Nuclear forces and their impact on structure, reactions and astrophysics

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Ohio State University

July, 2013

Lectures for Week 2

M. Chiral EFT 1 (as); χ-symmetry in NN scattering, QCD 2 (rjf)

T. Chiral EFT 2 (rjf); Three-nucleon forces 1 (as)

W. Renormalization group 1 (rjf);
Forces from LQCD (zd)

Th. Renormalization group 2 (rjf);
Three-nucleon forces 2 (as)

F. Many-body overview (rjf); Nuclear forces and electroweak interactions (as)

Outline

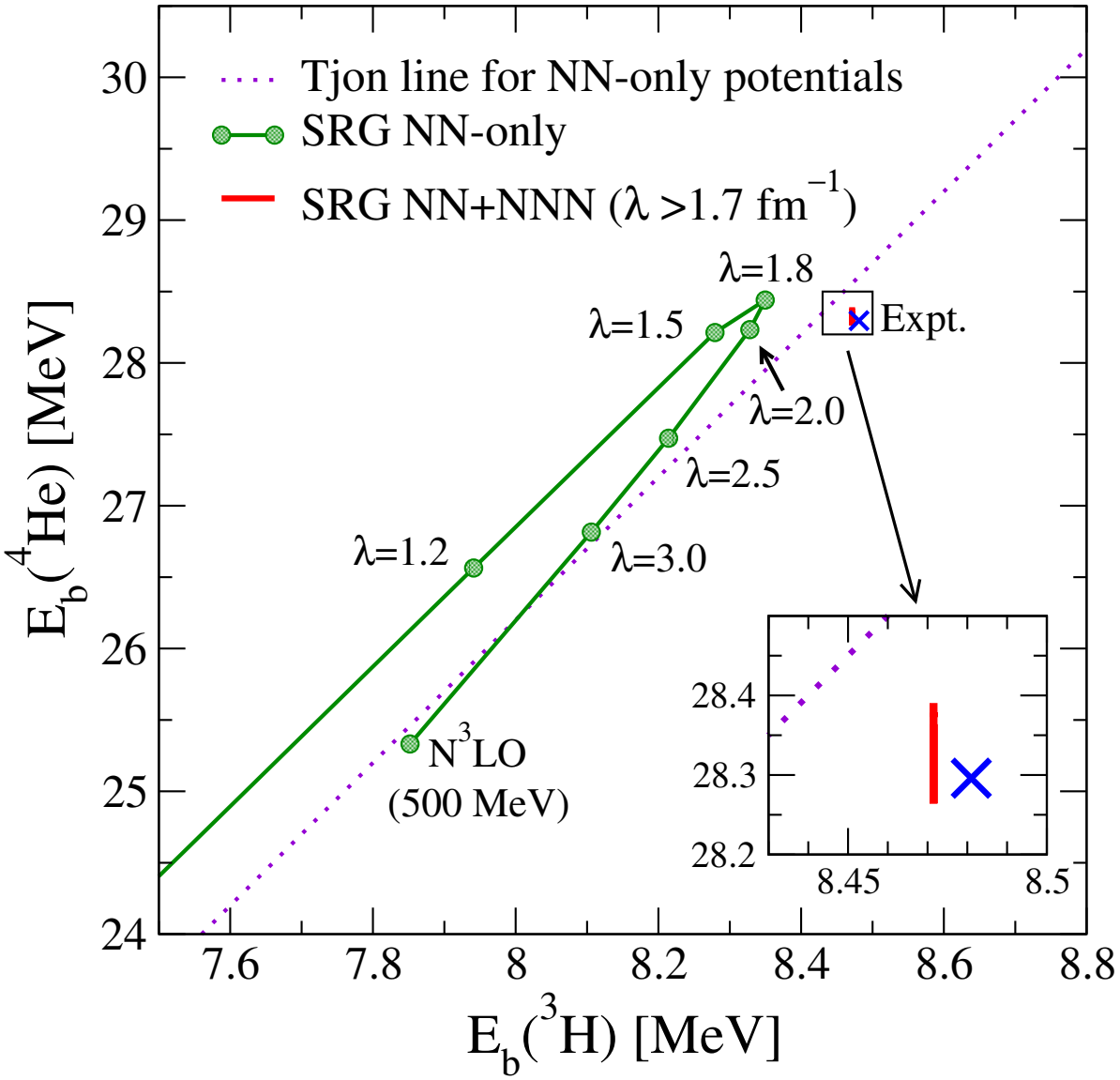
SRG leftovers

Overview of nuclear many-body problem

Many-body methods

Nuclear lattice simulations

Tjon line revisited



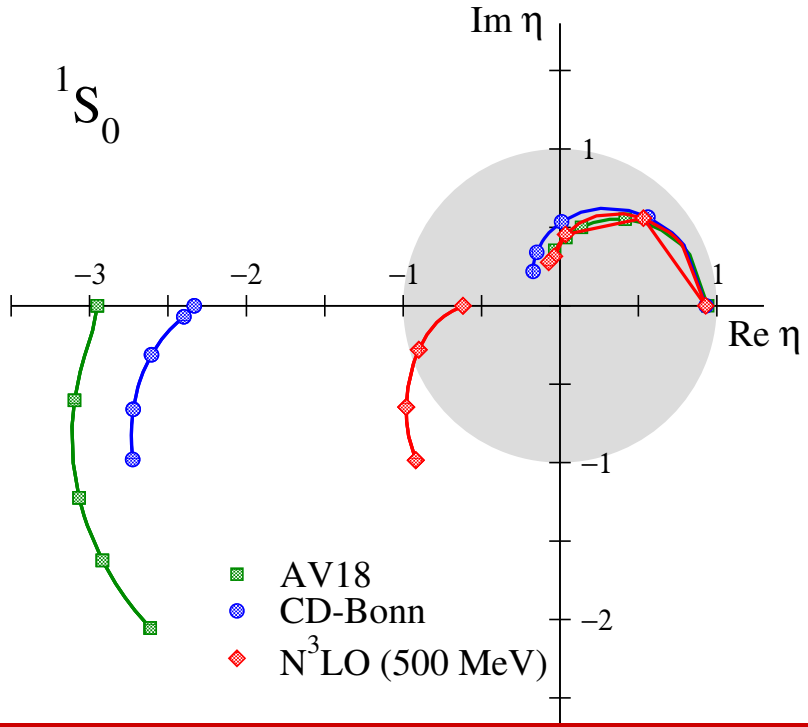
Weinberg eigenvalue analysis of convergence

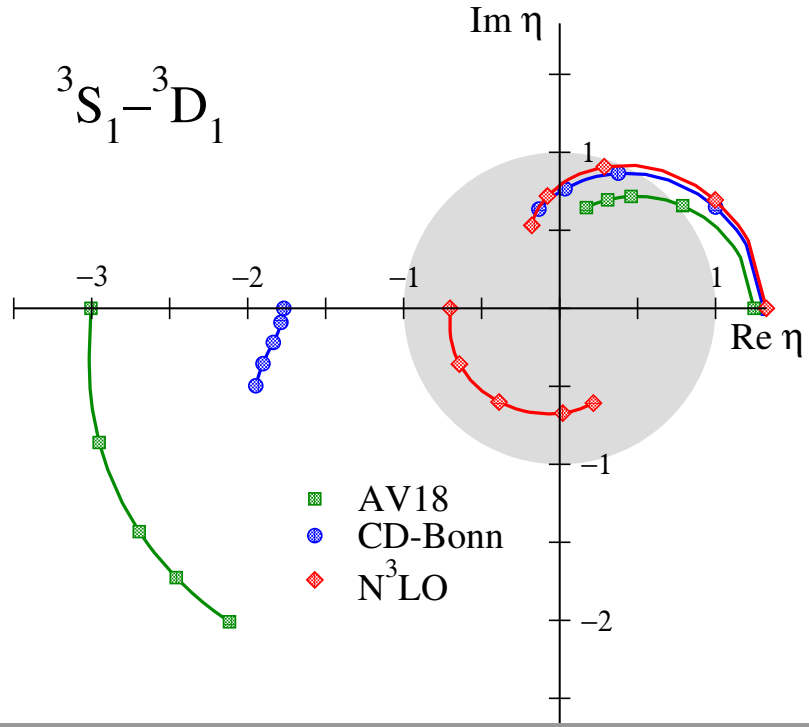
Born Series: $T(E) = V + V\frac{1}{E-H_0}V + V\frac{1}{E-H_0}V\frac{1}{E-H_0}V + \cdots$

- For fixed E, find (complex) eigenvalues $\eta_\nu(E)$ [Weinberg]

$$\frac{1}{E-H_0}V|\Gamma_\nu\rangle = \eta_\nu|\Gamma_\nu\rangle \quad \Longrightarrow \quad T(E)|\Gamma_\nu\rangle = V|\Gamma_\nu\rangle(1+\eta_\nu+\eta_\nu^2+\cdots)$$

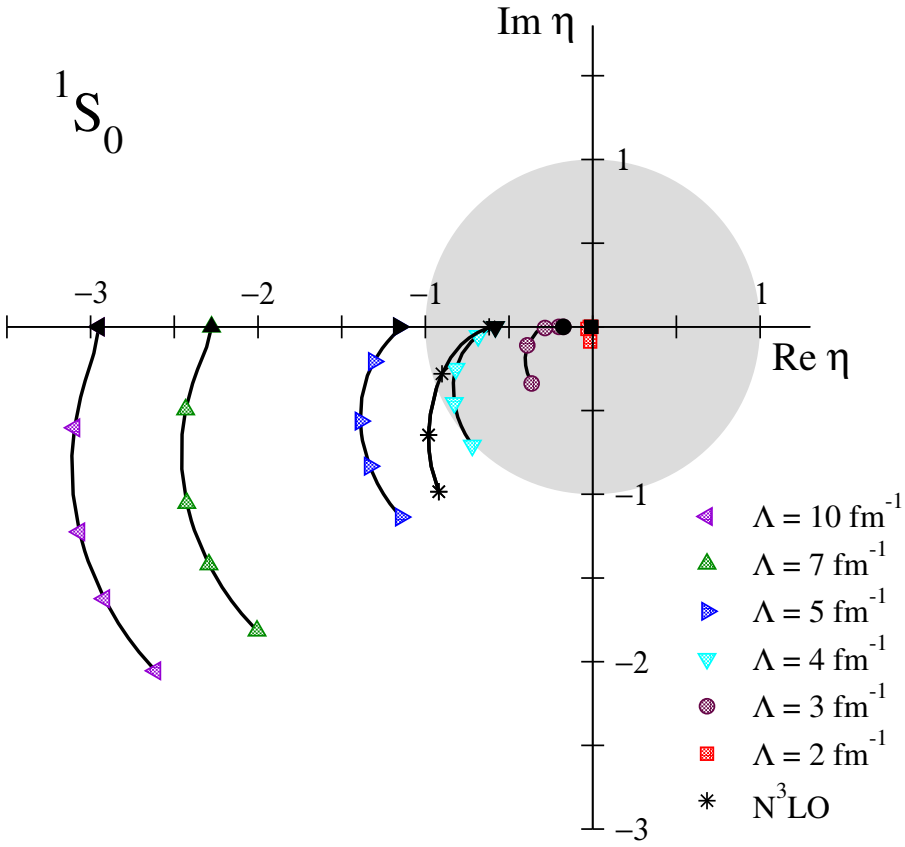
$\Longrightarrow$ T diverges if *any* $|\eta_\nu(E)| \geq 1$ [nucl-th/0602060]

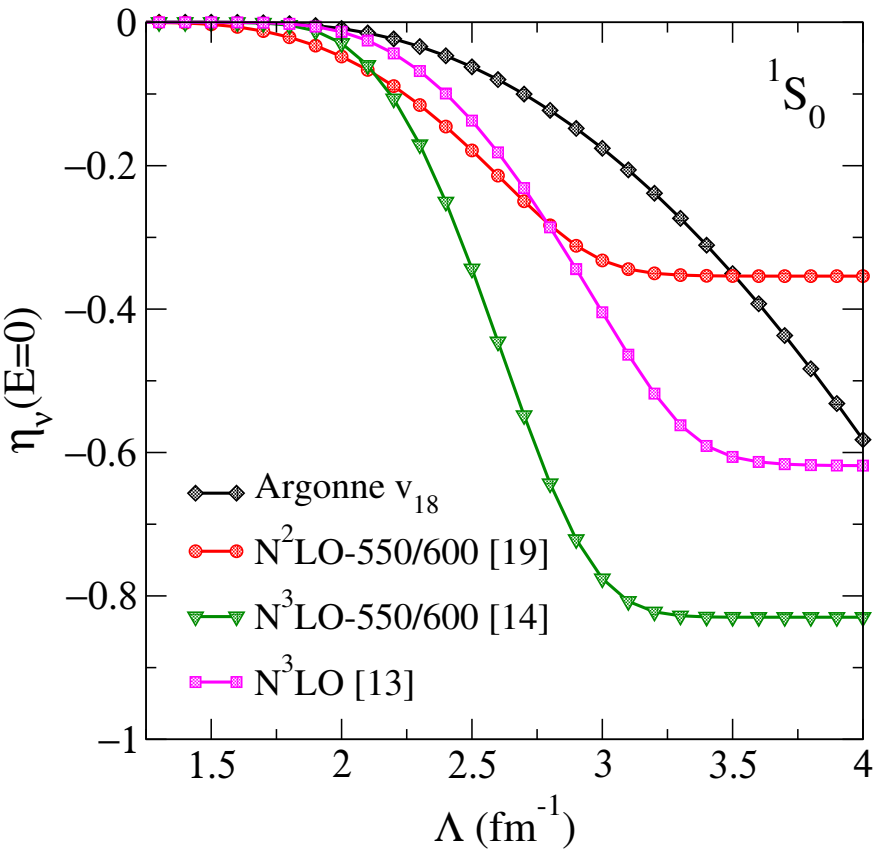




Lowering the cutoff increases "perturbativeness"

- Weinberg eigenvalue analysis (repulsive) [nucl-th/0602060]





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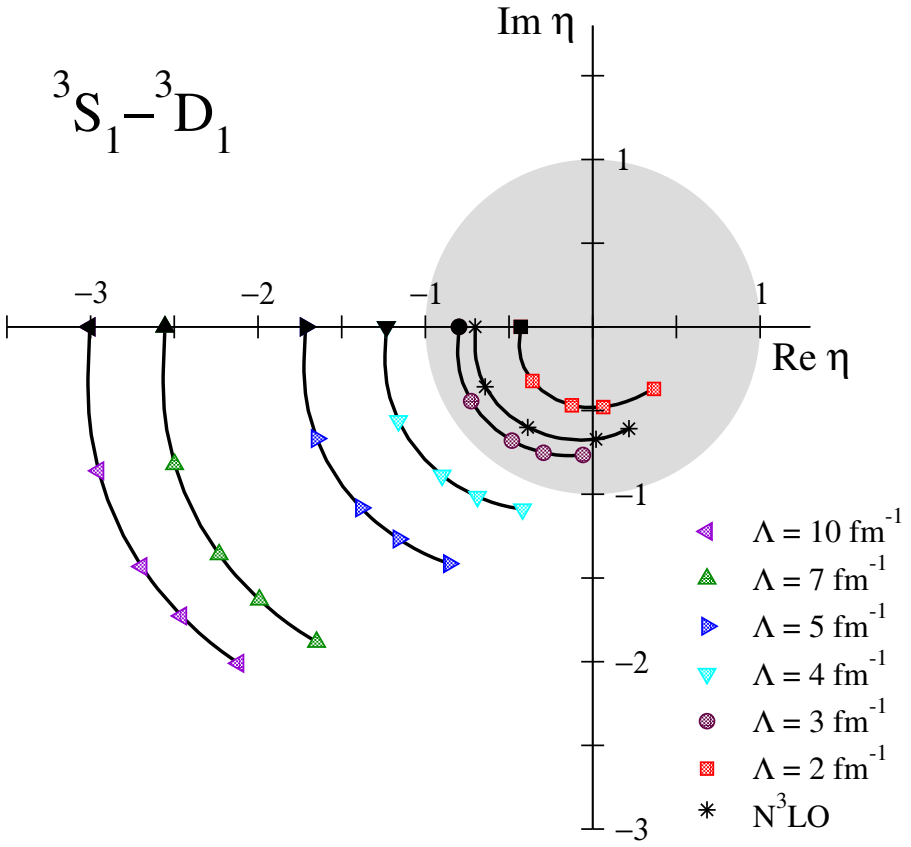
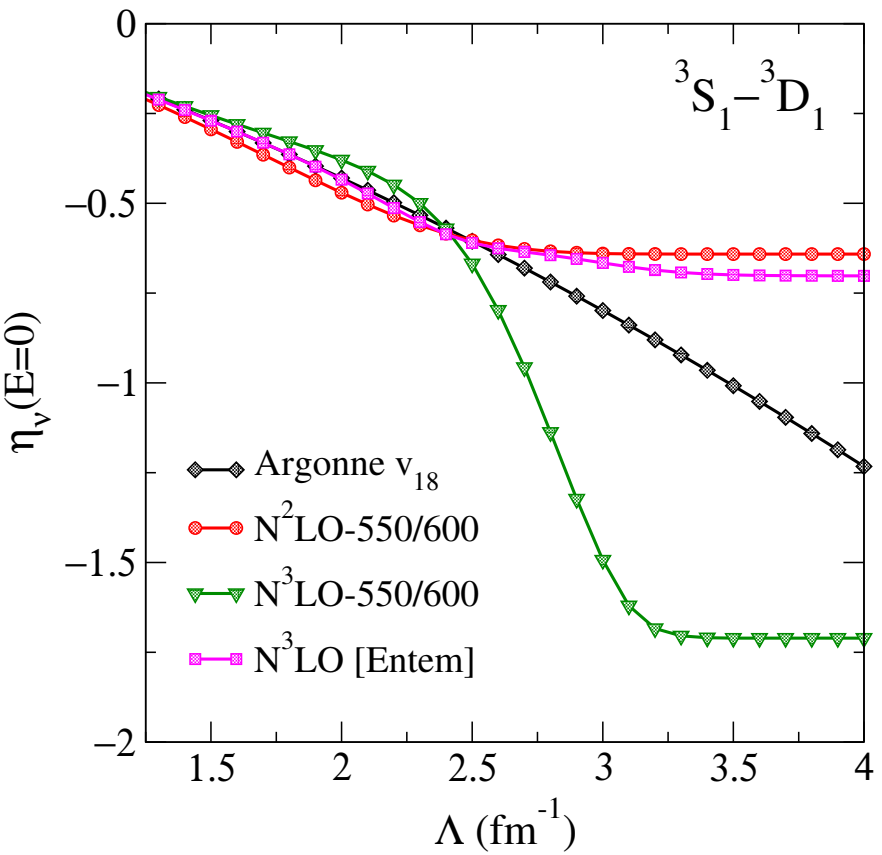
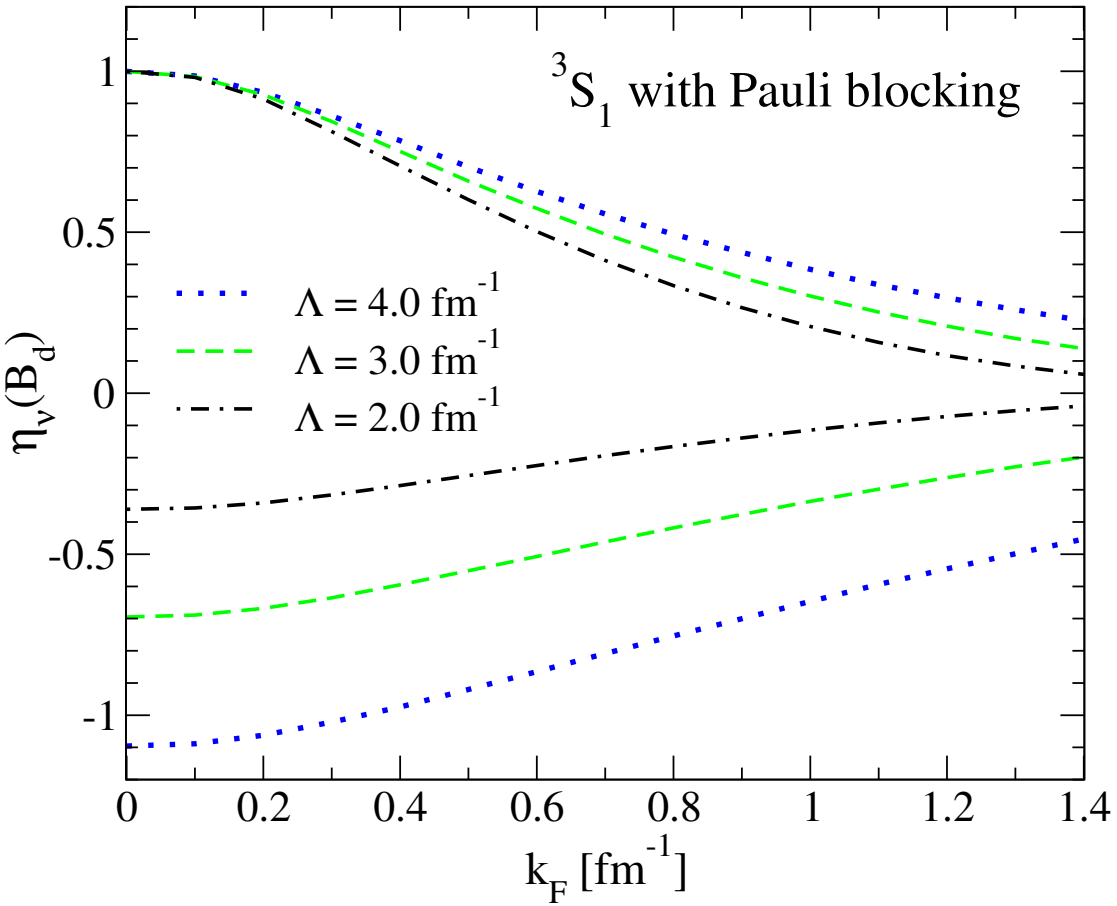




Lowering the cutoff increases "perturbativeness"

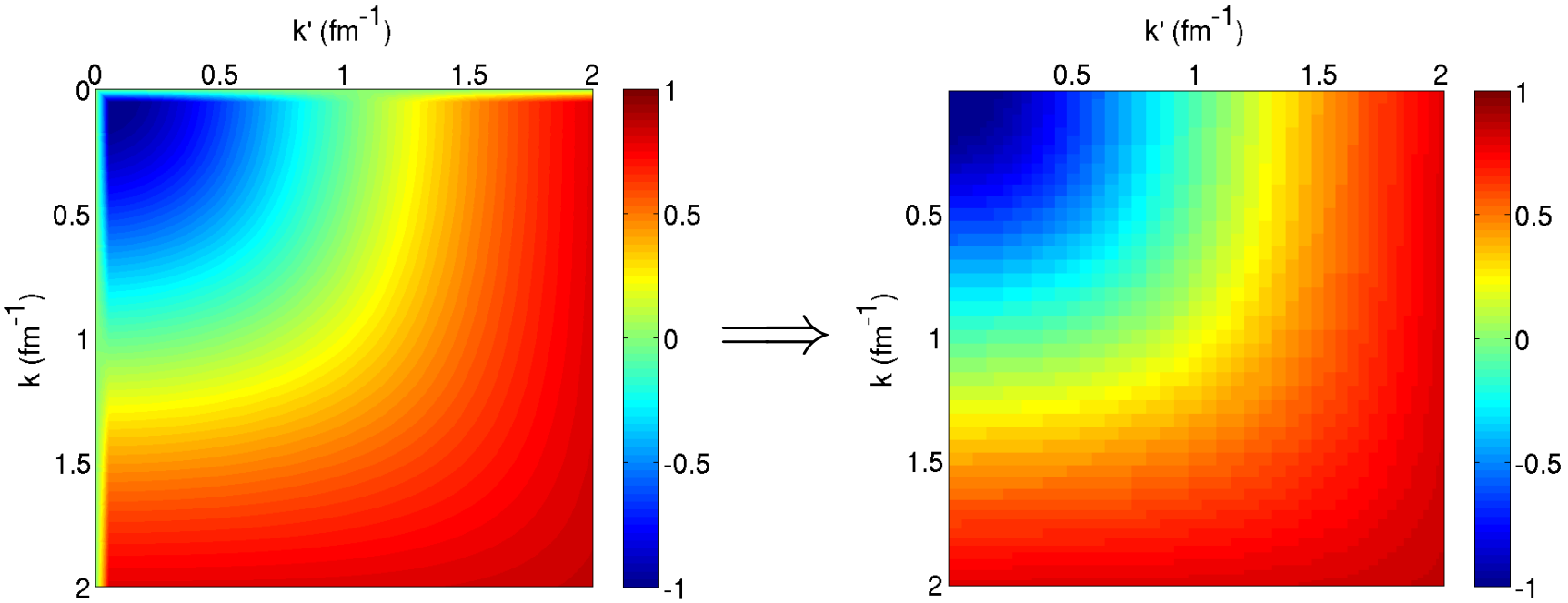
- Weinberg eigenvalue analysis (η_ν at -2.22 MeV vs. density)



- Pauli blocking in nuclear matter increases it even more!
  - at Fermi surface, pairing revealed by $|\eta_\nu| > 1$

Comments on computational aspects

- Although momentum is continuous in principle, in practice represented as discrete (gaussian quadrature) grid:



- Calculations become just matrix multiplications! E.g.,

$$\langle k|V|k\rangle + \sum_{k'} \frac{\langle k|V|k'\rangle\langle k'|V|k\rangle}{(k^2 - k'^2)/m} + \cdots \Longrightarrow V_{ii} + \sum_j V_{ij} V_{ji} \frac{1}{(k_i^2 - k_j^2)/m} + \cdots$$

- 100×100 resolution is sufficient for two-body potential

Discretization of integrals $\Longrightarrow$ matrices!

- Momentum-space flow equations have integrals like:

$$I(p,q) \equiv \int dk\, k^2\, V(p,k) V(k,q)$$

- Introduce gaussian nodes and weights $\{k_n, w_n\}$ $(n = 1, N)$

$$\Longrightarrow \quad \int dk\, f(k) \approx \sum_n w_n\, f(k_n)$$

- Then $I(p,q) \to I_{ij}$, where $p = k_i$ and $q = k_j$, and

$$I_{ij} = \sum_n k_n^2 w_n\, V_{in} V_{nj} \to \sum_n \widetilde{V}_{in} \widetilde{V}_{nj} \quad \text{where} \quad \widetilde{V}_{ij} = \sqrt{w_i} k_i\, V_{ij}\, k_j \sqrt{w_j}$$

- Lets us solve SRG equations, integral equation for phase shift, Schrödinger equation in momentum representation, ...
- In practice, N=100 gauss points more than enough for accurate nucleon-nucleon partial waves

MATLAB Code for SRG is a direct translation!

