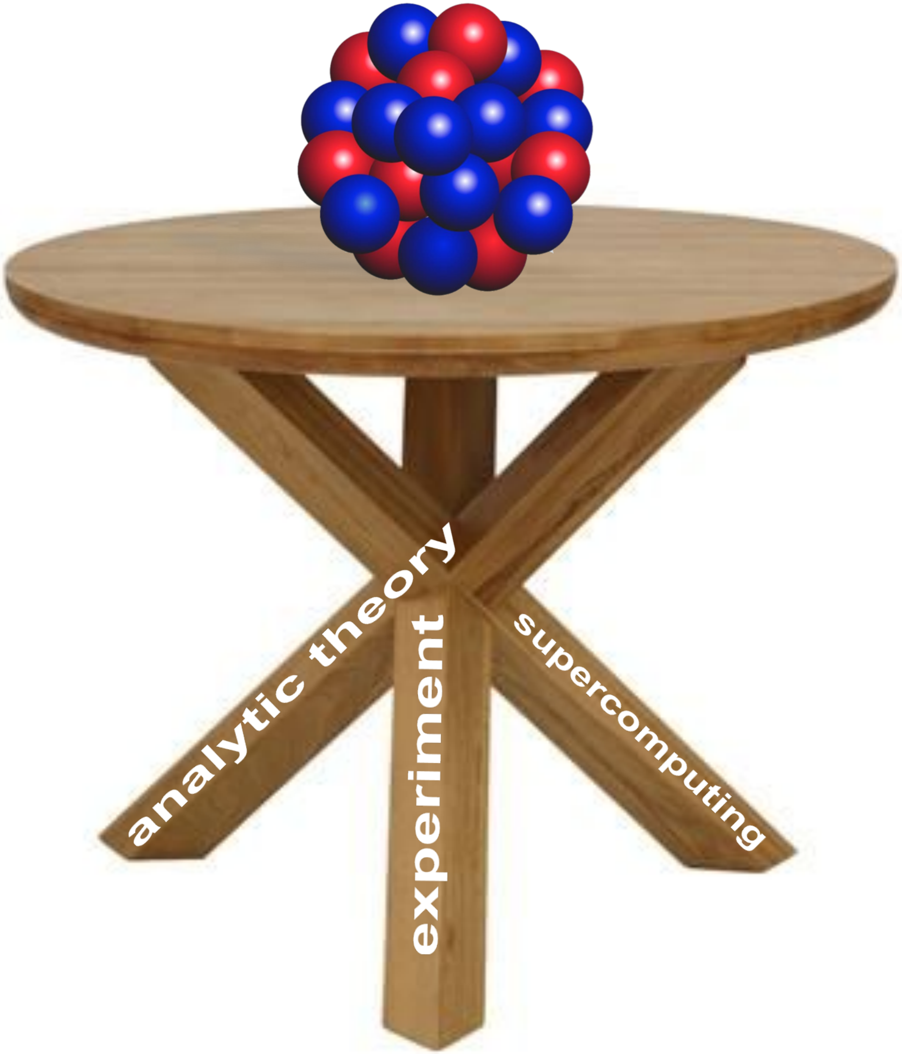


Data



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: $R(1.4M_\odot)$=10 km and R_{skin}= 0.17 fm.

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