- The flow equation $\frac{d}{ds} V_s = [[T, H_s], H_s]$ is solved by discretizing, so it is just matrix multiplication.
- If the matrix V_s is converted to a vector by "reshaping", it can be fed to a differential equation solver, with the right side:

```
% V_s is a vector of the current potential; convert to square matrix
V_s_matrix = reshape(V_s, tot_pts, tot_pts);
H_s_matrix = T_matrix + V_s_matrix;  % form the Hamiltontian

% Matrix for the right side of the SRG differential equation
if (strcmp(evolution,'T'))
  rhs_matrix = my_commutator( my_commutator(T_matrix, H_s_matrix), ...
                              H_s_matrix );

elseif (strcmp(evolution,'Wegner'))
  rhs_matrix = my_commutator( my_commutator(diag(diag(H_s_matrix)), ...
                                            H_s_matrix), H_s_matrix );
```

[etc.]

```
% convert the right side matrix to a vector to be returned
dVds = reshape(rhs_matrix, tot_pts*tot_pts, 1);
```

Pseudocode for SRG evolution

1. Set up basis (e.g., momentum grid with gaussian quadrature or HO wave functions with $N_{\max}$)
2. Calculate (or input) the initial Hamiltonian and G_s matrix elements (including any weight factors)
3. Reshape the right side $[[G_s, H_s], H_s]$ to a vector and pass it to a coupled differential equation solver
4. Integrate V_s to desired s (or $\lambda = s^{-1/4}$)
5. Diagonalize H_s with standard symmetric eigensolver $\Longrightarrow$ energies and eigenvectors
6. Form $U = \sum_i |\psi_s^{(i)}\rangle\langle\psi_{s=0}^{(i)}|$ from the eigenvectors
7. Output or plot or calculate observables

Many versions of SRG codes are in use

- Mathematica, MATLAB, Python, C++, Fortran-90
  - Instructive computational project for undergraduates!
- Once there are discretized matrices, the solver is the same with any size basis in any number of dimensions!
- Still the same solution code for a many-particle basis
- Any basis can be used
  - For 3NF, harmonic oscillators, discretized partial-wave momentum, and hyperspherical harmonics are available
  - An accurate 3NF evolution in HO basis takes $\sim$ 20 million matrix elements $\Longrightarrow$ that many differential equations

Outline

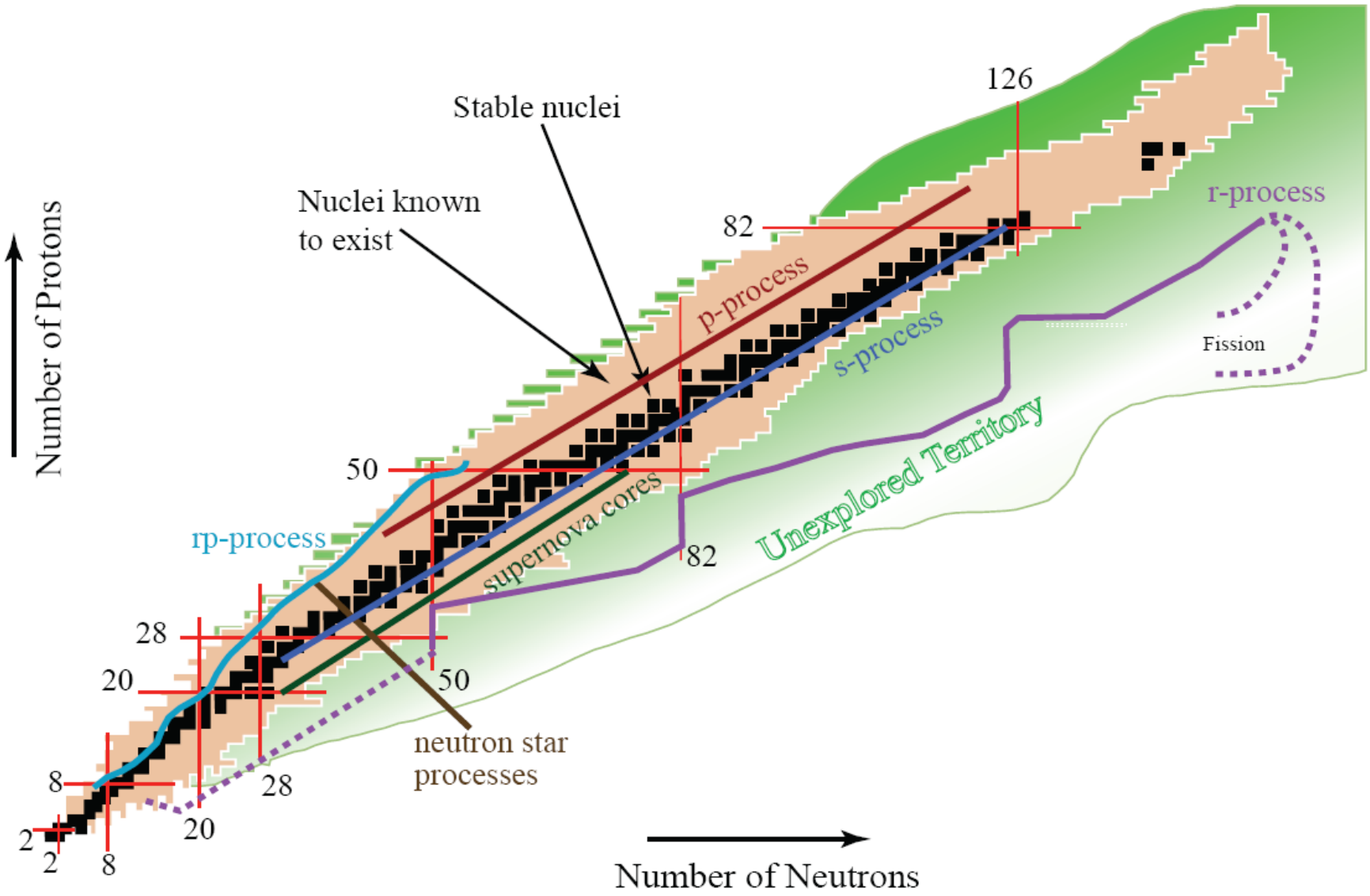
SRG leftovers

Overview of nuclear many-body problem

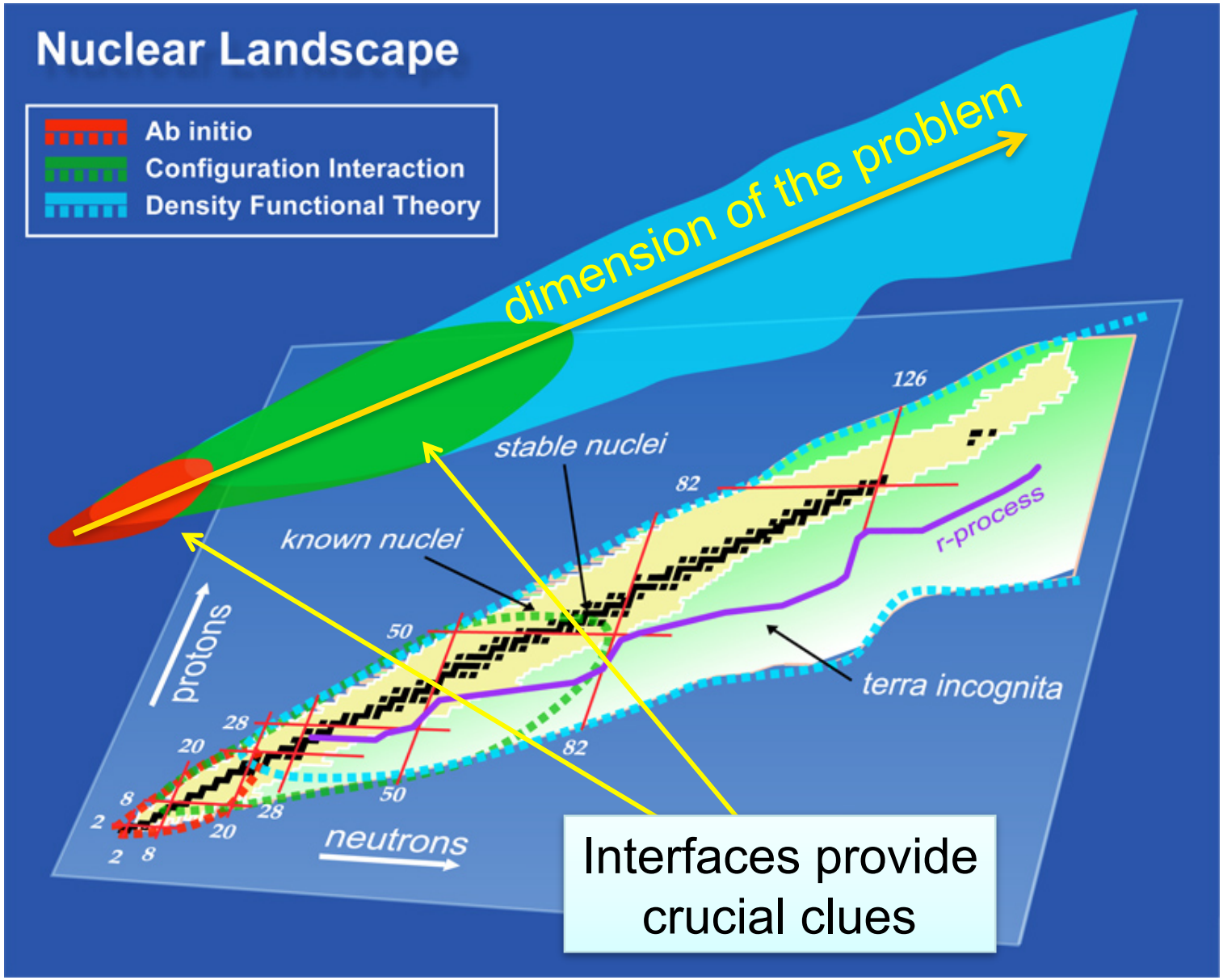
Many-body methods

Nuclear lattice simulations

Low-energy playground: Table of the nuclides



Overlapping theory methods cover all nuclei



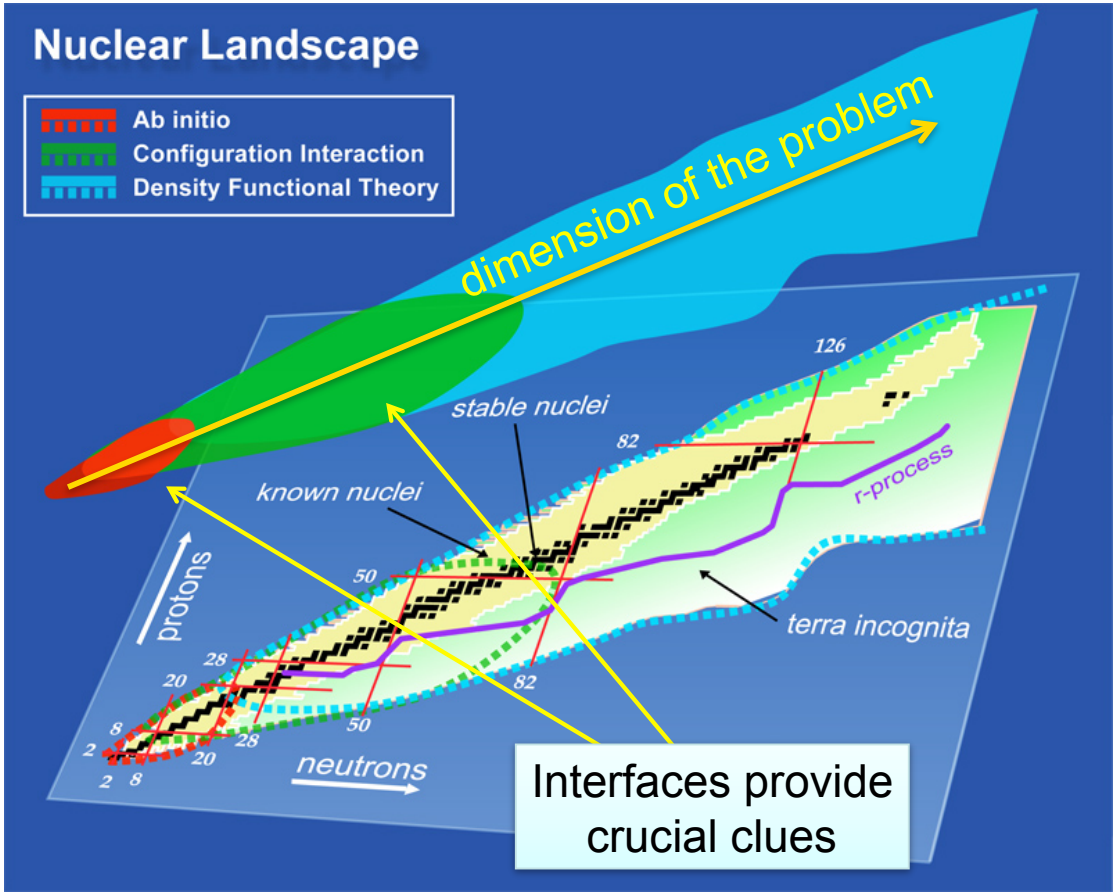
What is "new" about theory methods? (examples)

Really an explosion of new things!

- New methods for theoretical inputs (Hamiltonians and operators)
  - Three-body (and higher) forces (N3LO chiral 3NF, RG methods)
- New extensions of established microscopic techniques
  - e.g., IT-NCSM, MBPT, Berggren basis, LIT
  - Spectroscopic factors, ANCs, . . . (e.g., with GFMC, CC)
- New microscopic many-body techniques
  - e.g., Lattice EFT, IM-SRG, NCSM/RGM
- New analysis methods/philosophy (theory error bars!!)
  - Correlation analysis of energy functionals
  - Power counting, benchmarking, . . .
- New computational reach (e.g., from SciDAC projects)
  - Better scaling: massively parallel codes, load balancing
  - Improved algorithms: e.g., optimization (POUNDERS)

Why do we need so many different methods?

- Each method has strengths and limitations
- Need to cross-check results
- Exploit overlapping domains
- Trade-offs: Superior scaling vs. accuracy or more microscopic or . . .



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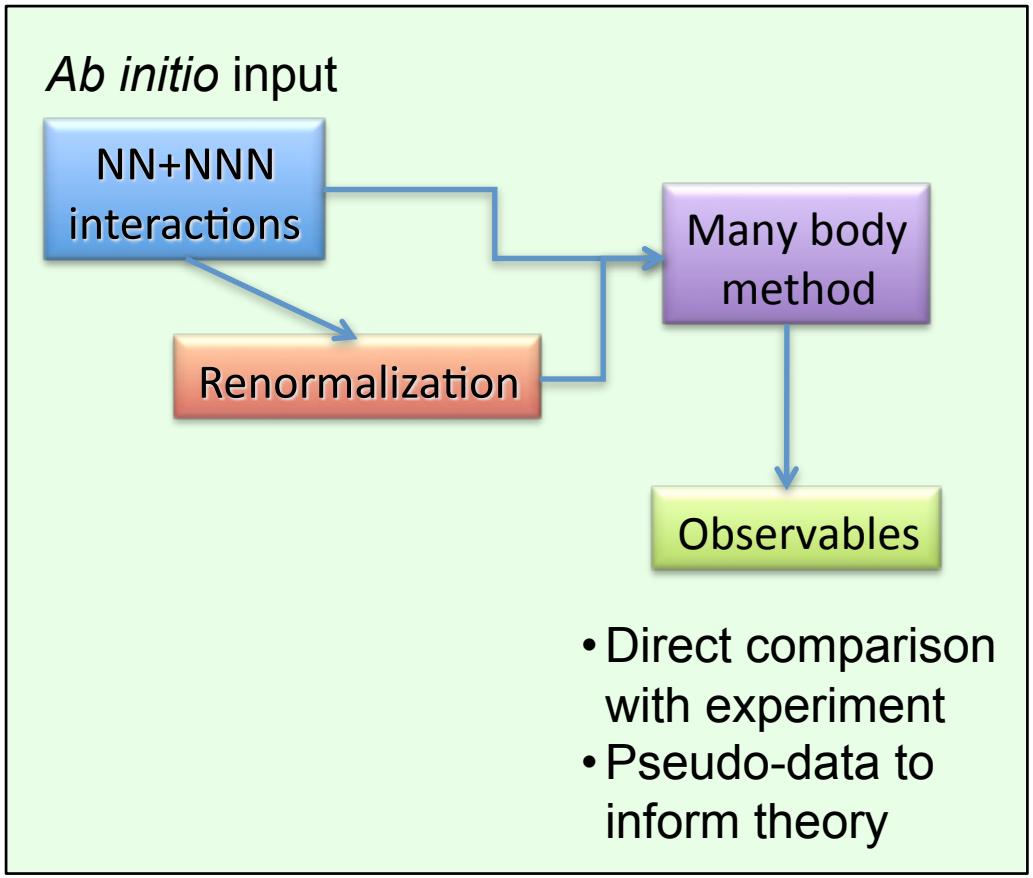
Fully microscopic (from input NN + NNN)

Ab initio theory for light nuclei and uniform matter

Ab initio: QMC, NCSM, CC,…

(nuclei, neutron droplets, nuclear matter)



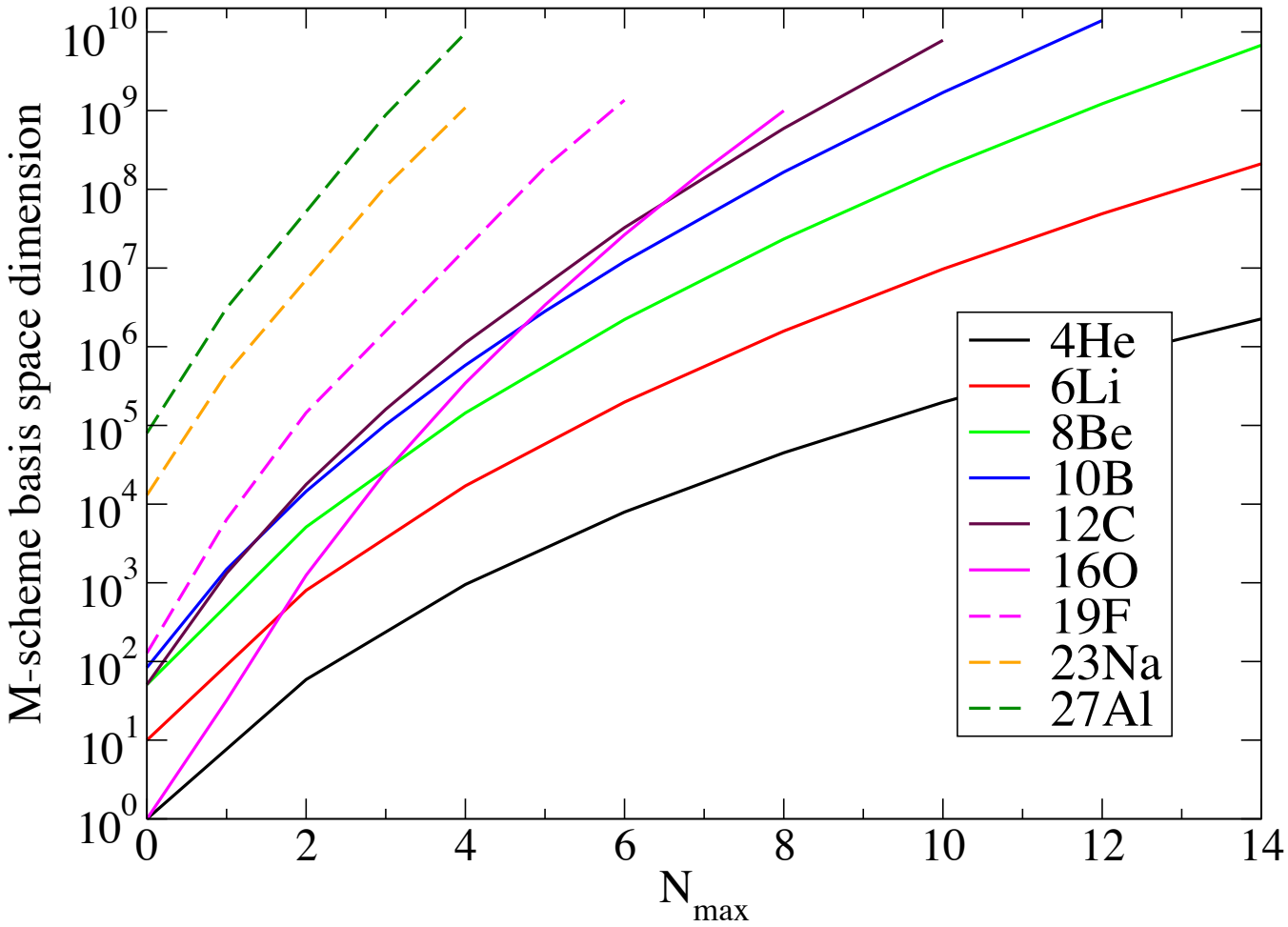
Input choices:

- Accurate forces based on phase shift analysis and few-body data
- EFT-based nonlocal chiral NN and NNN potentials
- RG-softened potentials evolved from NN+NNN interactions

- Quantum Monte Carlo (GFMC, lattice EFT) ^{12}C
- No-Core Shell Model ^{14}F, ^{14}C
- Coupled-Cluster Techniques ^{17}F, ^{48}Ca

Size and sparsity of Hamiltonian matrices [from P. Maris]

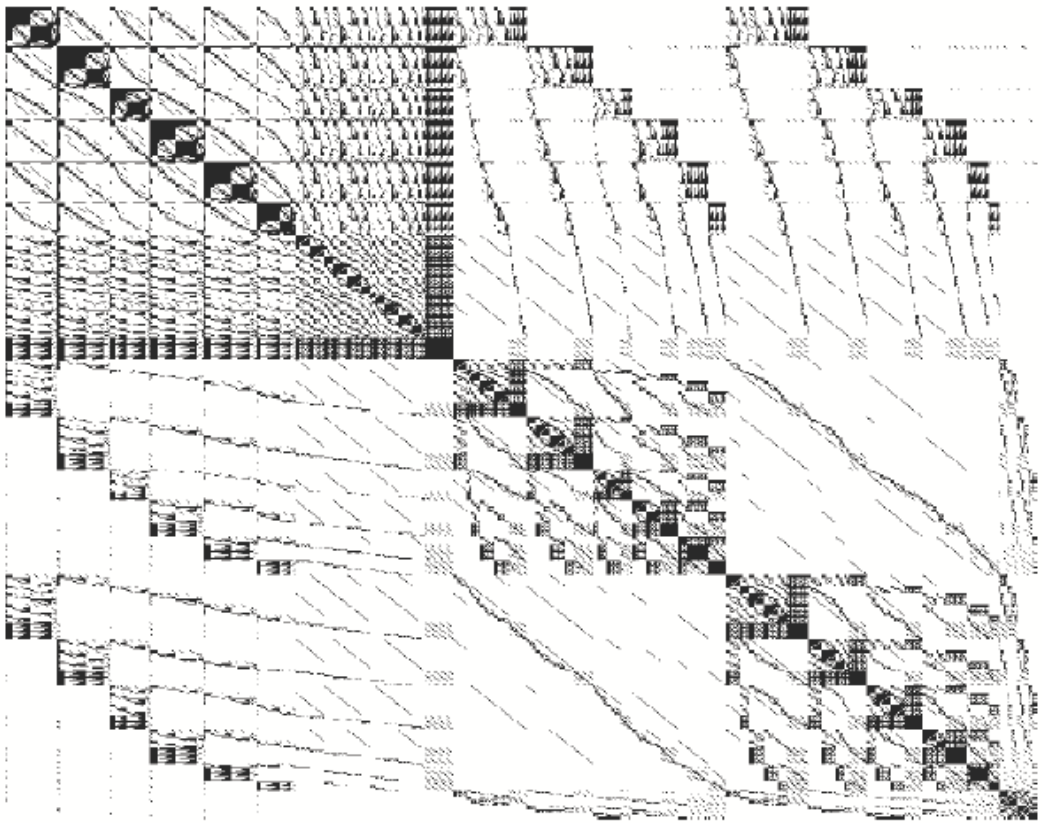
- Hamiltonian matrices grow rapidly with basis size ($N_{\max}$) and $A = N + Z$ from combinatorics:



Size and sparsity of Hamiltonian matrices [from P. Maris]

- But fortunately there are many zero elements so storage is large but feasible. How can we take advantage of sparsity?

Sparsity Structure for ^{6}Li



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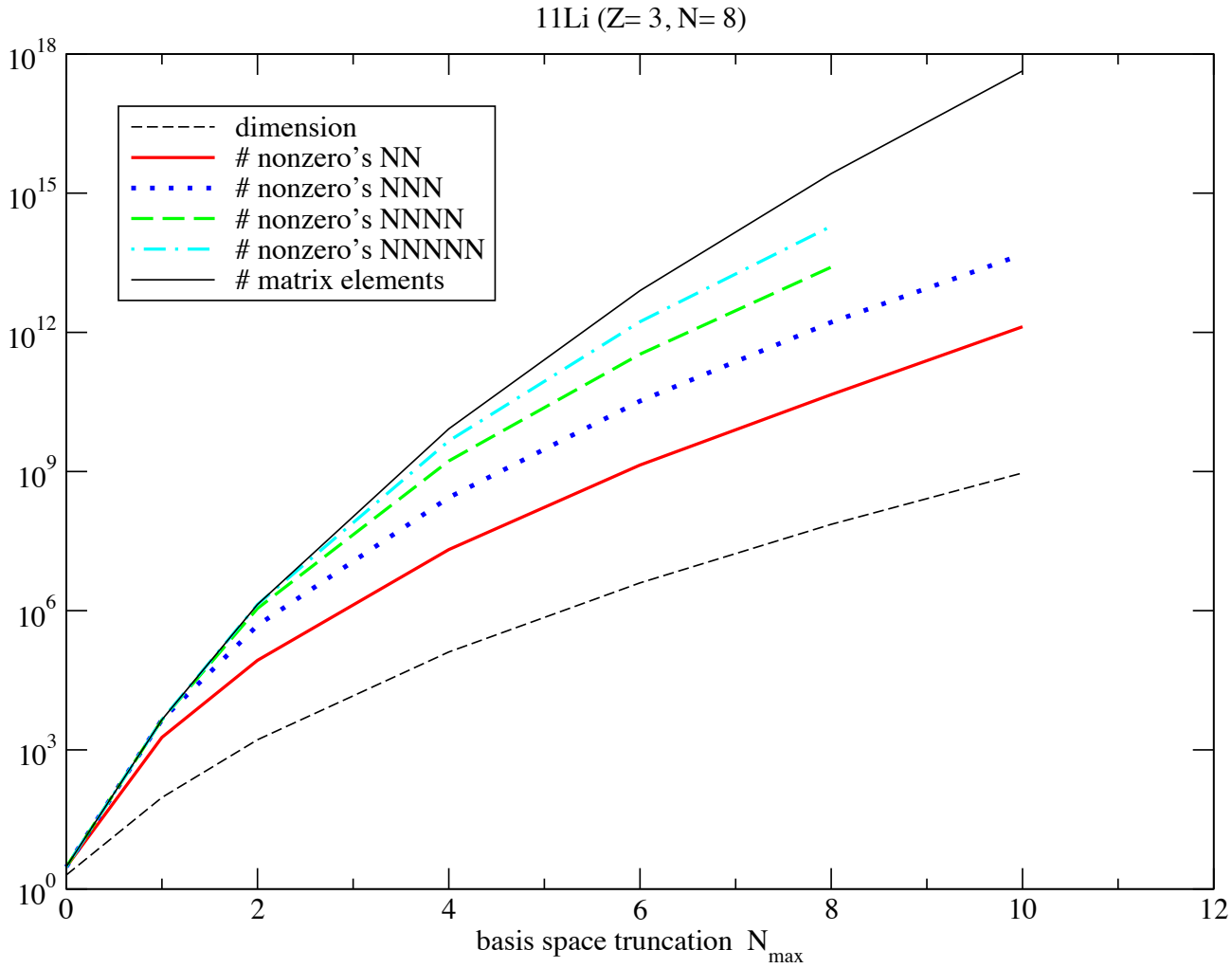


Lanczos method in short

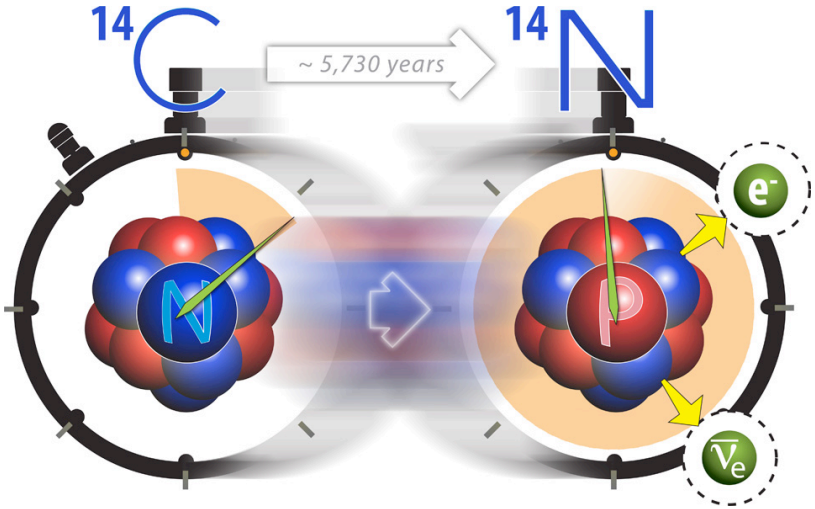
- Consider an arbitrary vector $|\Psi\rangle$ and its expansion in eigenstates of H, where $H|\psi_k\rangle = E_k|\psi_k\rangle$. Then $H^m|\Psi\rangle = \sum_k C_k E_k^m |\psi_k\rangle$
  - If m large enough, largest $|E_k|$ will dominate the sum $\Longrightarrow$ project out the corresponding eigenvector
  - To get lowest eigenvalue, use $(H - \sigma I)^m$ with $\sigma > 0$ large enough so that $|E_0 - \sigma| > |E_{\rm max} - \sigma|$
- More efficient to diagonalize H in the basis spanned by $H|\psi_k\rangle$, $H^2|\psi_k\rangle, \ldots, H^m|\psi_k\rangle$
  - Called the "Krylov space"
  - Lanczos: orthogonalize basis states as you go, generating H in tri-diagonal form, which is efficiently diagonalized
  - Re-orthonormalization for numerical stability
- Many computational advantages to treating sparse matrices with Lanczos [see J. Vary et al., arXiv:0907.0209]

U.S. DEPARTMENT OF ENERGY | Office of Science

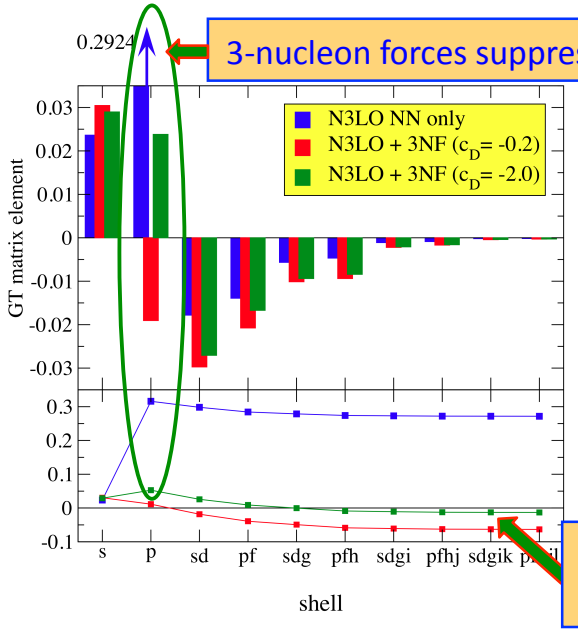
"Why does Carbon-14 live so long?"

Carbon-14 dating relies on ~5,730 year half-life, but other light nuclei undergo similar beta decay with half-lives less than a day!

UNEDF SciDAC Collaboration
Universal Nuclear Energy Density Functional



- Members of UNEDF collaboration made microscopic nuclear structure calculations to solve the puzzle
- Used systematic chiral Hamiltonian from low-energy effective field theory of QCD
- Key feature: consistent *3-nucleon* interactions



3-nucleon forces suppress critical component compared to 2-nucleon forces only

net decay rate is very small

- Solutions of ^{14}C and ^{14}N through Hamiltonian diagonalization
- 100-fold reduction in Gamow-Teller transition matrix element

Calculations enabled by high-performance computing through INCITE program

- Dimension of matrix solved for 8 lowest states: ~ 1×10^9
- Solution took ~ 6 hours on 215,000 cores on Cray XT5 Jaguar at ORNL

Office of Science INCITE Advancing America's Science and Industrial Competitiveness

Science ref.: Physical Review Letters **106**, 202502 (2011)
Computational ref.: Procedia Computer Science **1**, 97 (2010)

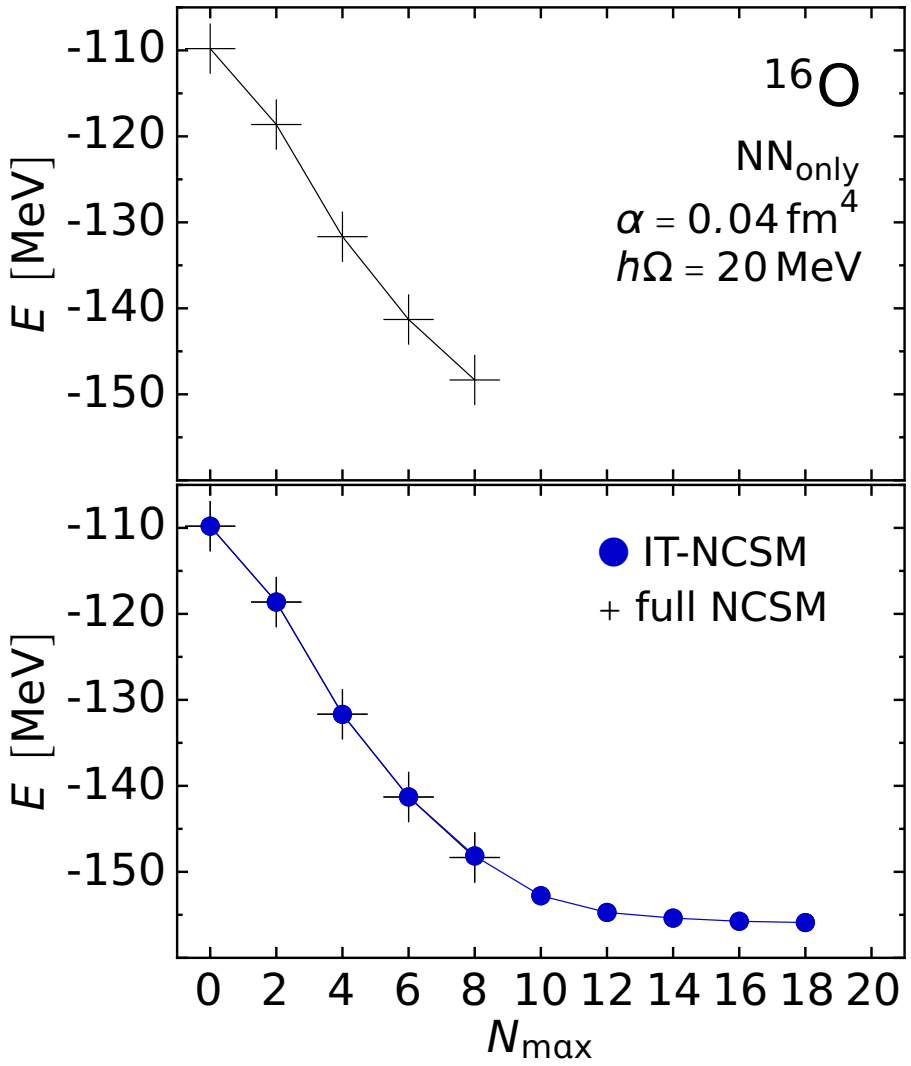
Importance Truncated NCSM [Roth et al.]

Roth, PRC 79, 064324 (2009); PRL 99, 092501 (2007)

- converged NCSM calculations essentially restricted to lower/mid p-shell
- full $N_{max} = 10$ calculation for ^{16}O very difficult (basis dimension $> 10^{10}$)

Importance Truncation

reduce model space to the relevant basis states using an **a priori importance measure** derived from MBPT



Coupled cluster method [from D. Dean, G. Hagen, T. Papenbrock]

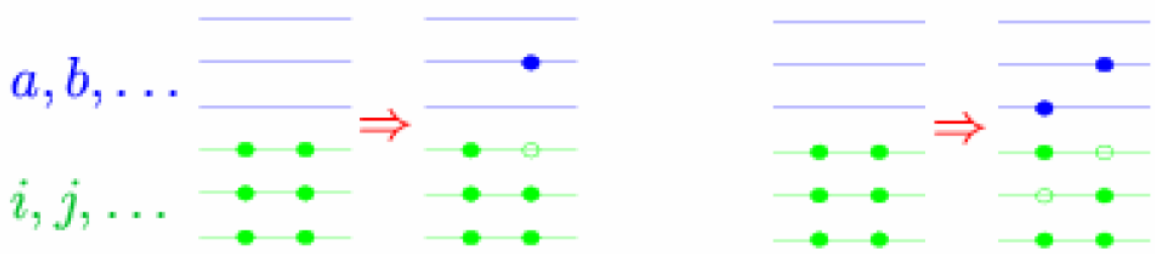
Coupled-cluster method (in CCSD approximation)

Ansatz:

$$
\begin{aligned}
|\Psi\rangle &= e^{T}|\Phi\rangle \\
T &= T_1 + T_2 + \dots \\
T_1 &= \sum_{ia} t_i^a a_a^\dagger a_i \\
T_2 &= \sum_{ijab} t_{ij}^{ab} a_a^\dagger a_b^\dagger a_j a_i
\end{aligned}
$$

- ☺ Scales gently (polynomial) with increasing problem size o^2u^4 .
- ☺ Truncation is the only approximation.
- ☺ Size extensive (error scales with A)
- ☹ Most efficient for doubly magic nuclei

Correlations are *exponentiated* 1p-1h and 2p-2h excitations. Part of np-nh excitations included!



Coupled cluster equations

$$
\begin{aligned}
E &= \langle\Phi|\overline{H}|\Phi\rangle \\
0 &= \langle\Phi_i^a|\overline{H}|\Phi\rangle \\
0 &= \langle\Phi_{ij}^{ab}|\overline{H}|\Phi\rangle
\end{aligned}
$$

Alternative view: CCSD generates similarity transformed Hamiltonian with no 1p-1h and no 2p-2h excitations.

$$
\overline{H} \equiv e^{-T} H e^{T} = \left(He^{T}\right)_c = \left(H + HT_1 + HT_2 + \frac{1}{2}HT_1^2 + \dots\right)_c
$$

Coupled cluster method [from D. Dean, G. Hagen, T. Papenbrock]

Asymmetry dependence and spectroscopic factors

- Spectroscopic factors are not observables
- They are extracted from a cross section based on a specific structure and reaction model
- Structure and reaction models needs to be consistent!

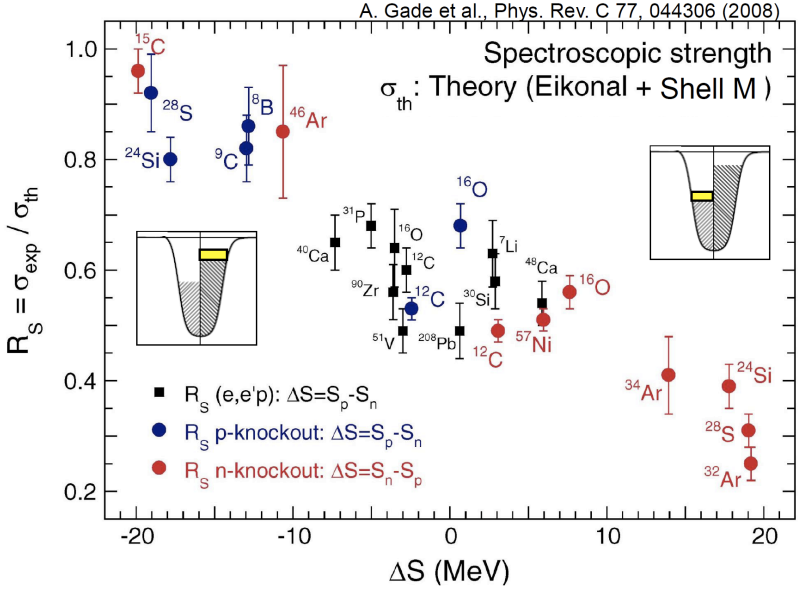
Theoretical cross section:

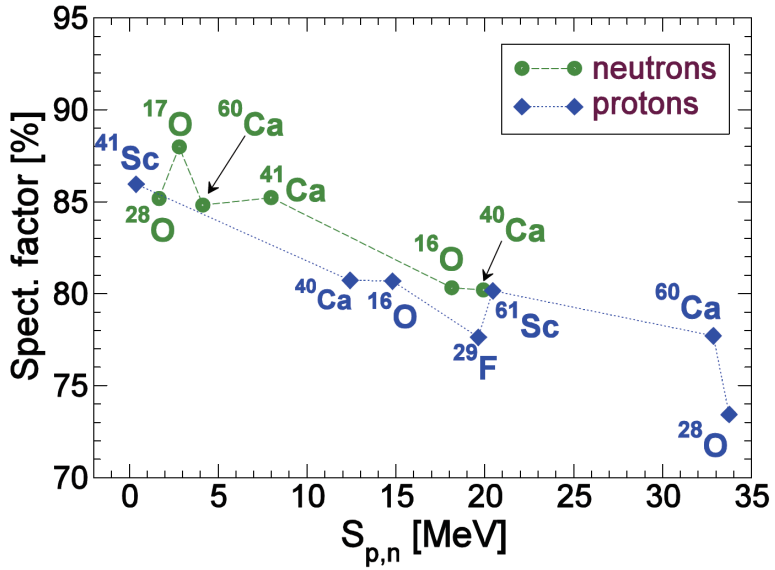
$$\sigma(j^\pi) = \left(\frac{A}{A-1}\right)^N C^2 S(j^\pi) \sigma_{sp}(j, S_N + E_x[j^\pi])$$

Reaction theory

Structure theory

A. Gade et al., Phys. Rev. C 77, 044306 (2008)



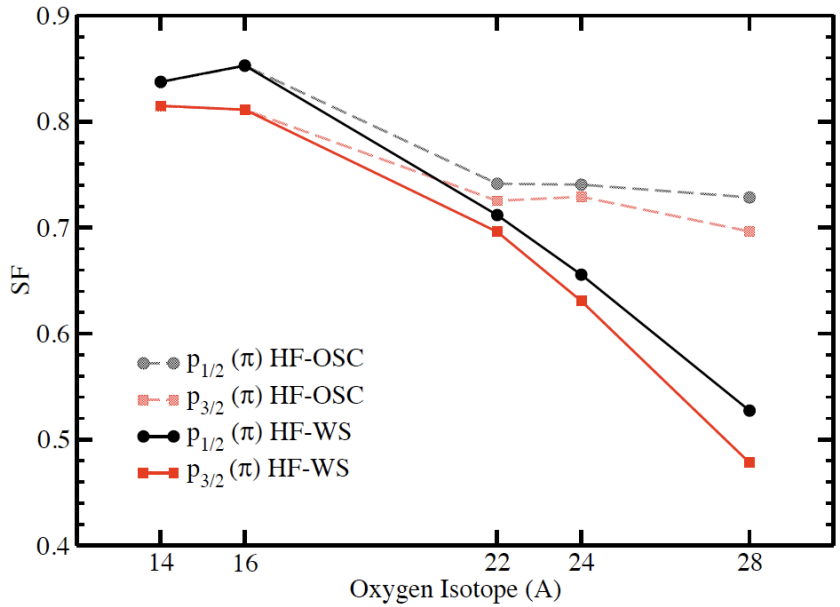


C. Barbieri, W.H.Dickhoff, Int. Jour. Mod. Phys. A24, 2060 (2009).

Self-consistent green's function method show rather weak asymmetry dependence for the spectroscopic factor.

Coupled cluster method [from D. Dean, G. Hagen, T. Papenbrock]

Quenching of spectroscopic factors for proton removal in neutron rich oxygen isotopes

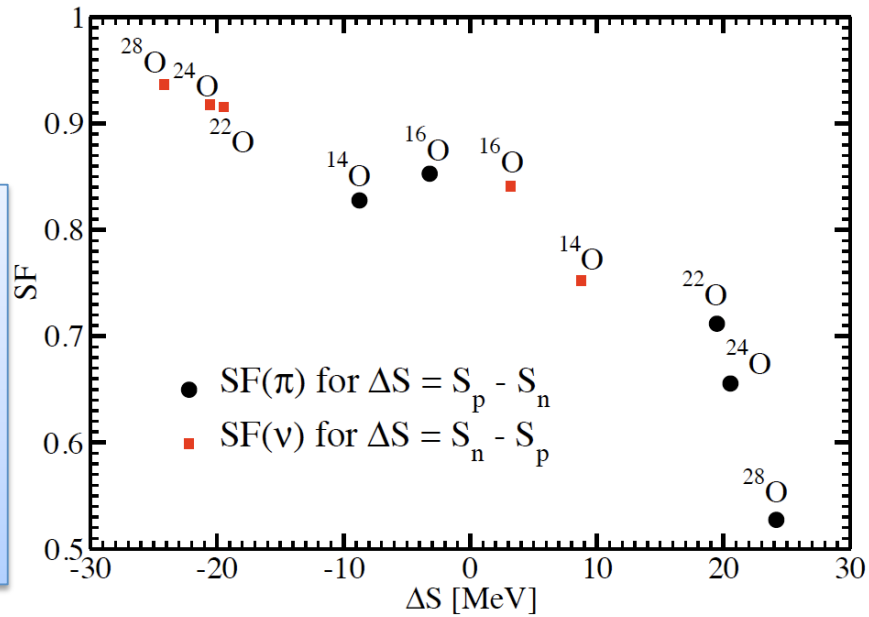


Spectroscopic factor is a useful tool to study correlations towards the dripline.

SF for proton removal in neutron rich ^{24}O show strong "quenching" pointing to large deviations from a mean-field like picture.
G. Hagen et al Phys. Rev. Lett. 107, 032501 (2011).

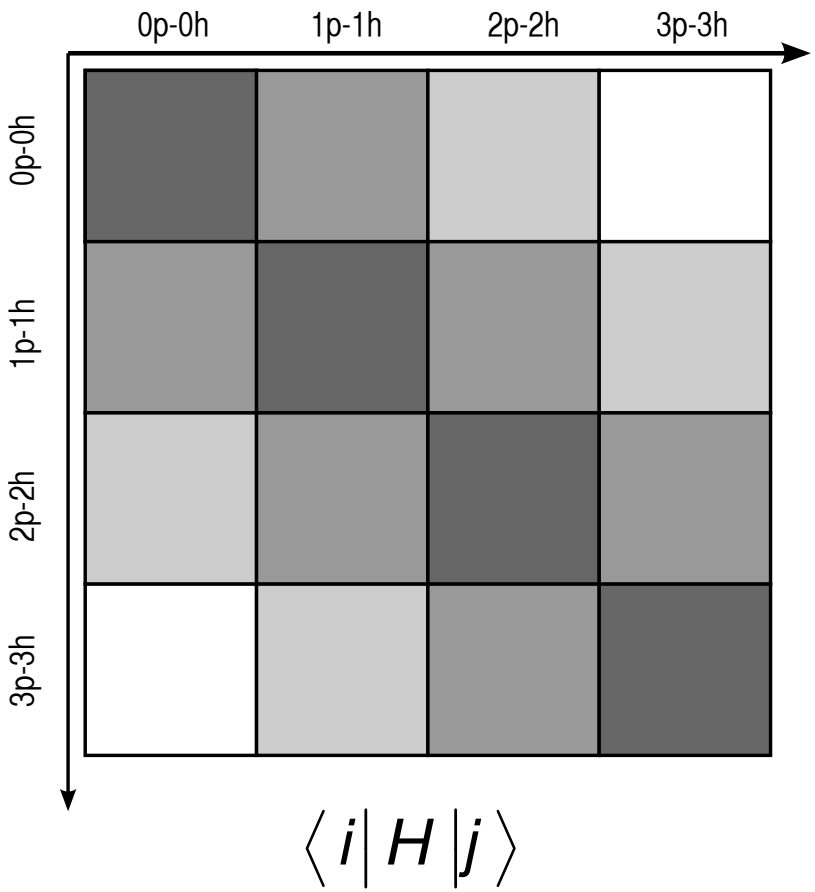
Strong asymmetry dependence on the SF for proton and neutron removal in neutron rich oxygen isotopes.

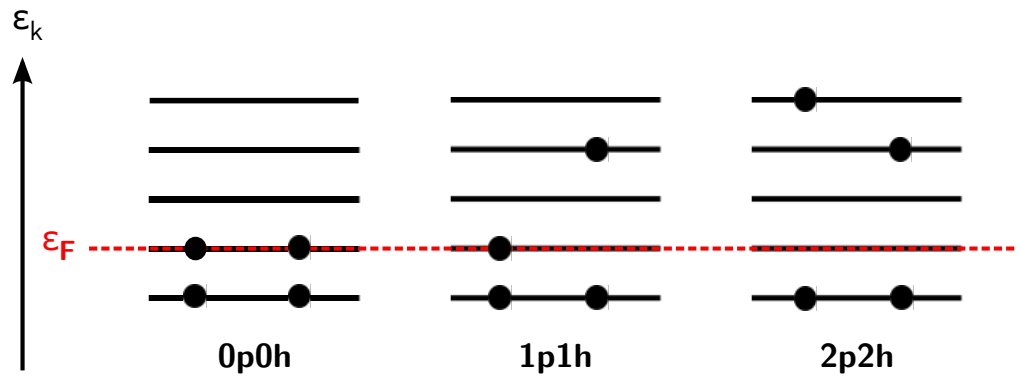
SF~1 for neutron removal while protons are strongly correlated SF ~0.6-0.7 in ^{22,24,28}O



In-medium SRG decoupling [slides from H. Hergert]

Consider SRG with 0*p*–0*h* reference state (instead of vacuum)

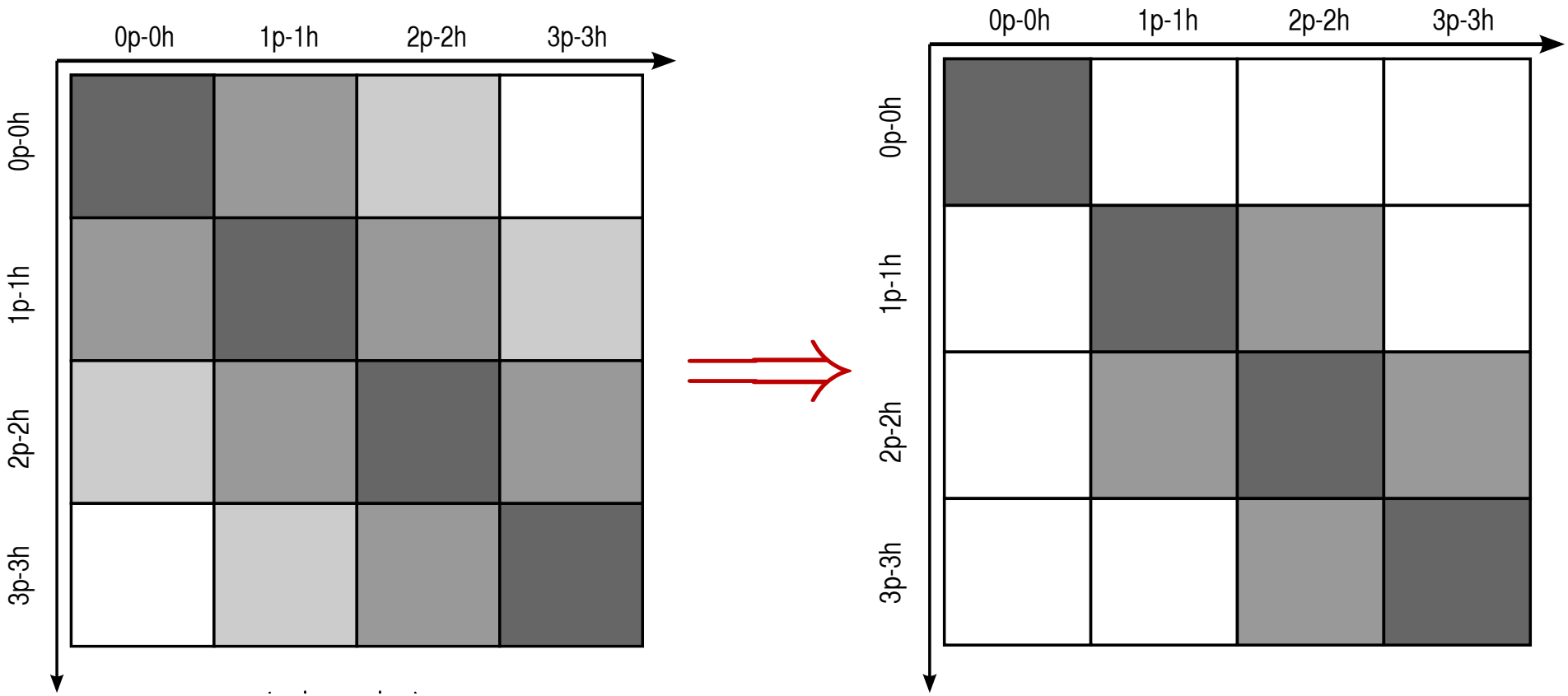




K. Tsukiyama, S. K. Bogner, and A. Schwenk, PRL **106**, 222502 (2011)

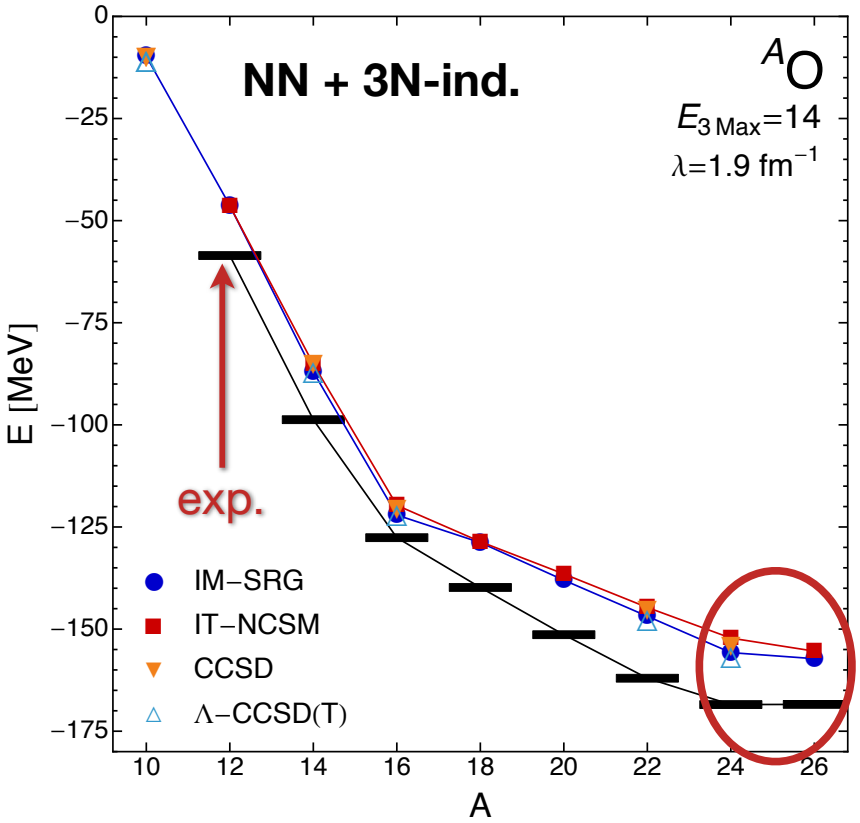
In-medium SRG decoupling [H. Hergert]

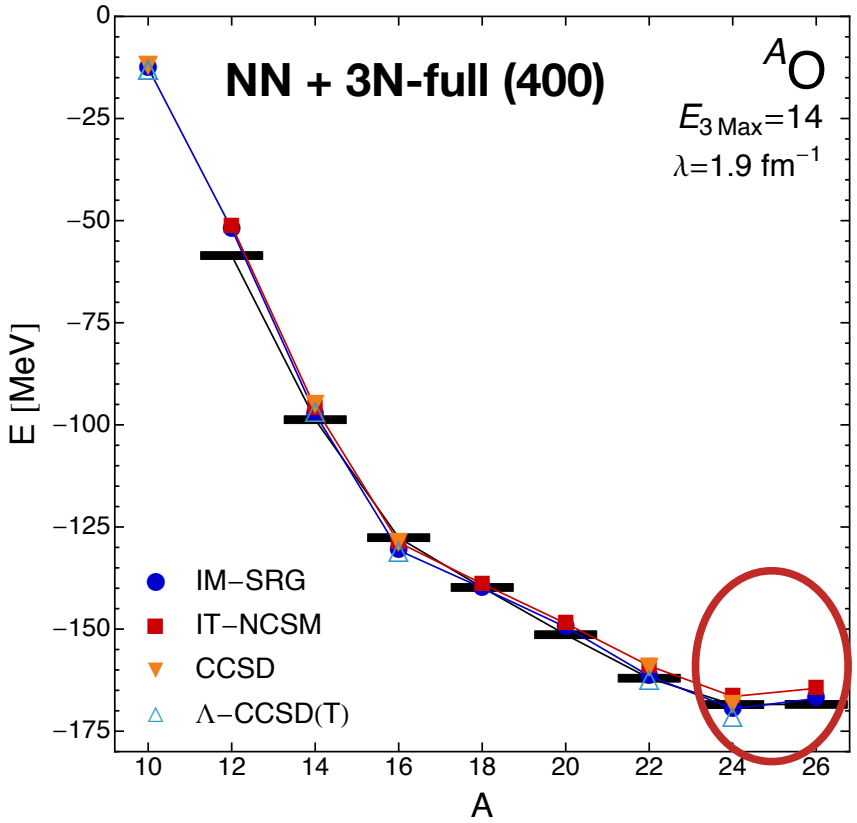
Aim: decouple reference state (0*p*–0*h*) from excitations



K. Tsukiyama, S. K. Bogner, and A. Schwenk, PRL **106**, 222502 (2011)

Oxygen chain with multi-reference IM-SRG [H. Hergert]





- ref. state: number-projected Hartree-Fock-Bogoliubov vacuum
- results (mostly) insensitive to choice of generator for same H^{od}
- **consistency between different many-body methods**

Outline

SRG leftovers

Overview of nuclear many-body problem

Many-body methods

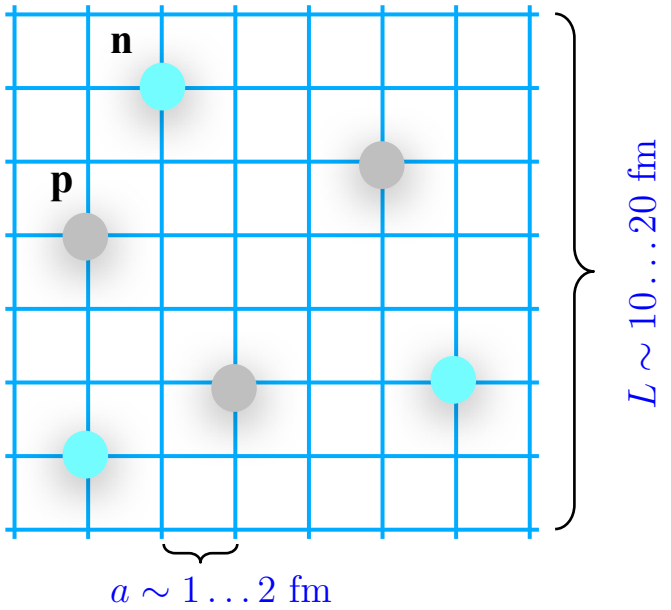
Nuclear lattice simulations

Lattice EFT collaboration [E. Epelbaum]

Nuclear Lattice Effective Field Theory

The Collaboration: E.E., Hermann Krebs (Bochum), Timo Lähde (Jülich), Dean Lee (NC State), Ulf-G. Meißner (Bonn/Jülich), Gautam Rupak (Mississippi State)

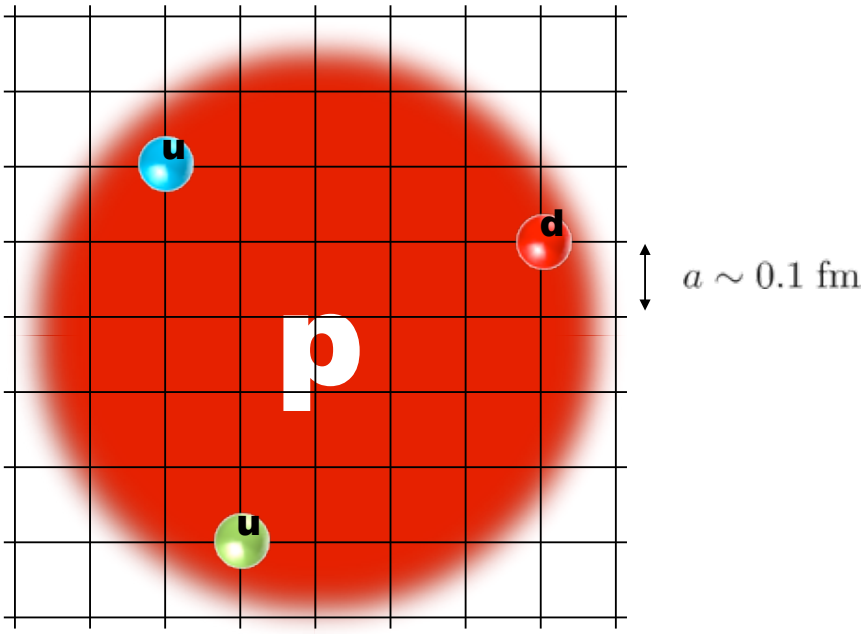
Borasoy, E.E., Krebs, Lee, Meißner, Eur. Phys. J. A31 (07) 105,
Eur. Phys. J. A34 (07) 185,
Eur. Phys. J. A35 (08) 343,
Eur. Phys. J. A35 (08) 357,
E.E., Krebs, Lee, Meißner, Eur. Phys. J A40 (09) 199,
Eur. Phys. J A41 (09) 125,
Phys. Rev. Lett 104 (10) 142501,
Eur. Phys. J. 45 (10) 335,
Phys. Rev. Lett. 106 (11) 192501,
E.E., Krebs, Lähde, Lee, Meißner Phys. Rev. Lett. 109 (12) 252501,
Phys. Rev. Lett. 110 (13) 112502,
arXiv:1303.4856



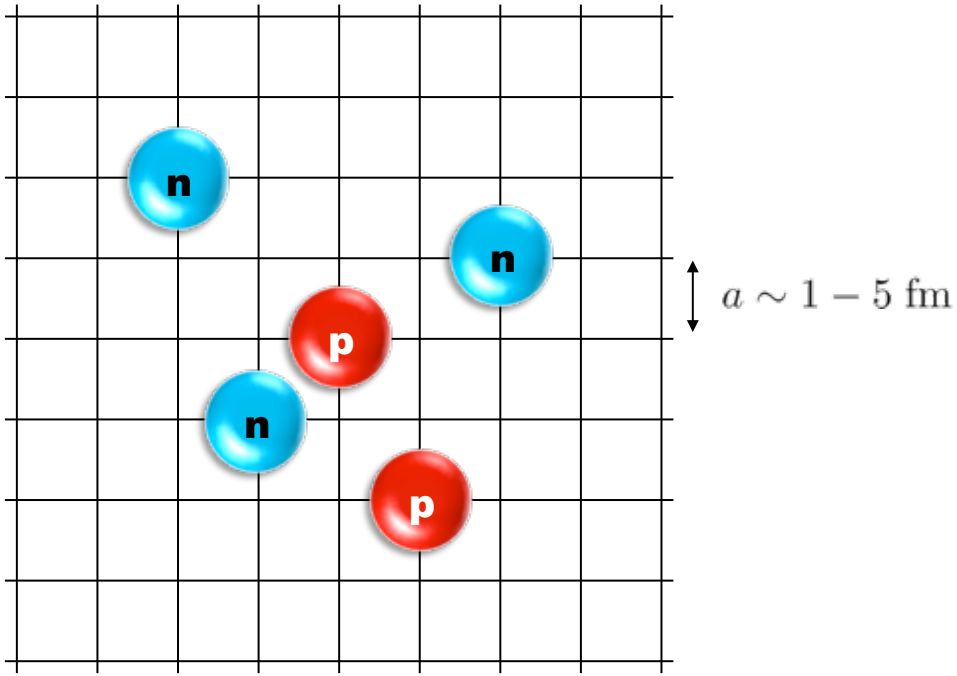
Lattice QCD versus lattice EFT [from Dean Lee]

Compare variables and lattice spacing *a*:

Lattice quantum chromodynamics



Lattice effective field theory

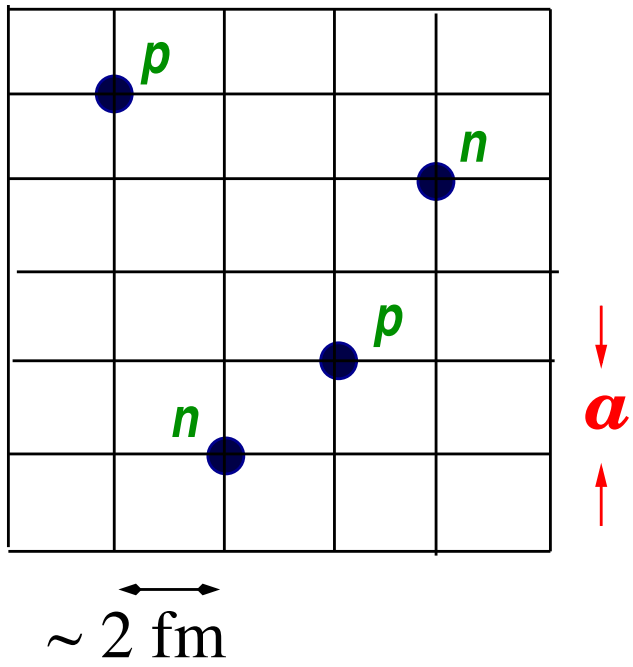


Lattice EFT basics [from U. Meißner]

Frank, Brockmann (1992), Koonin, Müller, Seki, van Kolck (2000) , Lee, Schäfer (2004), . . .
Borasoy, Krebs, Lee, UGM, Nucl. Phys. **A768** (2006) 179; Borasoy, Epelbaum, Krebs, Lee, UGM, Eur. Phys. J. **A31** (2007) 105

- *new method* to tackle the nuclear many-body problem
- discretize space-time $V = L_s \times L_s \times L_s \times L_t$:
  nucleons are point-like fields on the sites
- discretized chiral potential w/ pion exchanges
  and contact interactions
- typical lattice parameters

$$\Lambda = \frac{\pi}{a} \simeq 300\,\text{MeV [UV cutoff]}$$

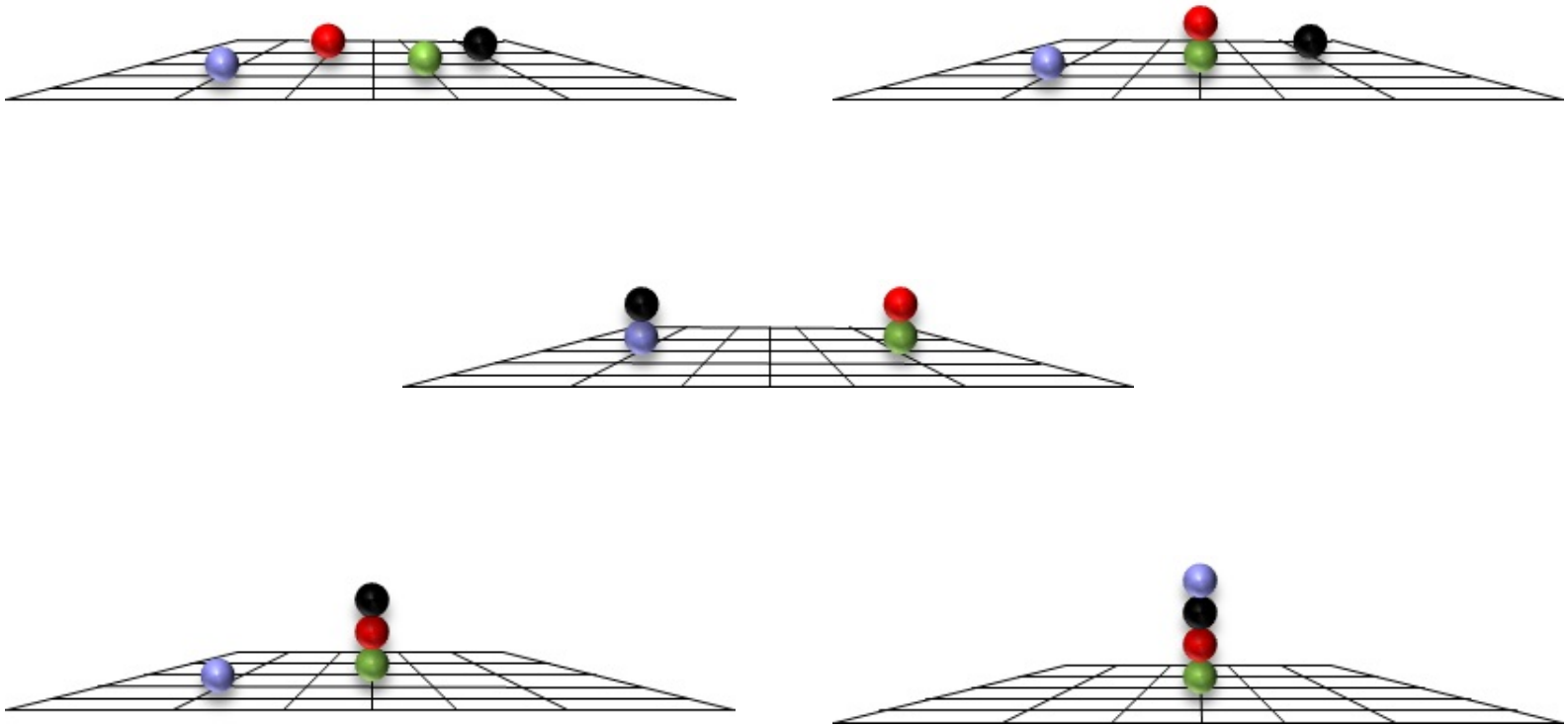


- strong suppression of sign oscillations due to approximate Wigner SU(4) symmetry

J. W. Chen, D. Lee and T. Schäfer, Phys. Rev. Lett. **93** (2004) 242302

- hybrid Monte Carlo & transfer matrix (similar to LQCD)

Lattice EFT basics [from U. Meißner]



$\Rightarrow$ all *possible* configurations are sampled

$\Rightarrow$ *clustering* emerges *naturally*

Lattice EFT basics [from U. Meißner]

- Correlation–function for A nucleons: $Z_A(t) = \langle \Psi_A | \exp(-tH) | \Psi_A \rangle$

  with Ψ_A a Slater determinant for A free nucleons

Euclidean time

- Ground state energy from the time derivative of the correlator

$$E_A(t) = -\frac{d}{dt} \ln Z_A(t)$$

$\rightarrow$ ground state filtered out at large times: $E_A^0 = \lim_{t\to\infty} E_A(t)$

- Expectation value of any normal–ordered operator $\mathcal{O}$

$$Z_A^{\mathcal{O}} = \langle \Psi_A | \exp(-tH/2)\, \mathcal{O}\, \exp(-tH/2) \, | \Psi_A \rangle$$

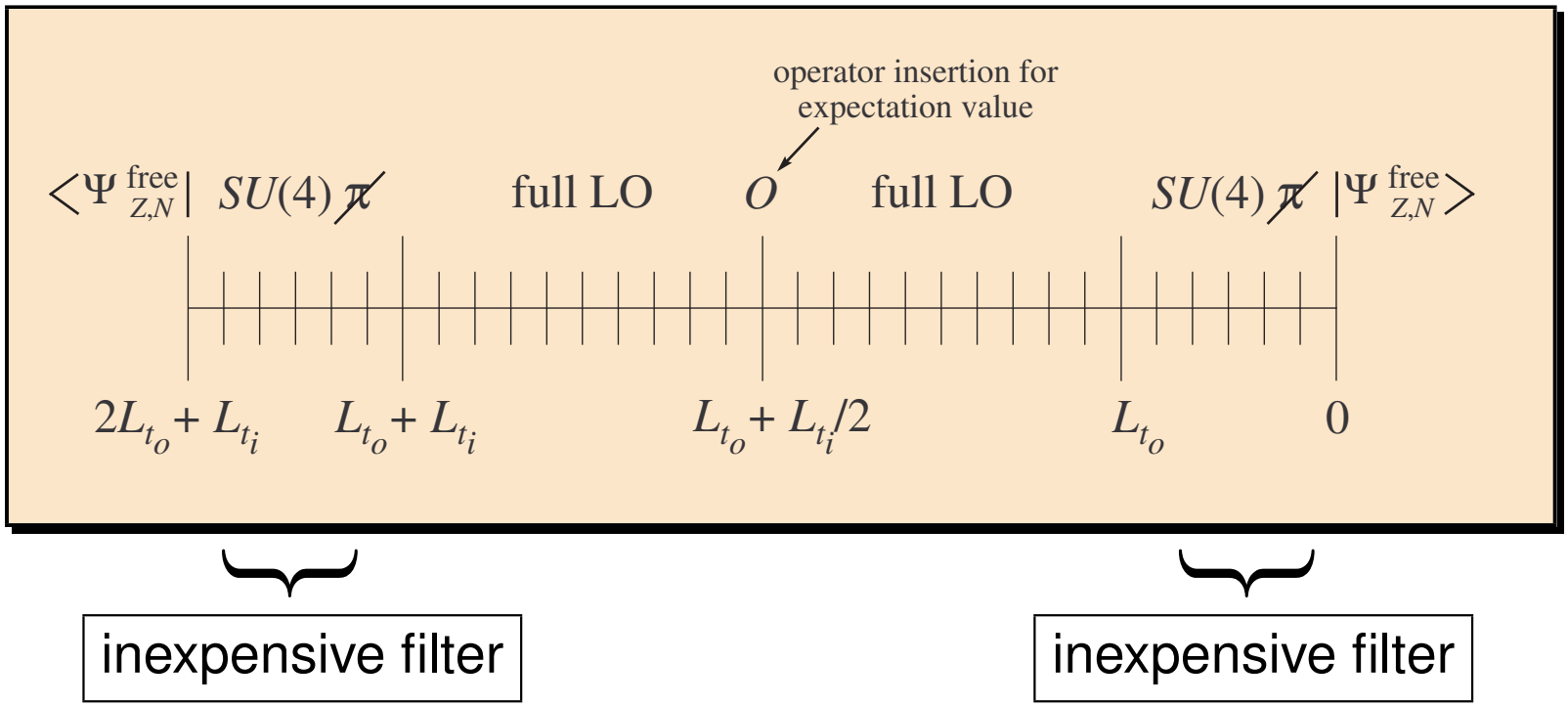
$$\lim_{t\to\infty} \frac{Z_A^{\mathcal{O}}(t)}{Z_A(t)} = \langle \Psi_A | \mathcal{O} \, | \Psi_A \rangle$$

Lattice EFT basics [from U. Meißner]

- Expectation value of any normal–ordered operator $\mathcal{O}$

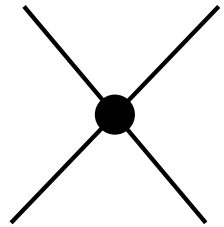
$$\langle \Psi_A | \mathcal{O} | \Psi_A \rangle = \lim_{t\to\infty} \frac{\langle \Psi_A | \exp(-tH/2)\, \mathcal{O}\, \exp(-tH/2) | \Psi_A \rangle}{\langle \Psi_A | \exp(-tH) | \Psi_A \rangle}$$

- Anatomy of the transfer matrix



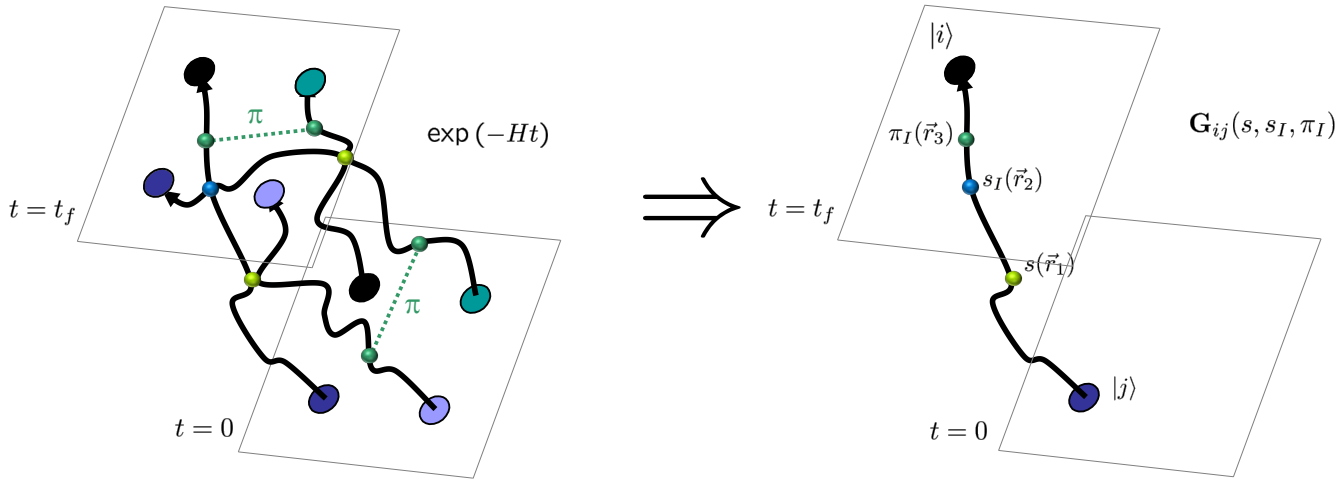
Lattice EFT basics [from U. Meißner]

- Contact interactions represented by auxiliary fields s, s_I



$$\exp(\rho^2/2) \propto \int_{-\infty}^{+\infty} ds \, \exp(-s^2/2 - s\rho) \, , \quad \rho \sim N^\dagger N$$

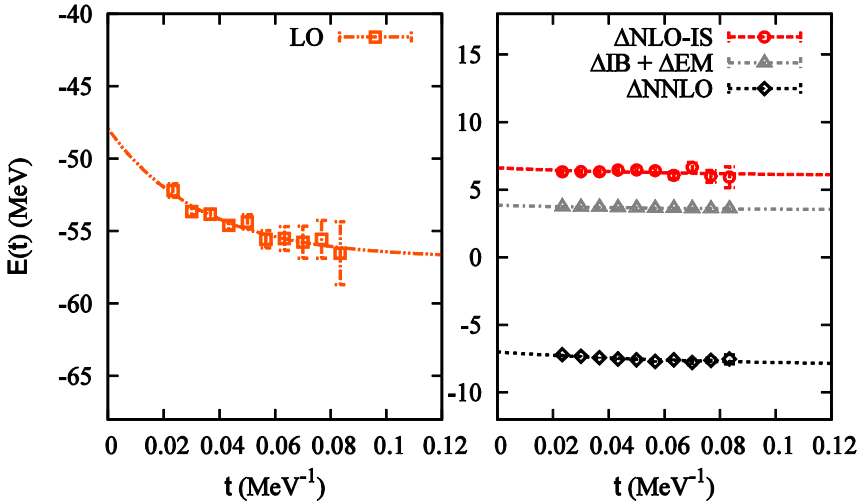
- Correlation function = path-integral over pions & auxiliary fields

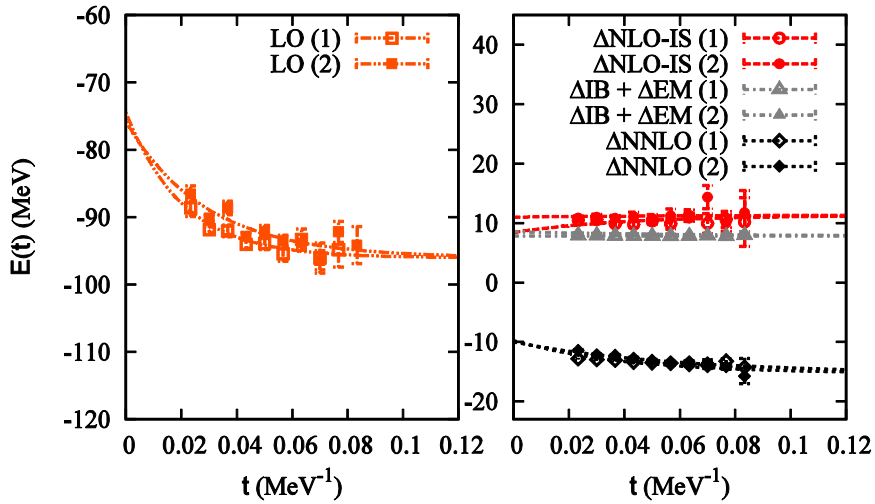


Ground states of ^{8}Be and ^{12}C [E. Epelbaum]

E.E., Krebs, Lee, Meißner, PRL 106 (11) 192501

Simulations for ^{8}Be and ^{12}C, L=11.8 fm





Ground state energies (L=11.8 fm) of ^{4}He, ^{8}Be, ^{12}C & ^{16}O

	^{4}He	^{8}Be	^{12}C	^{16}O
LO $[Q^0]$, in MeV	$-28.0(3)$	$-57(2)$	$-96(2)$	$-144(4)$
NLO $[Q^2]$, in MeV	$-24.9(5)$	$-47(2)$	$-77(3)$	$-116(6)$
NNLO $[Q^3]$, in MeV	$-28.3(6)$	$-55(2)$	$-92(3)$	$-135(6)$
Experiment, in MeV	-28.30	-56.5	-92.2	-127.6

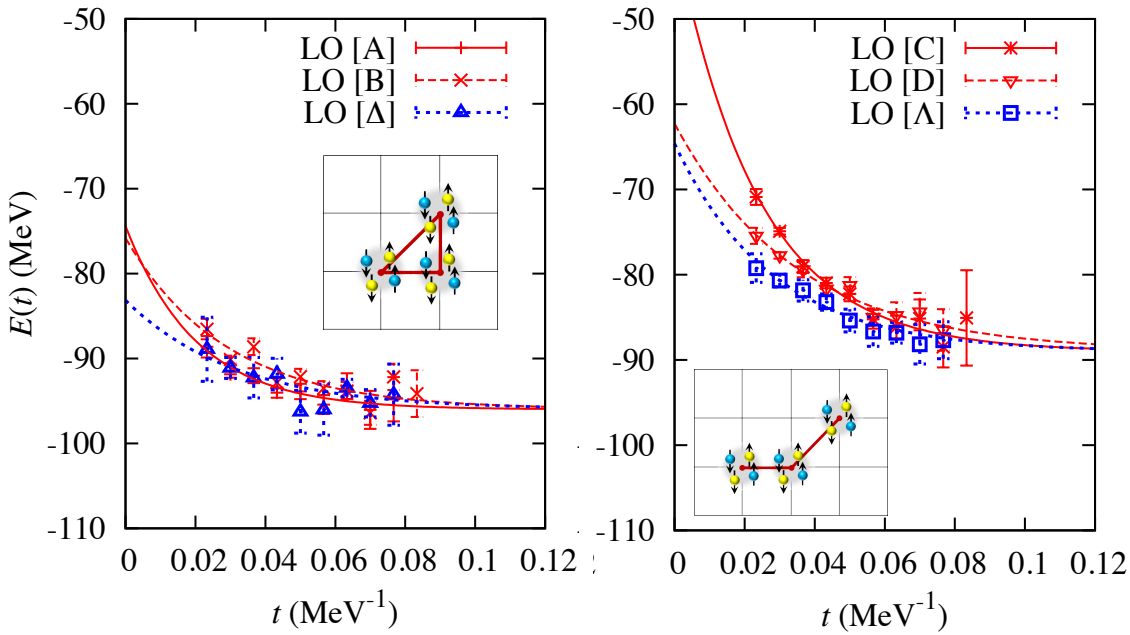
Hoyle State [E. Epelbaum]

EE, Krebs, Lähde, Lee, Meißner, PRL 106 (2011) 192501; PRL 109 (2012) 252501

Lattice results for low-lying even-parity states of ^{12}C

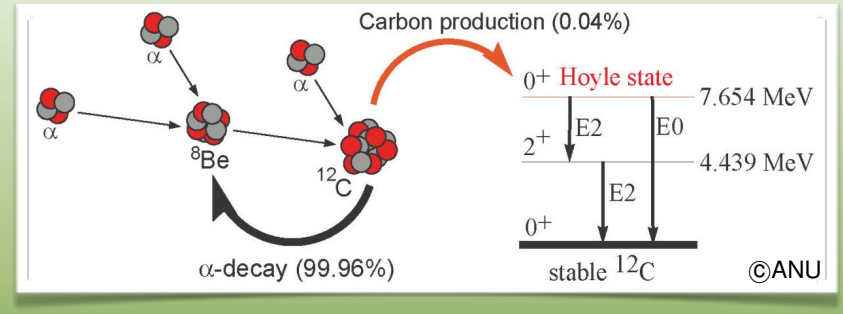
	0_1^+	$2_1^+(E^+)$	0_2^+	$2_2^+(E^+)$
LO	−96(2)	−94(2)	−89(2)	−88(2)
NLO	−77(3)	−74(3)	−72(3)	−70(3)
NNLO	−92(3)	−89(3)	−85(3)	−83(3)
Exp	−92.16	−87.72	−84.51	−82(1)

Probing (α-cluster) structure of the 0_1^+, 0_2^+ states



RMS radii and quadrupole moments

	LO	Experiment
$r(0_1^+)$ [fm]	2.2(2)	2.47(2) [26]
$r(2_1^+)$ [fm]	2.2(2)	–
$Q(2_1^+)$ [e fm^2]	6(2)	6(3) [27]
$r(0_2^+)$ [fm]	2.4(2)	–
$r(2_2^+)$ [fm]	2.4(2)	–
$Q(2_2^+)$ [e fm^2]	−7(2)	–



The triple alpha reaction rate as a function of the quark mass

Production of ^{12}C in stars depends sensitively on the energy differences: $\Delta E_b \equiv E_8 - 2E_4\,,$

$\Delta E_h \equiv E_{12}^\star - E_8 - E_4$

Reaction rate for the triple alpha process: $r_{3\alpha} \simeq 3^{\frac{3}{2}} N_\alpha^3 \left(\frac{2\pi\hbar^2}{M_\alpha k_{\rm B} T}\right)^3 \frac{\Gamma_\gamma}{\hbar} \exp\left(-\frac{\varepsilon}{k_{\rm B} T}\right)$

Oberhummer, Csoto, Schlattl, Science 289 (2000) 88

where $\varepsilon \equiv \Delta E_b + \Delta E_h = E_{12}^\star - 3E_4 = 379.47(18)\ \text{keV}$ - crucial control parameter

Changing ε by ~100 keV destroys production of either ^{12}C or ^{16}O Livio et al.'89; Oberhummer, et al.'00

How robust is ε with respect to variations of fundamental constants (QCD+QED)?

Quark mass dependence of the triple-α reaction rate

EE, Krebs, Lähde, Lee, Meißner, PRL 110 (2013) 112502; arXiv:1303.4856 (to appear in EPJA)

Input: M_π-dependence of the long-range force known, short-range M_π-dependence parametrized in terms of

spin-singlet ($^1S_0$): $\bar{A}_s \equiv \left.\frac{\partial a_s^{-1}}{\partial M_\pi}\right|_{M_\pi^{\rm phys}}$ spin-triplet ($^3S_1$): $\bar{A}_t \equiv \left.\frac{\partial a_t^{-1}}{\partial M_\pi}\right|_{M_\pi^{\rm phys}}$

1) Is ε a fine-tuned quantity (with respect to $\bar{A}_s$, $\bar{A}_t$)? Yes!

For example:

$$K^\pi_{\rm E_4} = 1.652(25)\,\bar{A}_s + 3.401(21)\,\bar{A}_t - 0.183(7)^{+0.029}_{-0.039}$$
$$K^\pi_{E_8} = 1.940(80)\,\bar{A}_s + 3.870(60)\,\bar{A}_t - 0.217(21)^{+0.027}_{-0.041}$$
$$K^\pi_{\rm E^\star_{12}} = 2.593(19)\,\bar{A}_s + 4.940(13)\,\bar{A}_t - 0.287(8)^{+0.034}_{-0.043}$$

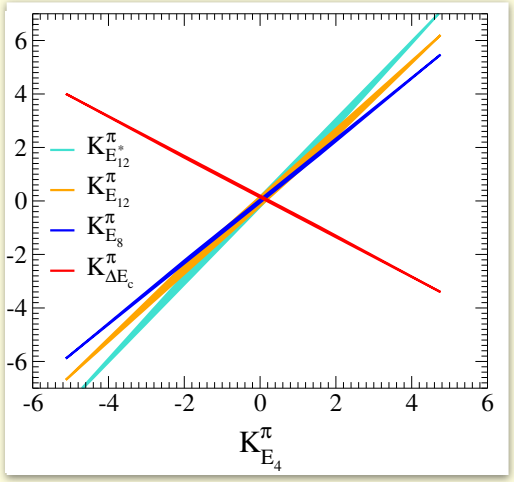
but:

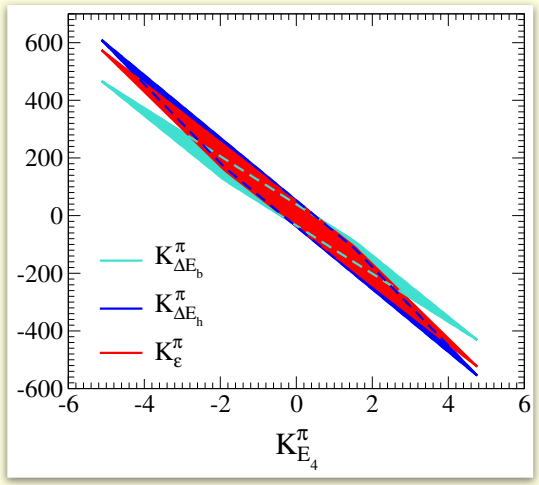
$$K^\pi_\varepsilon = -213(7)\,\bar{A}_s - 348(6)\,\bar{A}_t + 24(2)^{+3.7}_{-3.4}$$

nearly the same ratio for all energies

2) Strong correlations between different energies:

K-factors for all energies and energy differences are expressible in terms of that of ^{4}He





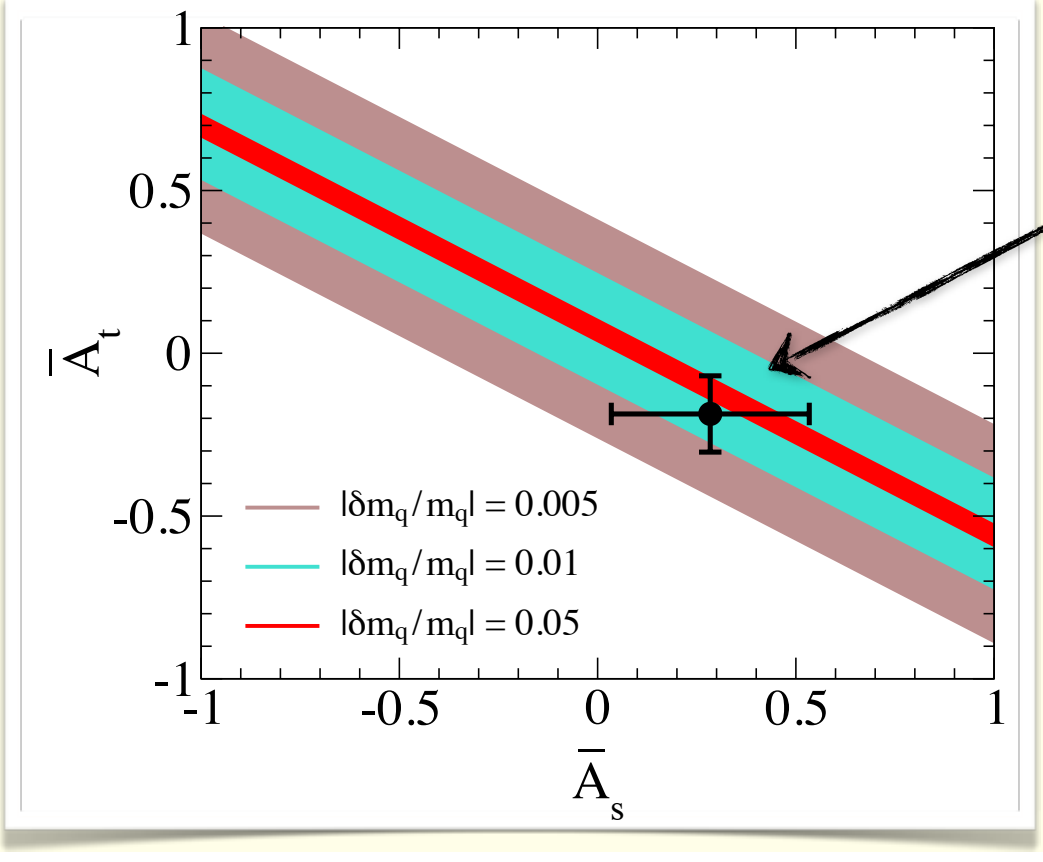
Quark mass dependence of the triple-α reaction rate

EE, Krebs, Lähde, Lee, Meißner, PRL 110 (2013) 112502; arXiv:1303.4856 (to appear in EPJA)

3) How much change in m_q can be accommodated to still have enough ^{12}C, ^{16}O production?

$$|\delta\varepsilon| < 100 \text{ keV} \longrightarrow \left| \left(0.771(14)\,\bar{A}_s + 0.934(11)\,\bar{A}_t - 0.069(6)\right) \frac{\delta m_q}{m_q} \right| < 0.0015$$

„Survivability bands" for carbon-oxygen based life due to 0.5%, 1%, 5% variation of m_q



up-to-date chiral EFT calculation (N²LO):

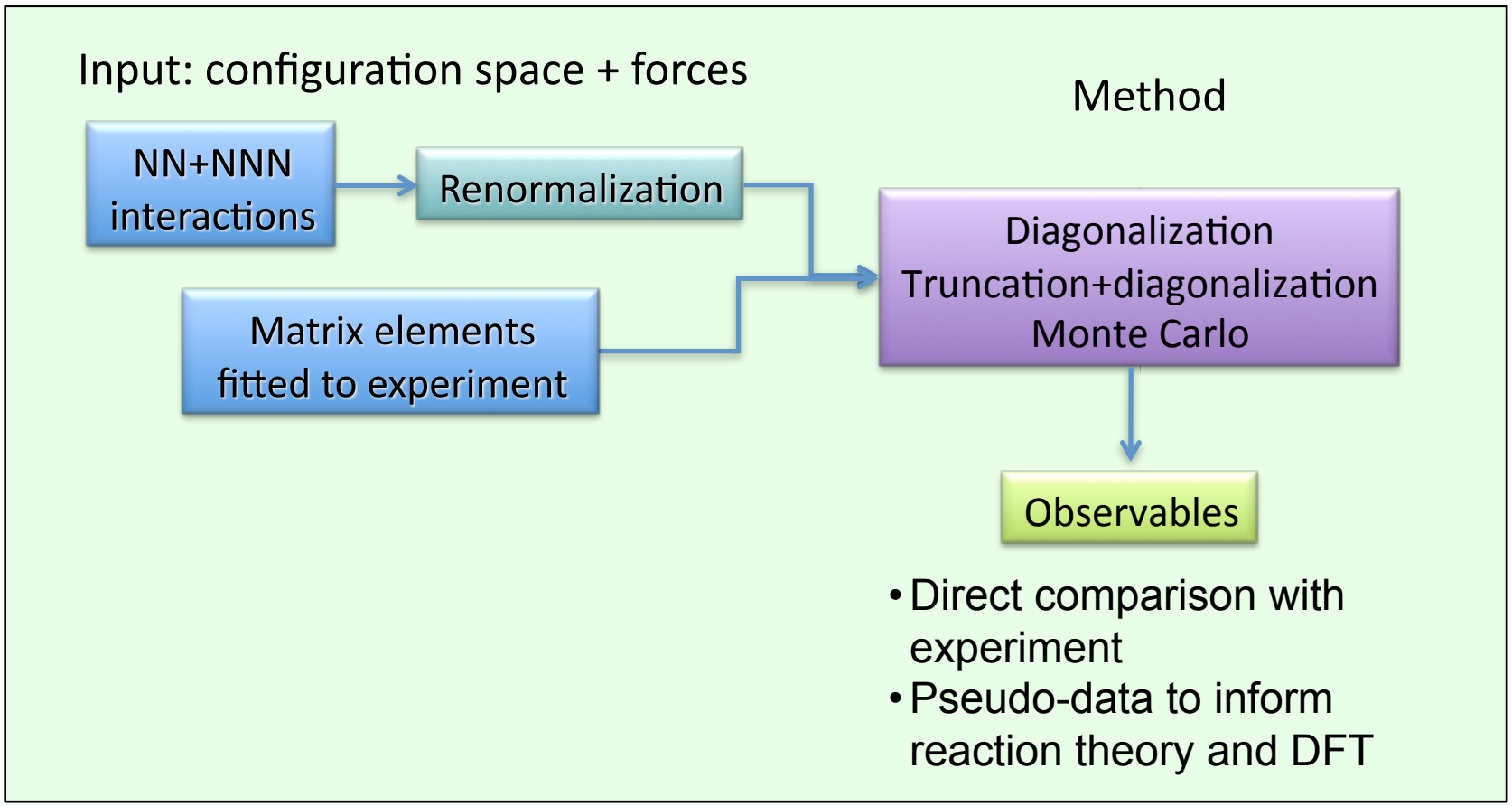
$$K^q_{a_s} = 2.3^{+1.9}_{-1.8}, \quad K^q_{a_t} = 0.32^{+0.17}_{-0.18}$$

Berengut et al., PRD 87 (2013)

The shell model revisited

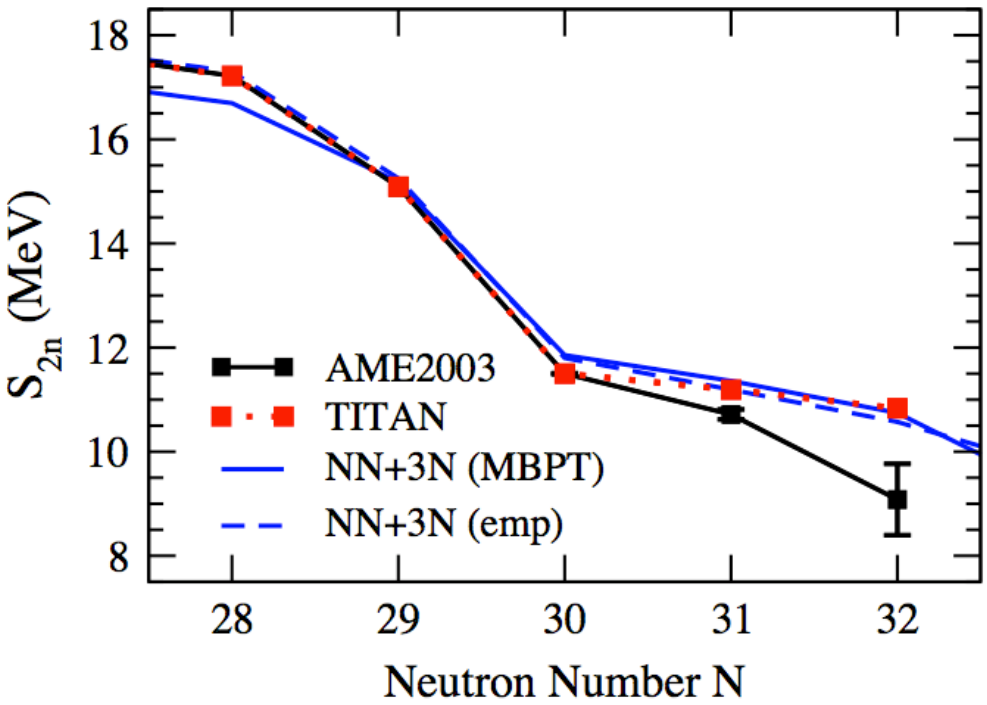
Configuration interaction techniques

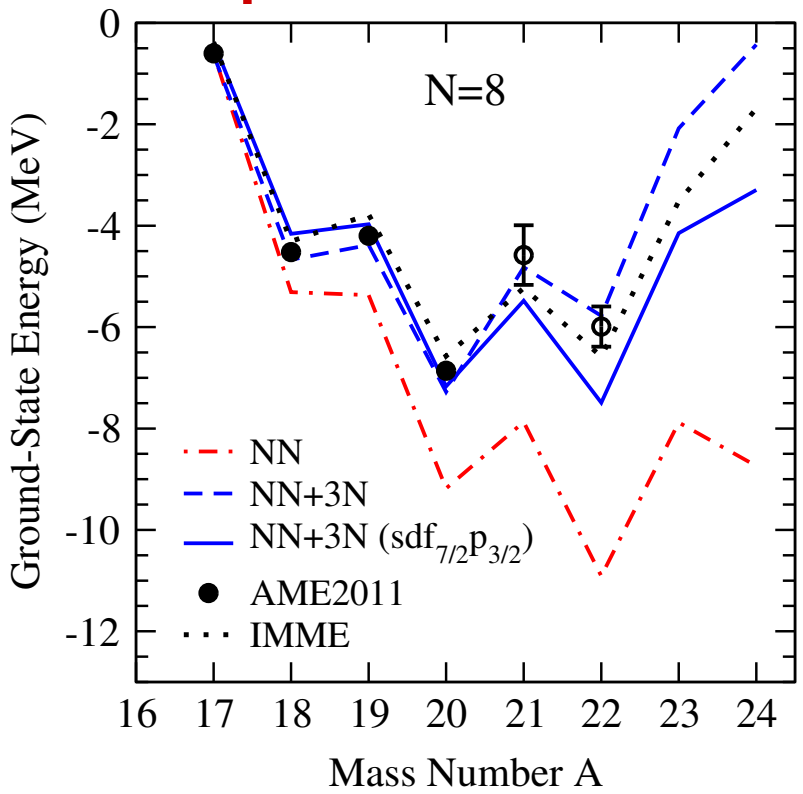
- light and heavy nuclei
- detailed spectroscopy
- quantum correlations (lab-system description)



Confronting theory and experiment to both driplines

- Precision mass measurements test impact of chiral 3NF
- Proton rich [Holt et al., arXiv:1207.1509]
- Neutron rich [Gallant et al., arXiv:1204.1987]
- Many new tests possible!





- Shell model description using chiral potential evolved to $V_{\mathrm{low}\,k}$ plus 3NF fit to $A = 3, 4$
- Excitations outside valence space included in 3rd order MBPT

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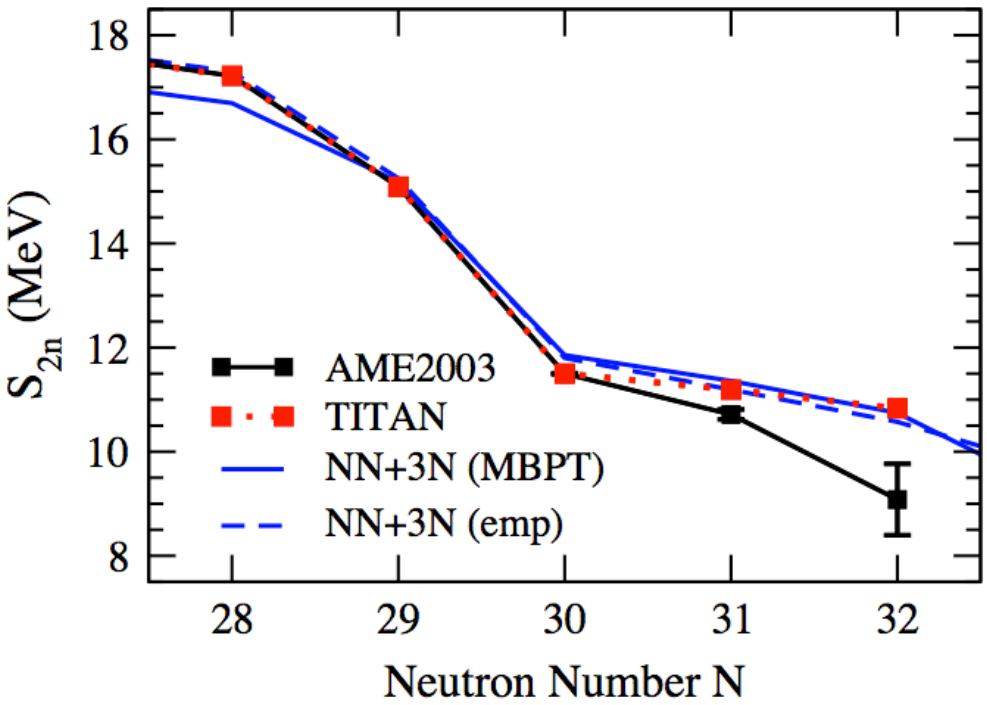

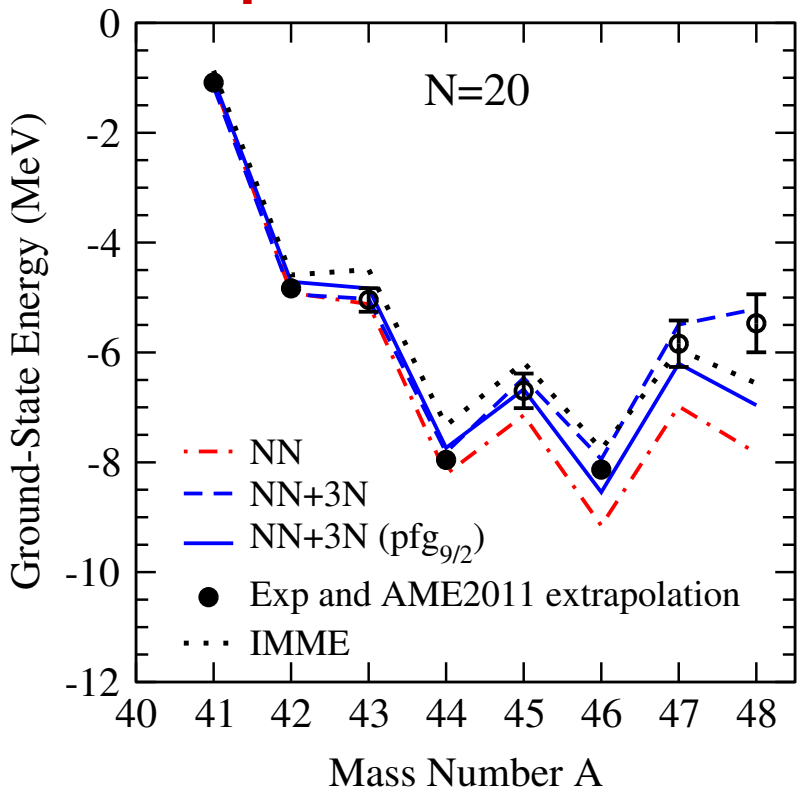

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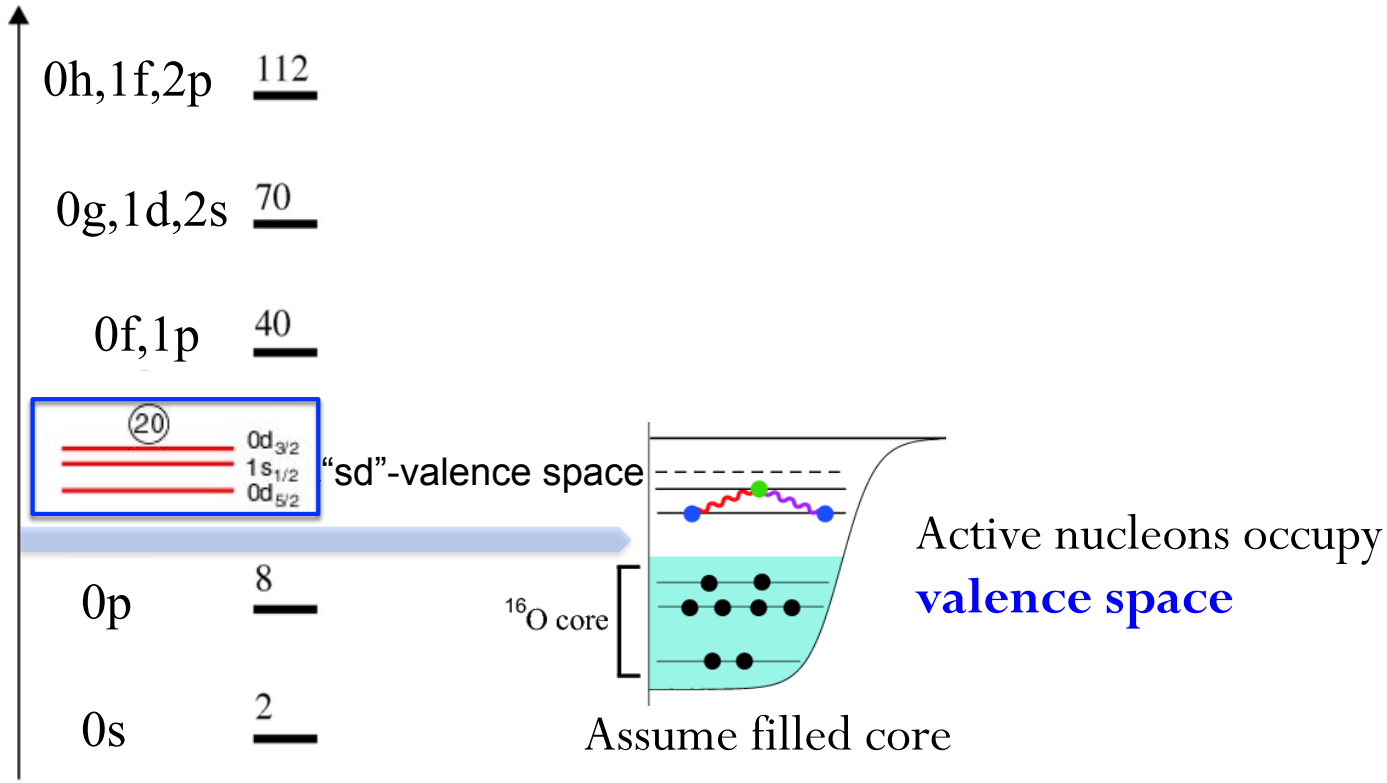
Non-empirical shell model [from J. Holt]

Solving the Nuclear Many-Body Problem

Nuclei understood as many-body system starting from closed shell, add nucleons

Interaction and energies of valence space orbitals from original $V_{\mathrm{low}\,k}$

This alone does not reproduce experimental data



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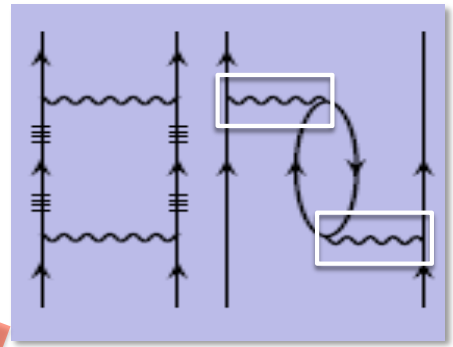
Hjorth-Jensen, Kuo, Osnes (1995)



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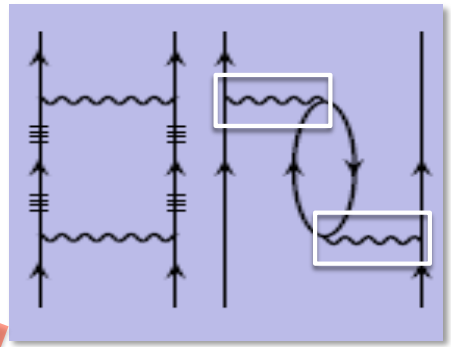
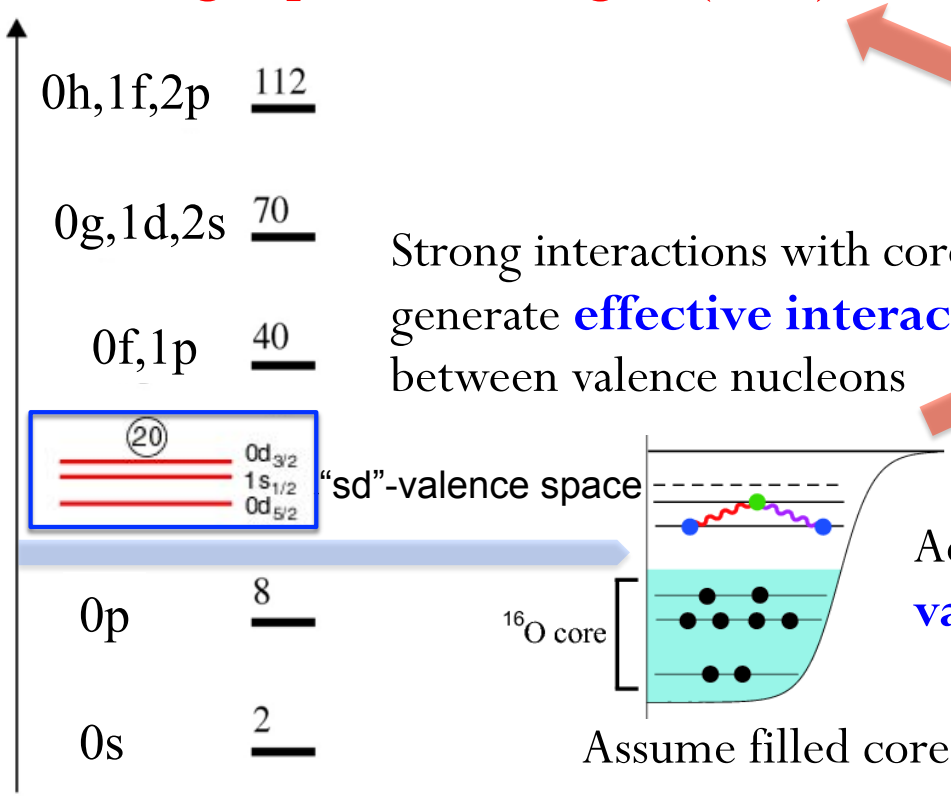
Effective two-body matrix elements

Single-particle energies (SPEs)

Hjorth-Jensen, Kuo, Osnes (1995)





Strong interactions with core generate **effective interaction** between valence nucleons

Active nucleons occupy **valence space**

Assume filled core

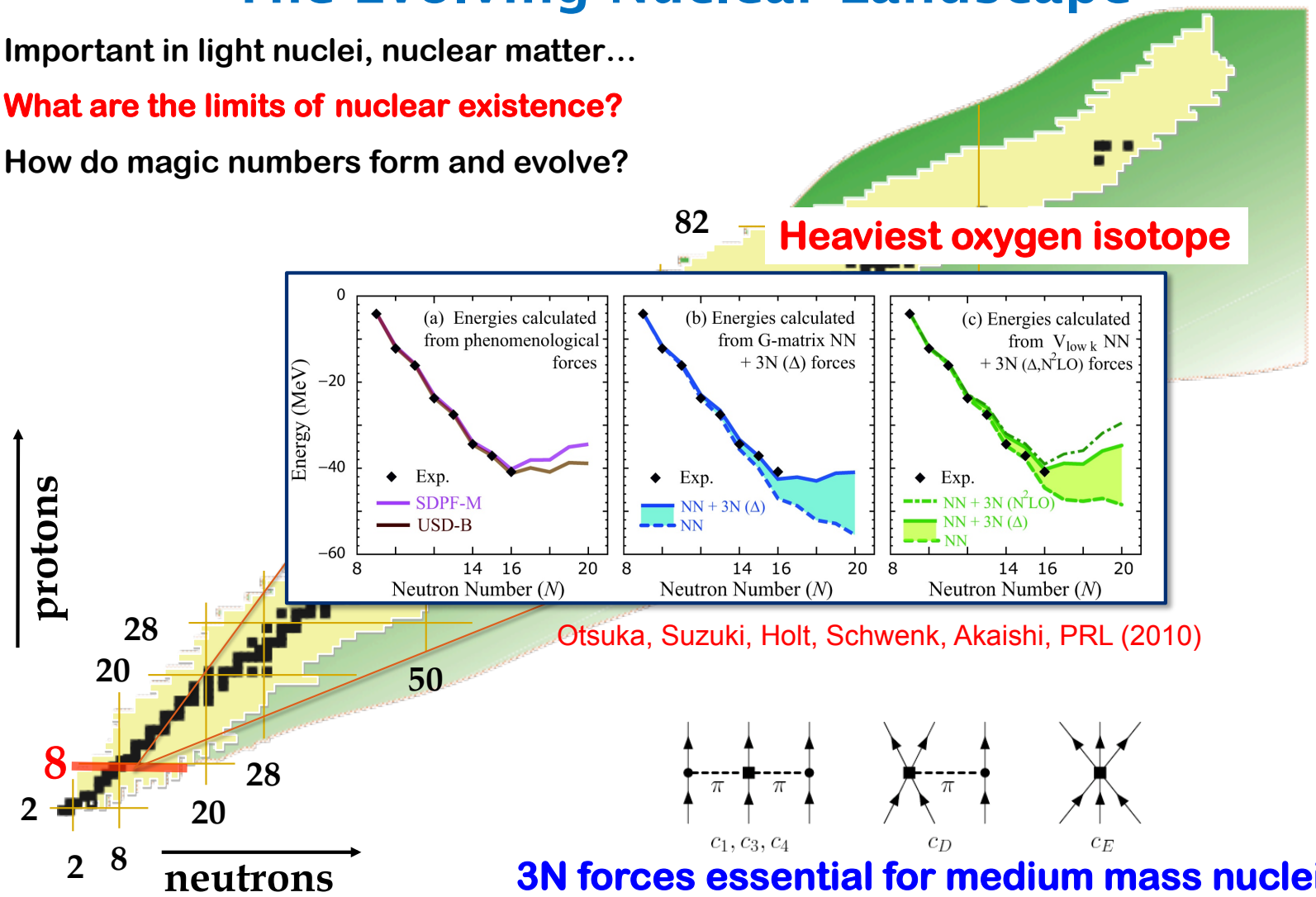
Chiral 3NFs meet the shell model [from J. Holt]

Drip Lines and Magic Numbers: The Evolving Nuclear Landscape

Important in light nuclei, nuclear matter…

What are the limits of nuclear existence?

How do magic numbers form and evolve?

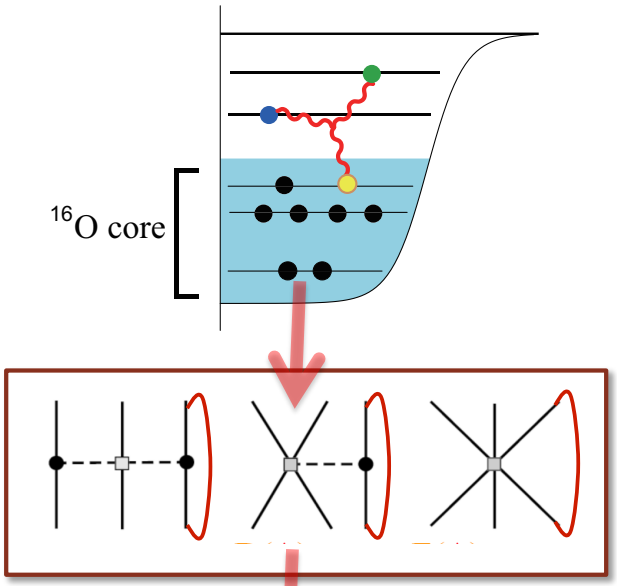


Chiral 3NFs meet the shell model [from J. Holt]

3N Forces for Valence-Shell Theories

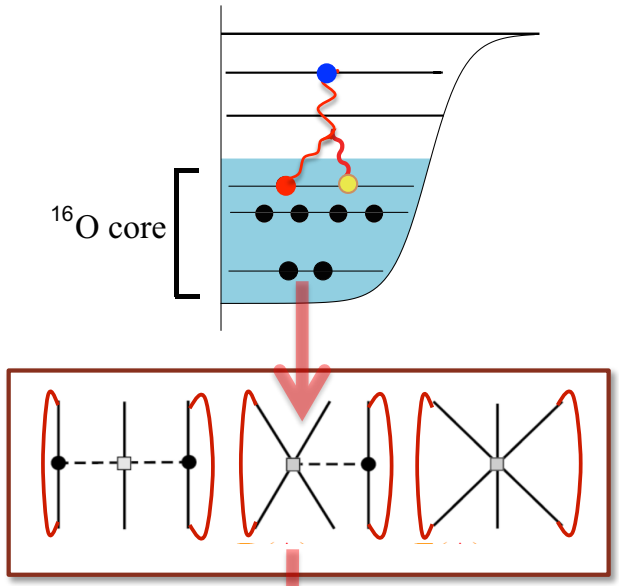
Normal-ordered 3N: contribution to valence neutron interactions

Effective two-body



$$\langle ab|\, V_{3N,\mathrm{eff}}\,|a'b'\rangle = \sum_{\alpha=core}\langle \alpha ab|\, V_{3N}\,|\alpha a'b'\rangle$$

Effective one-body



$$\langle a|\, V_{3N,\mathrm{eff}}\,|a'\rangle = \frac{1}{2}\sum_{\alpha\beta=core}\langle \alpha\beta a|\, V_{3N}\,|\alpha\beta a'\rangle$$

Combine with microscopic NN: eliminate empirical adjustments

Chiral 3NFs meet the shell model [from J. Holt]

Drip Lines and Magic Numbers: 3N Forces in Medium-Mass Nuclei

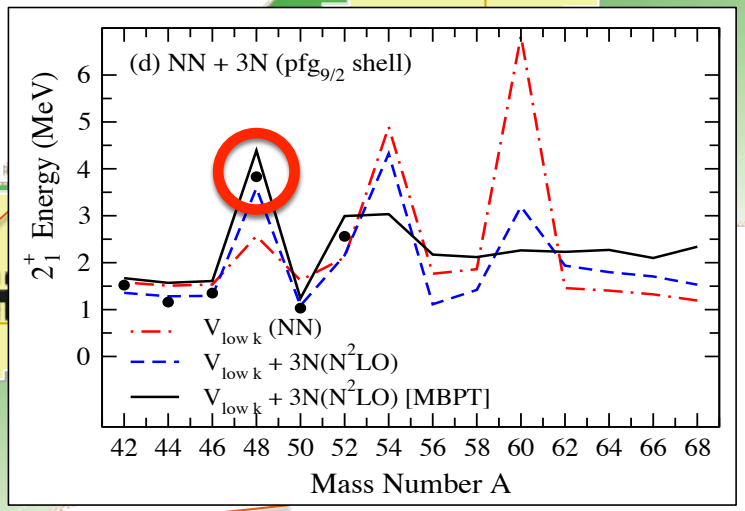
Important in light nuclei, nuclear matter…

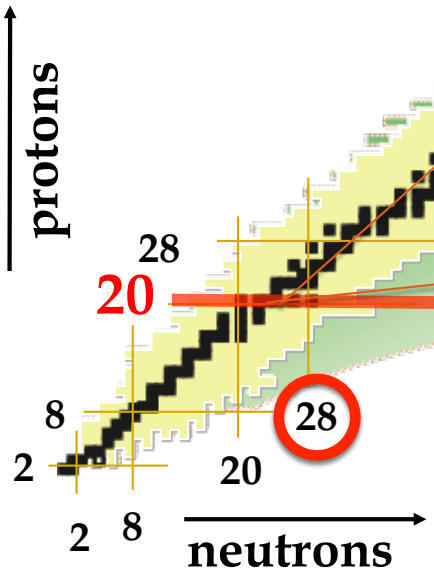
What are the limits of nuclear existence?

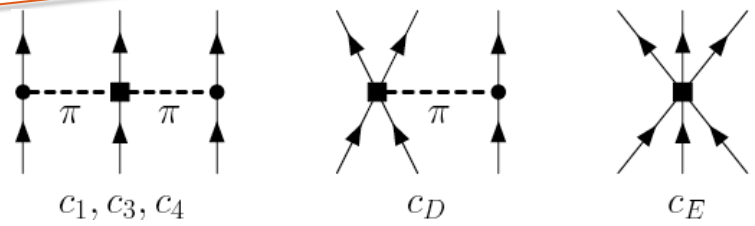
How do magic numbers form and evolve?

N=28 magic number in calcium

Holt, Otsuka, Schwek, Suzuki, arXiv:1009.5984

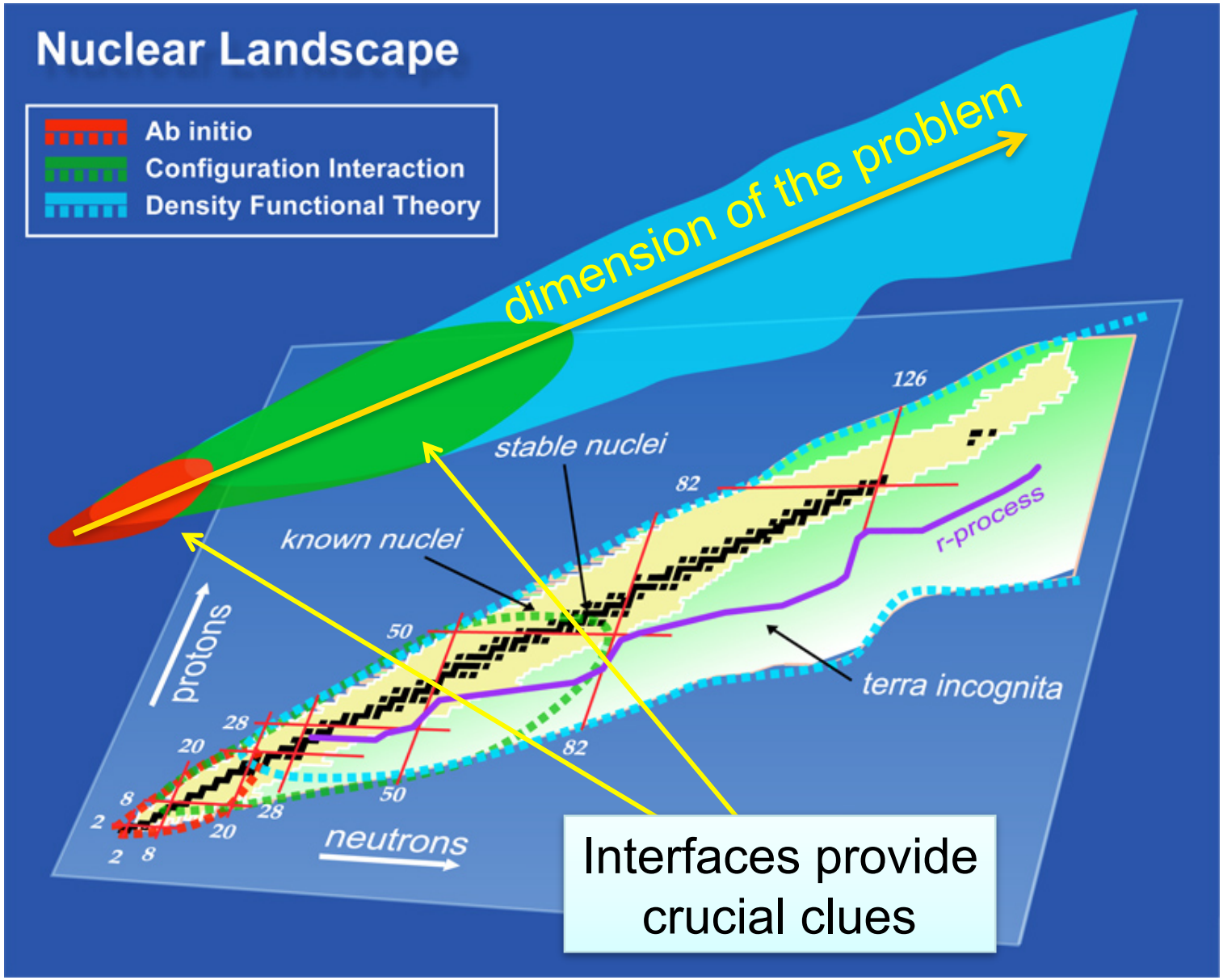






3N forces essential for medium mass nuclei

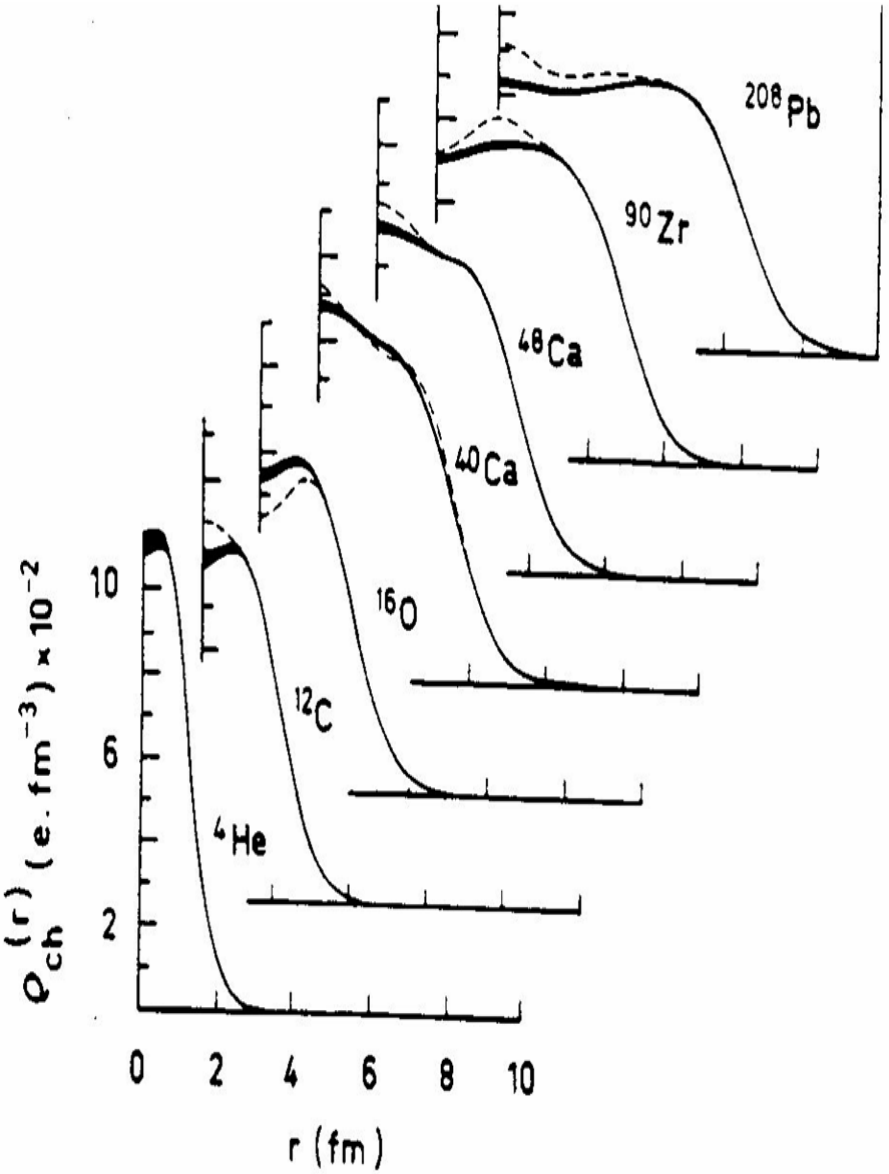
Overlapping theory methods cover all nuclei



What do (ordinary) nuclei look like?

- Charge densities of magic nuclei (mostly) shown
- Proton density has to be "unfolded" from $\rho_{\text{charge}}(r)$, which comes from elastic electron scattering
- Roughly constant interior density with $R \approx (1.1\text{–}1.2\,\text{fm}) \cdot A^{1/3}$
- Roughly constant surface thickness

$\Longrightarrow$ Like a liquid drop!



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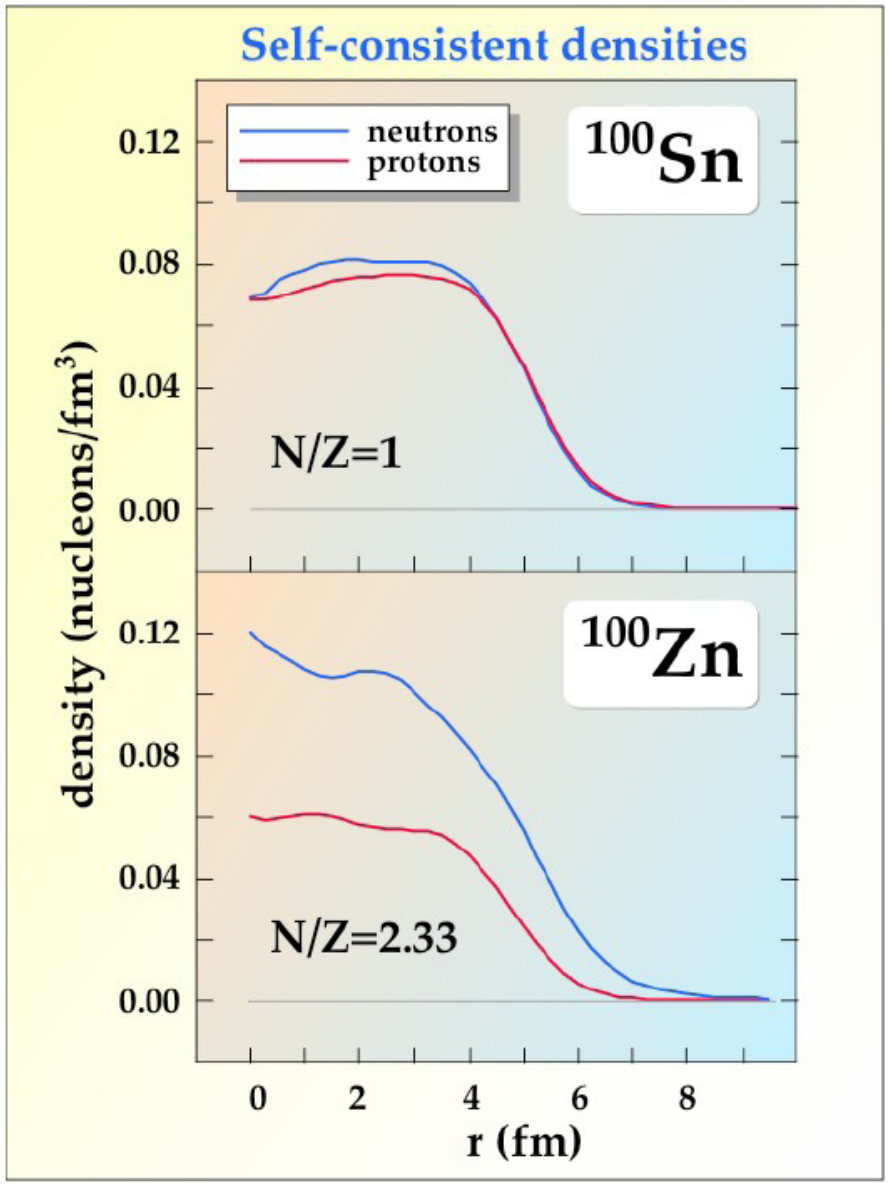
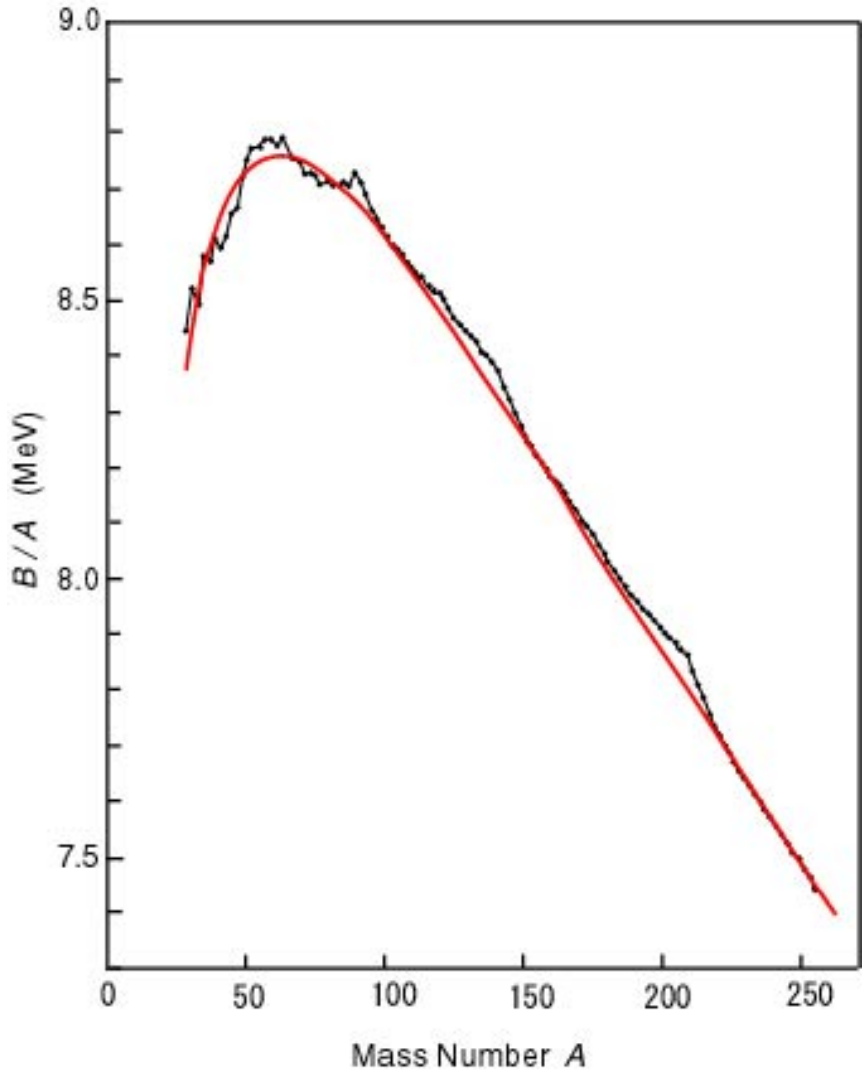


Semi-empirical mass formula ($A = N + Z$)

$$E_B(N,Z) = a_v A - a_s A^{2/3} - a_C \frac{Z^2}{A^{1/3}} - a_{\rm sym} \frac{(N-Z)^2}{A} + \Delta$$

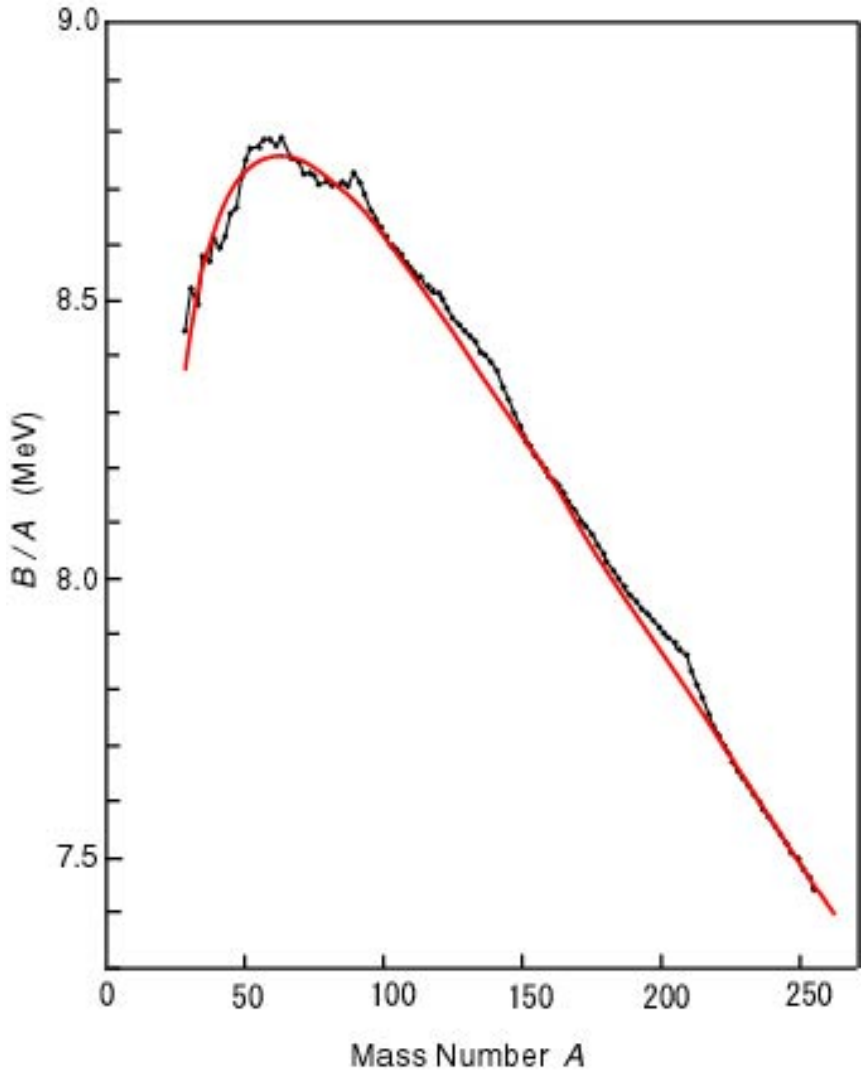
- Many predictions!
- Rough numbers: $a_v \approx 16\,\text{MeV}$, $a_s \approx 18\,\text{MeV}$, $a_C \approx 0.7\,\text{MeV}$, $a_{\rm sym} \approx 28\,\text{MeV}$
- Pairing $\Delta \approx \pm 12/\sqrt{A}\,\text{MeV}$ (even-even/odd-odd) or 0 [or $43/A^{3/4}$ MeV or . . .]
- Surface symmetry energy: $a_{\rm surf\ sym}(N-Z)^2/A^{4/3}$
- Much more sophisticated mass formulas include shell effects, etc.



Semi-empirical mass formula per nucleon

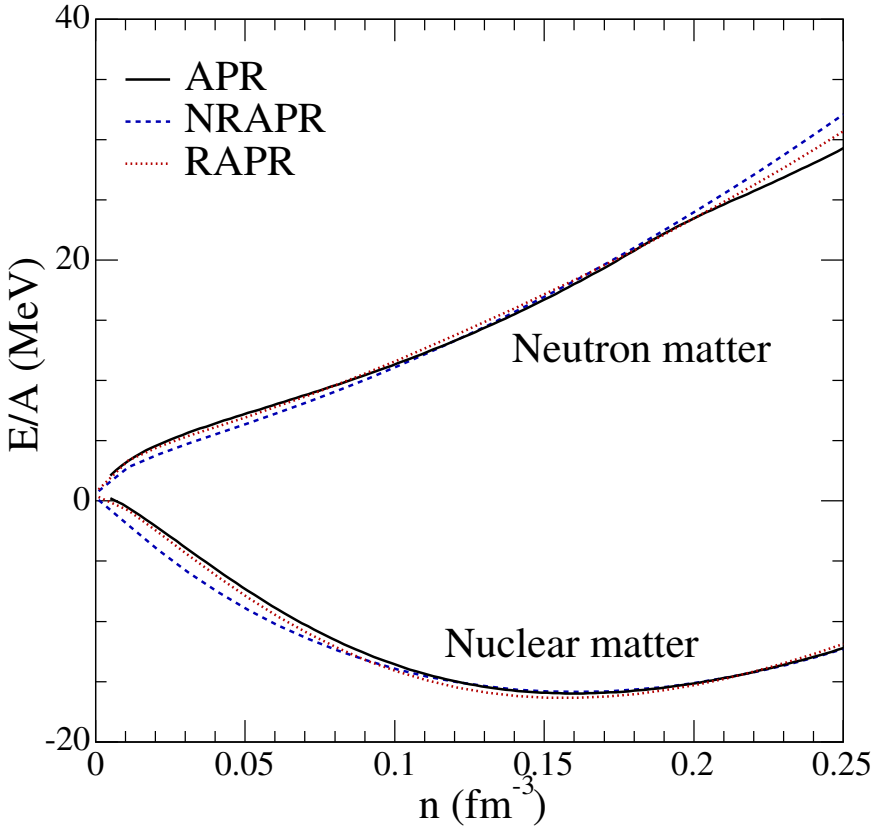
$$\frac{E_B(N,Z)}{A} = a_v - a_s A^{-1/3} - a_C \frac{Z^2}{A^{4/3}} - a_{\rm sym} \frac{(N-Z)^2}{A^2}$$

- Divide terms by $A = N + Z$
- Rough numbers:
  $a_v \approx 16\,\text{MeV}$, $a_s \approx 18\,\text{MeV}$,
  $a_C \approx 0.7\,\text{MeV}$, $a_{\rm sym} \approx 28\,\text{MeV}$
- Surface symmetry energy:
  $a_{\rm surf\ sym}(N-Z)^2/A^{7/3}$
- Now take $A \to \infty$ with Coulomb $\to 0$ and fixed N/A, Z/A
- Surface terms negligible



Nuclear and neutron matter energy vs. density

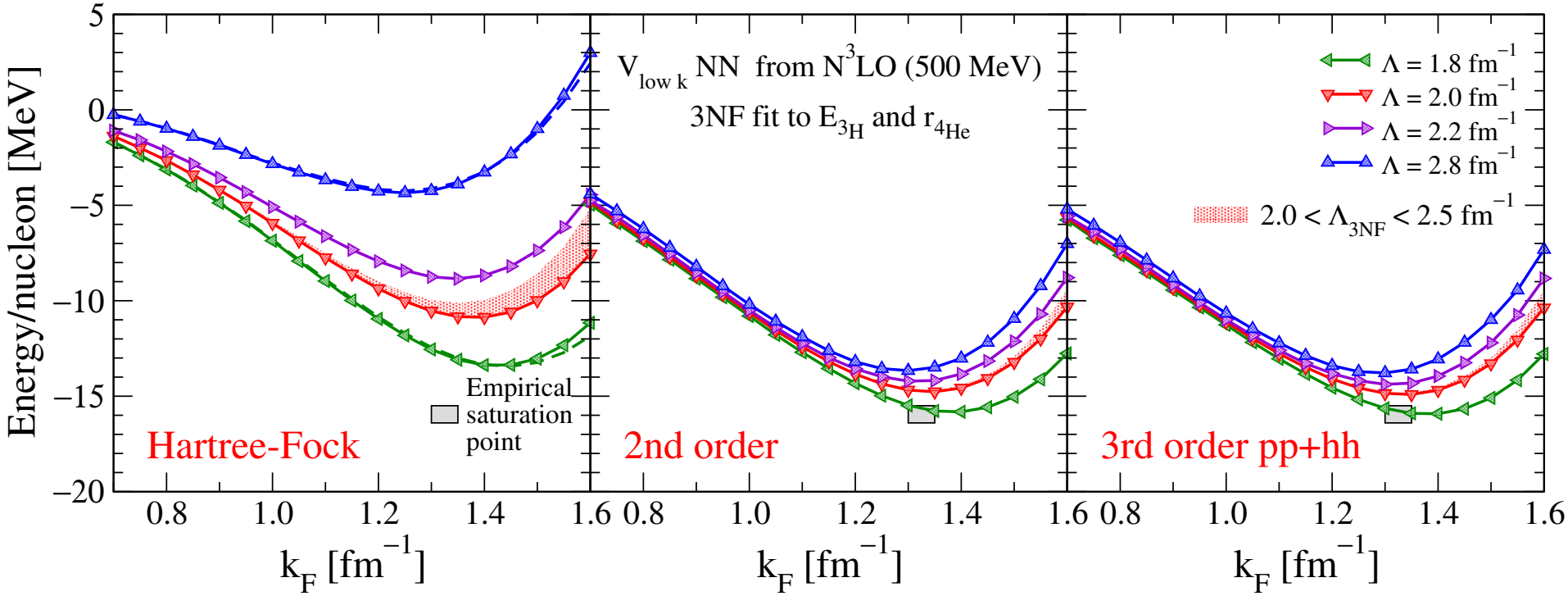
[Akmal et al. calculations shown]



- Uniform with Coulomb turned off
- Density n (or often ρ)
- Fermi momentum $n = (\nu/6\pi^2)k_{\rm F}^3$
- Neutron matter ($Z = 0$) has positive pressure
- Symmetric nuclear matter ($N = Z = A/2$) saturates
- *Empirical* saturation at about $E/A \approx -16\,\text{MeV}$ and $n \approx 0.17 \pm 0.03\,\text{fm}^{-3}$

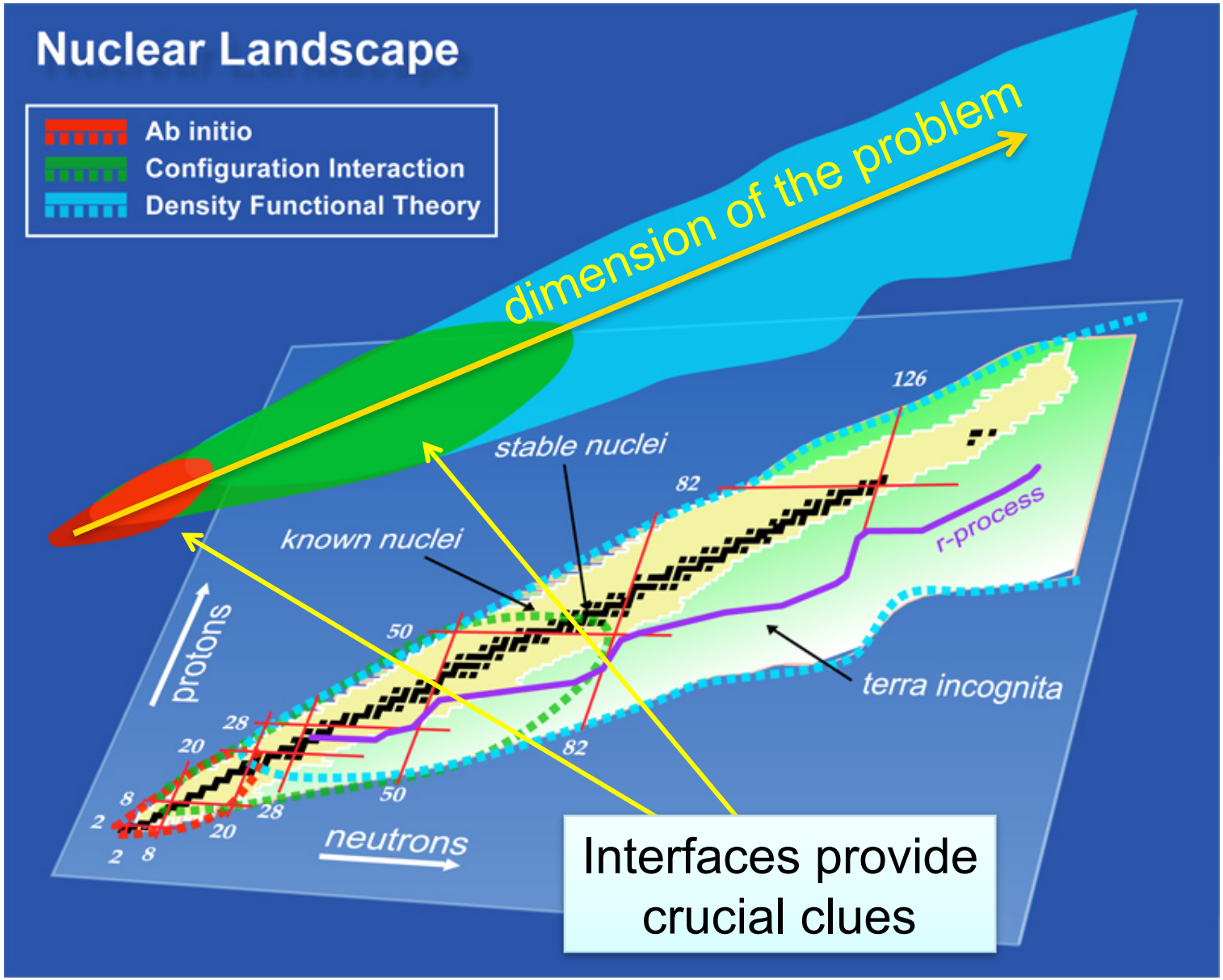
Low resolution calculations of nuclear matter

- Evolve NN by RG to low momentum, fit NNN to $A = 3, 4$
- Predict nuclear matter in MBPT [Hebeler et al. (2011)]



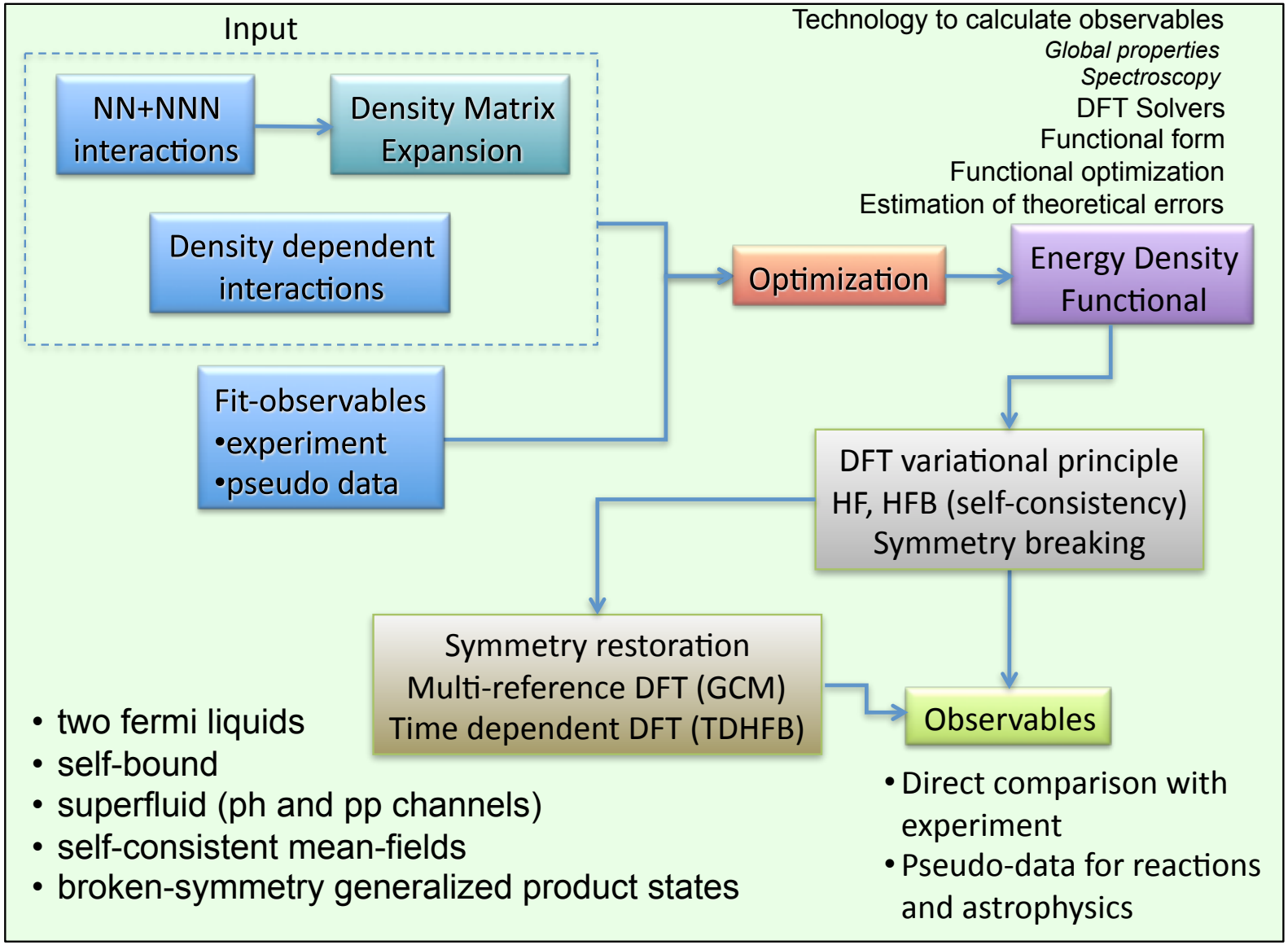
- Cutoff dependence at 2nd order significantly reduced
- 3rd order contributions are small
- Remaining cutoff dependence: many-body corrections, 4NF?

Overlapping theory methods cover all nuclei



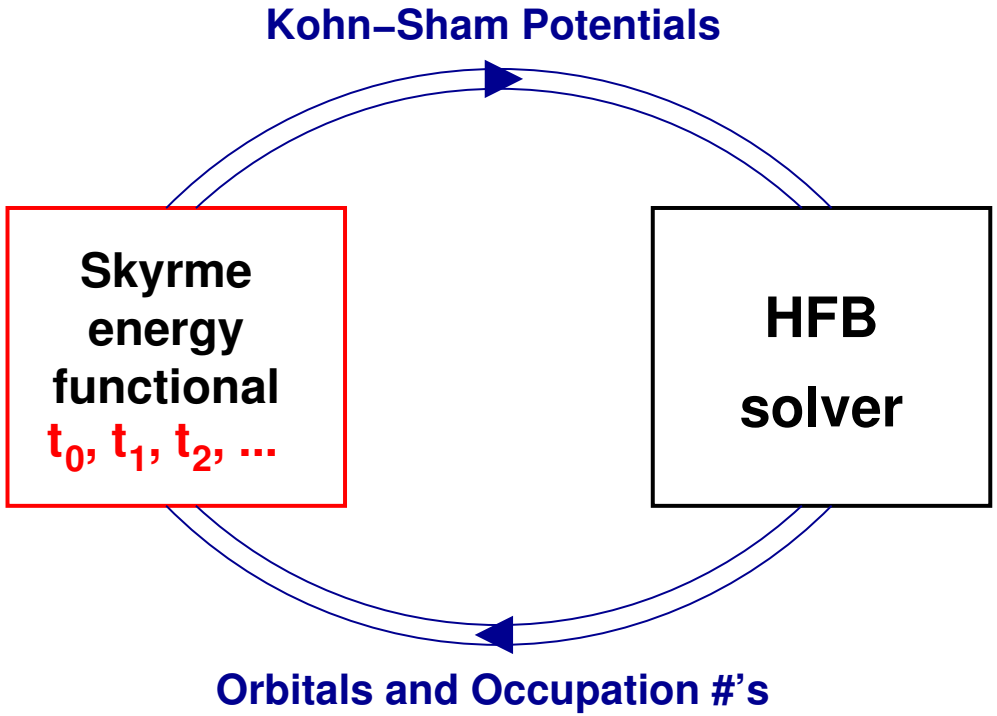
DFT for nuclei [UNEDF and NUCLEI projects]

Nuclear Density Functional Theory and Extensions



Skyrme EDF and beyond

$$\mathcal{E}_{Skyrme} = \frac{\tau}{2M} + \frac{3}{8}t_0\rho^2 + \frac{1}{16}t_3\rho^{2+\alpha} + \frac{1}{16}(3t_1 + 5t_2)\rho\tau + \frac{1}{64}(9t_1 - 5t_2)|\nabla\rho|^2 + \cdots$$



- Kohn-Sham density functional theory $\Longrightarrow$ iterate to self-consistency
- Pairing is critical
- Improve functional with same iteration scheme

Schematic equations to solve self-consistently:

$$V_{\rm KS}(\mathbf{r}) = \frac{\delta E_{\rm int}[\rho]}{\delta\rho(\mathbf{r})} \iff [-\frac{\nabla^2}{2m} + V_{\rm KS}(\mathbf{x})]\psi_\alpha = \varepsilon_\alpha\psi_\alpha \implies \rho(\mathbf{x}) = \sum_\alpha n_\alpha|\psi_\alpha(\mathbf{x})|^2$$

Skyrme EDF and beyond

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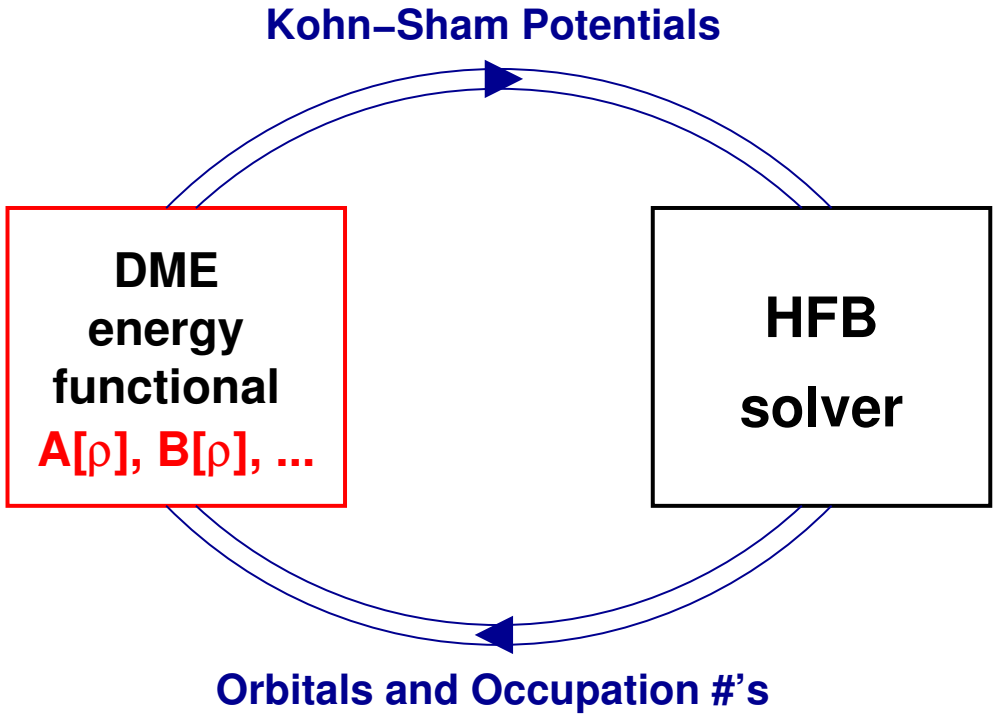

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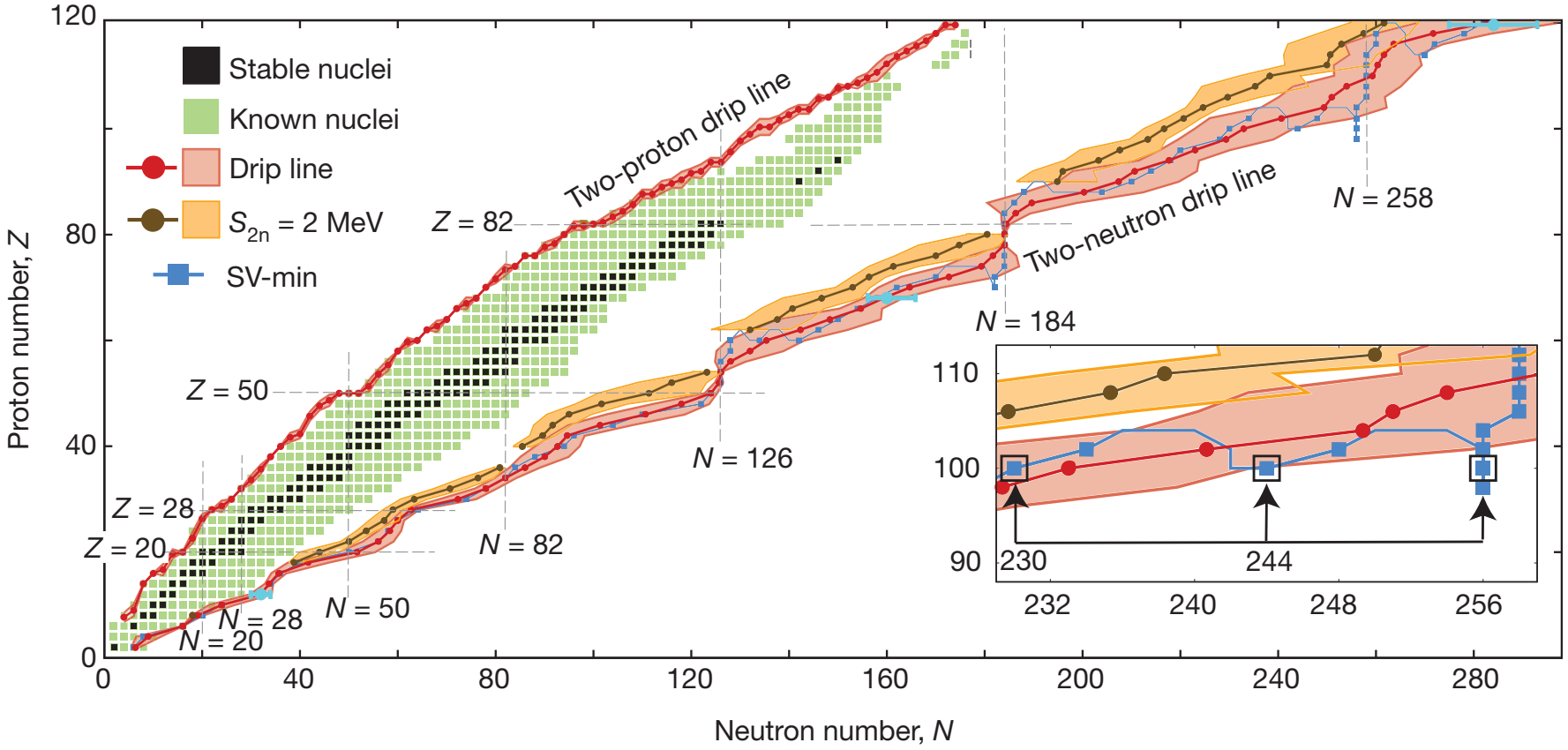
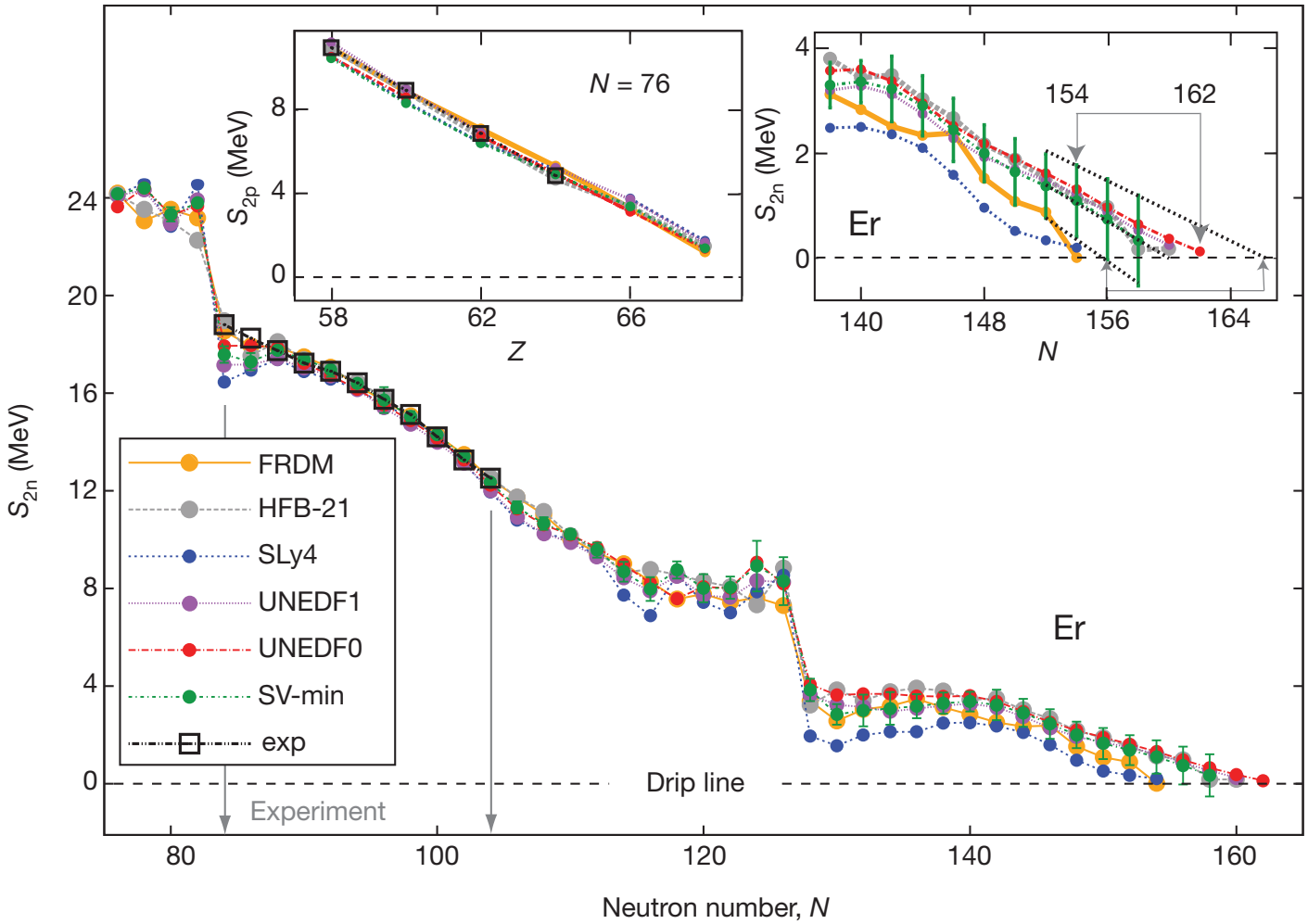
"The limits of the nuclear landscape"

J. Erler et al., Nature **486**, 509 (2012)



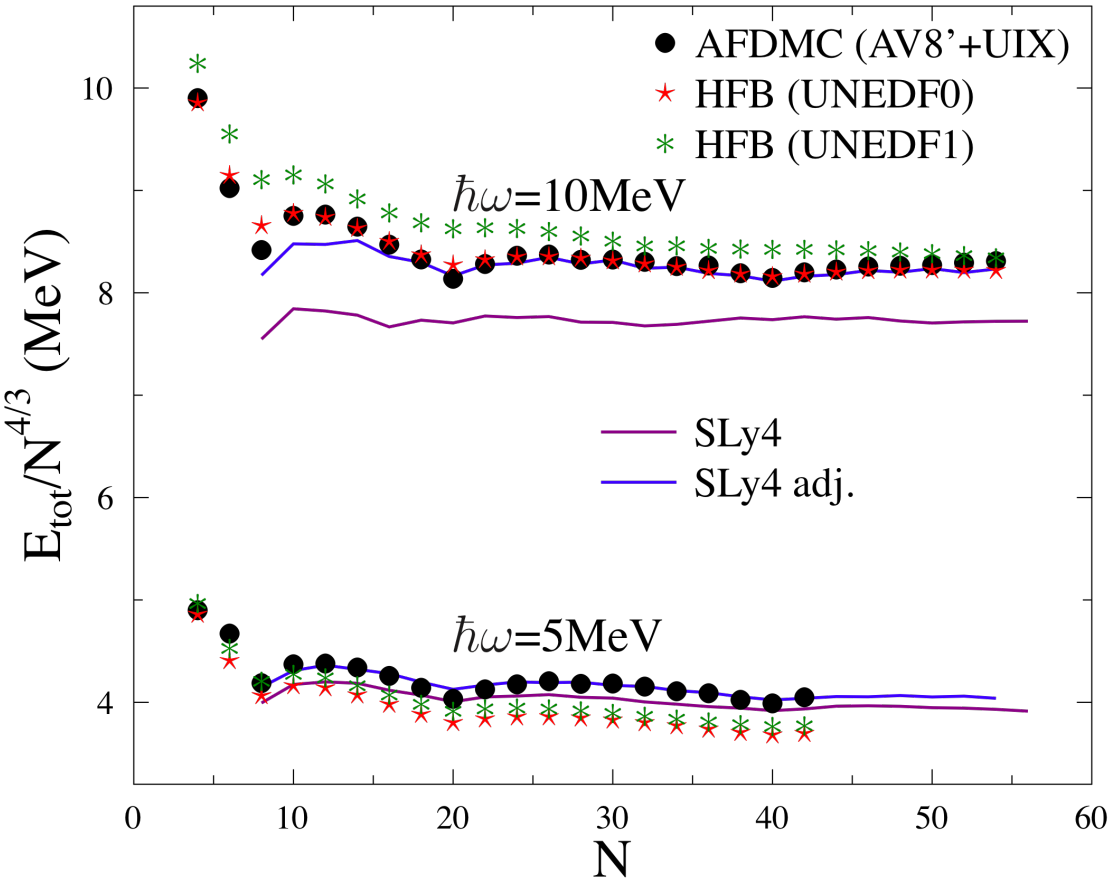
- Proton and neutron driplines predicted by Skyrme EDFs
  - Total: 6900 ± 500 nuclei with $Z \leq 120$ (≈ 3000 known)
  - Estimate systematic errors by comparing models

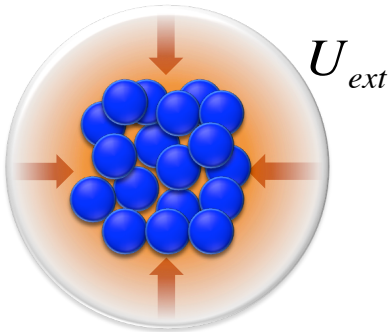
"The limits of the nuclear landscape"



- Two-neutron separation energies of even-even erbium isotopes
  - Compare different functionals, with uncertainties of fits
  - Dependence on neutron excess poorly determined (cf. driplines)

UNEDF Project: Use *ab initio* pseudo-data





- Put neutrons in a harmonic oscillator trap with $\hbar\omega$ (cf. cold atoms!)
- Calculate exact result with AFDMC [S. Gandolfi, J. Carlson, and S.C. Pieper, Phys. Rev. Lett. 106, 012501 (2011)] (or with other methods)
- UNEDF0 and UNEDF1 functionals improve over Skyrme SLy4!

Interaction with applied math experts

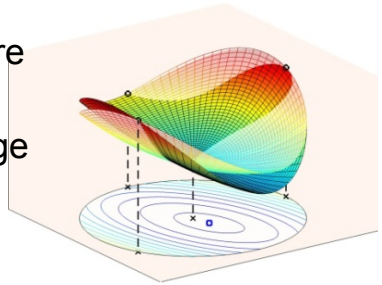
Optimization Algorithms for Calibrating Extreme Scale Simulations

Typical Challenges

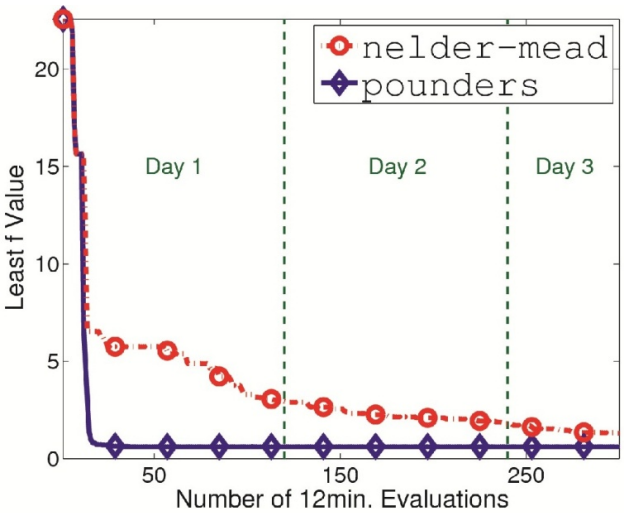
- Computational expense of simulation only allows for evaluating a few sets of parameter values
- Derivatives with respect to parameters can be unavailable or intractable to compute/approximate
- Experimental data incomplete or inaccurate
- Sensitivity analysis/confidence regions desired

New Algorithm POUNDERS

- Exploits mathematical structure in calibration problems
- Benefits from expert knowledge
  - data, weights, uncertainties, etc.
- Obtains good fits in minimal number of simulations



POUNDERS obtains better solutions faster

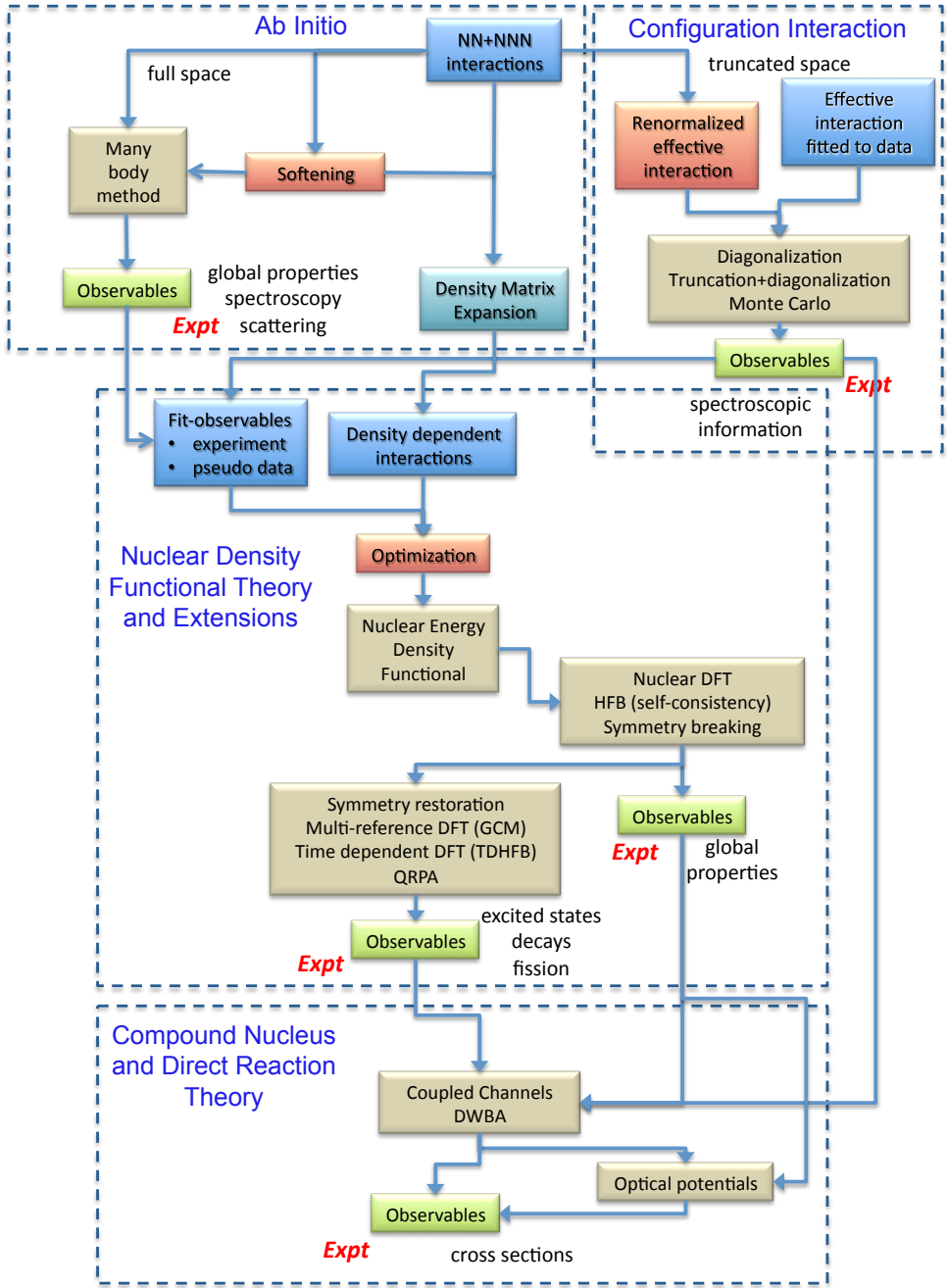


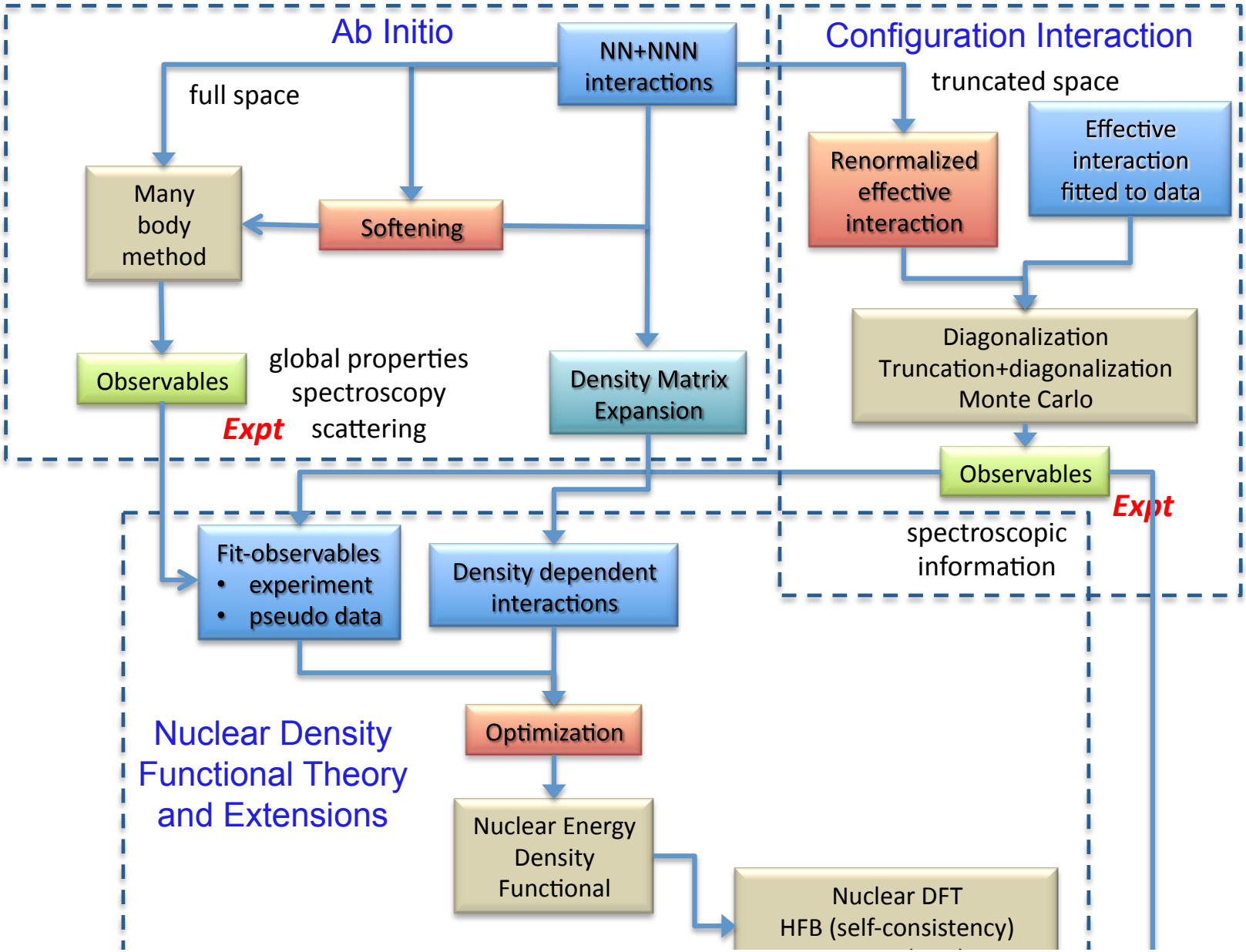
Energy density functionals (EDFs) for UNEDF

- Enables fitting of complex, state-of-the-art EDFs
  - Optimization previously avoided because too many evaluations required to obtain desirable features
- Substantial computational savings over alternatives
- Using resulting EDF parameterizations, the entire nuclear mass table was computed and is now distributed at **www.massexplorer.org**
  - *Nuclear Energy Density Optimization. Kortelainen et al., Physical Review C **82**, 024313, 2010*
  - *Three joint physics & optimization publications @ SciDAC11!*

- SciDAC-2 UNEDF project
- Universal Nuclear Energy Density Functional
- Collaboration of physicists, applied mathematicians, and computer scientists
- US funding but international collaborators also
- See unedf.org for highlights!

New SciDAC-3 NUCLEI project:
NUclear Computational Low-Energy Initiative




Ab Initio
NN+NNN interactions
full space
Many body method
Softening
Observables
global properties
spectroscopy
scattering
Expt
Density Matrix Expansion
Configuration Interaction
truncated space
Renormalized effective interaction
Effective interaction fitted to data
Diagonalization
Truncation+diagonalization
Monte Carlo
Observables
Expt
spectroscopic information
Fit-observables
• experiment
• pseudo data
Density dependent interactions
Optimization
Nuclear Density Functional Theory and Extensions
Nuclear Energy Density Functional
Nuclear DFT
HFB (self-consistency)

Interaction with computer science experts

"Load Balancing at Extreme Scale" – Ewing Lusk, Argonne National Laboratory

ASCR- SciDAC UNEDF Computer Science Highlight

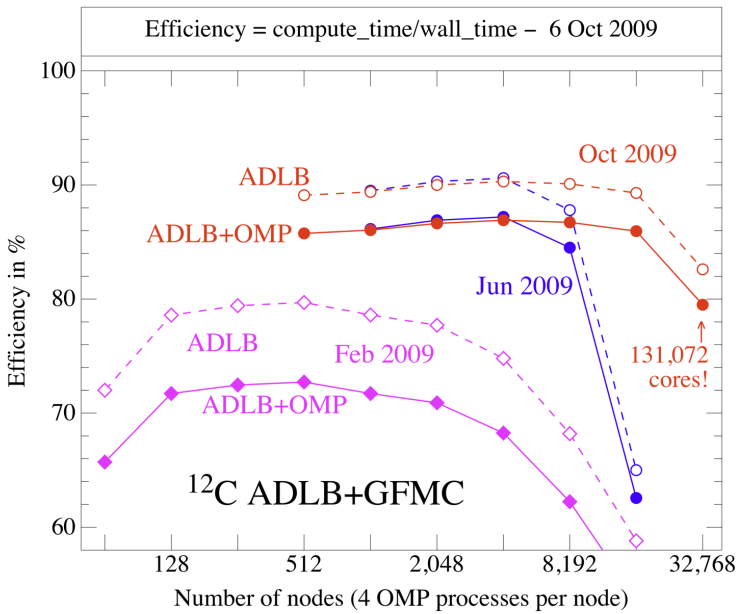
Objectives

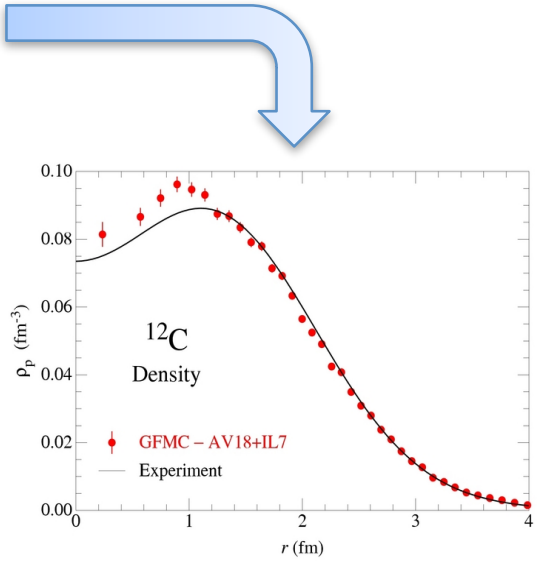
- **Enable Green's Function Monte Carlo calculations for ^{12}C on full BG/P as part of UNEDF project**
- **Simplify programming model**
- **Scale to leadership class machines**

Impact

- **Demonstrate capabilities of simple programming models at petascale and beyond**
- **Show path forward with hybrid programming models in library implementation**

Improved Efficiency (compute time/wall time) with more nodes





Progress

- **Initial load balancing was of CPU cycles**
- **Next it became necessary to balance memory utilization as well**
- **Finally ADLB acquired the capability to balance message flow**
- **"More Scalability, Less Pain" by E. Lusk, S.C. Pieper and R. Butler published in SciDAC Review 17, 30 (2010)**

SciDAC-3 NUCLEI Project