Progress and challenges in theory of nuclei (Snapshots)

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"The shell must break before the bird can fly." -- Tennyson

Nuclear Data and Standards

The systematic collection and availability of nuclear data and associated standards is a pre-requisite for various applications.

→ **Worldwide network of nuclear data centers:**
- → **Collect nuclear data (experiment and theory)**
- → **Evaluate the quality**
- → **Make the data available in the appropriate form for the user**

Present Status:

Evaluated Nuclear Data Files represent a consistent set of cross sections and associated quantities for all relevant reaction processes.

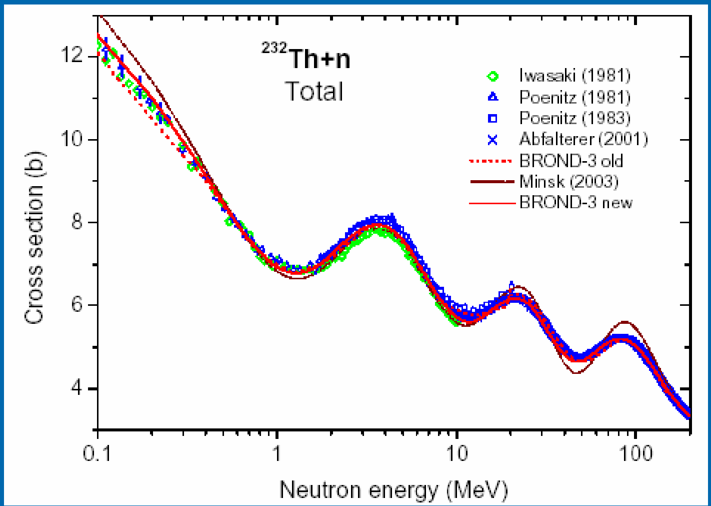
EXFOR, ENSDF
ENDF, Mass Data Library

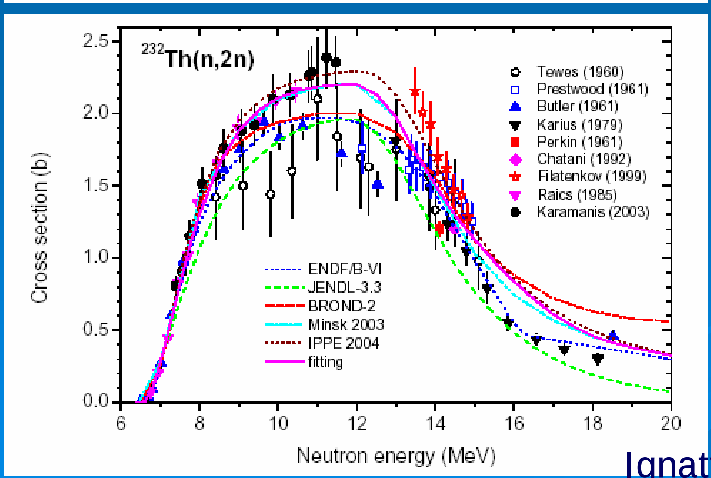
Maintained by Centers: IAEA, NNDC,…

Future requirement:
Data files should contain the values of the cross sections and appropriate information about the uncertainty and reliability of the nuclear data.
Directly impacts safty and economic issues.

Nuclear Data: Quality

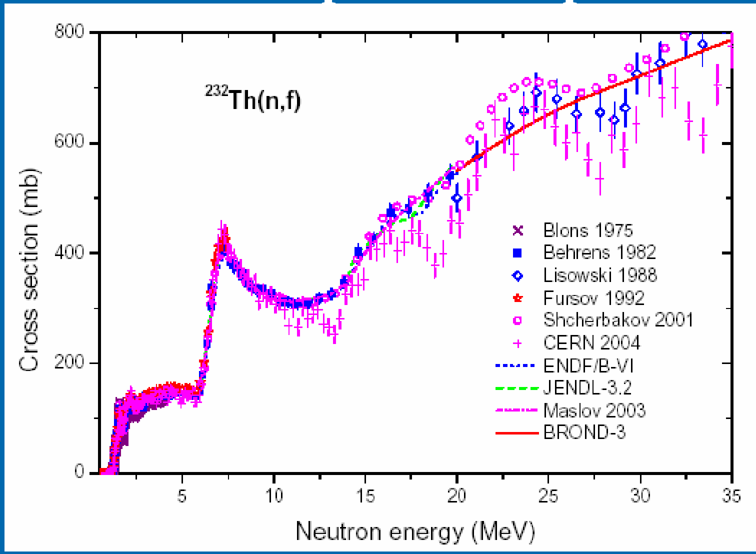
Nuclear data required for standard applications are of satisfactory quality – i.e. for thermal reactors and dosimetry

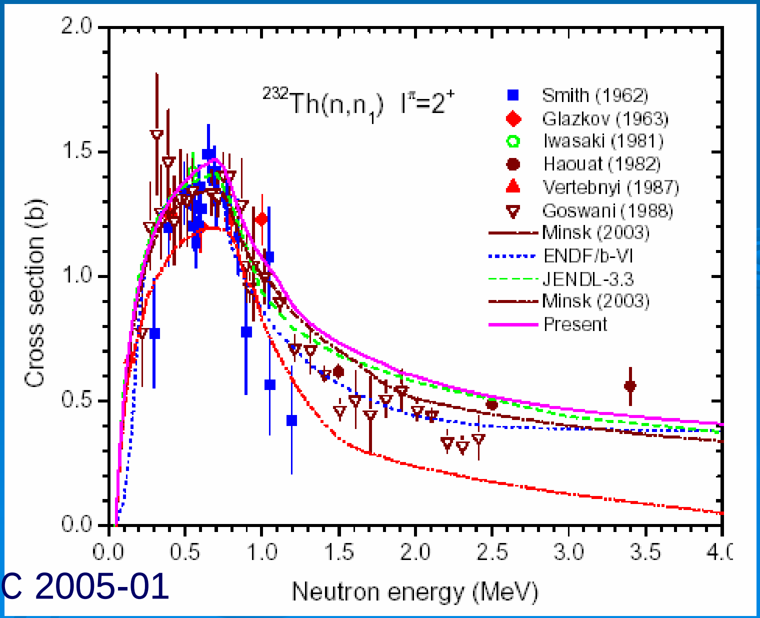




Nuclear Data Limitations

Standard evaluation techniques have a limited predictive power





Ignatyuk et al., ATI-NDC 2005-01

Emerging nuclear technologies and the data need

New nuclear technologies are emerging:
- **Generation IV reactors with high burnup**
- **Transmutation of radioactive waste**
- **Use of Thorium-Uranium cycle**
- **Aspects of Materials research**

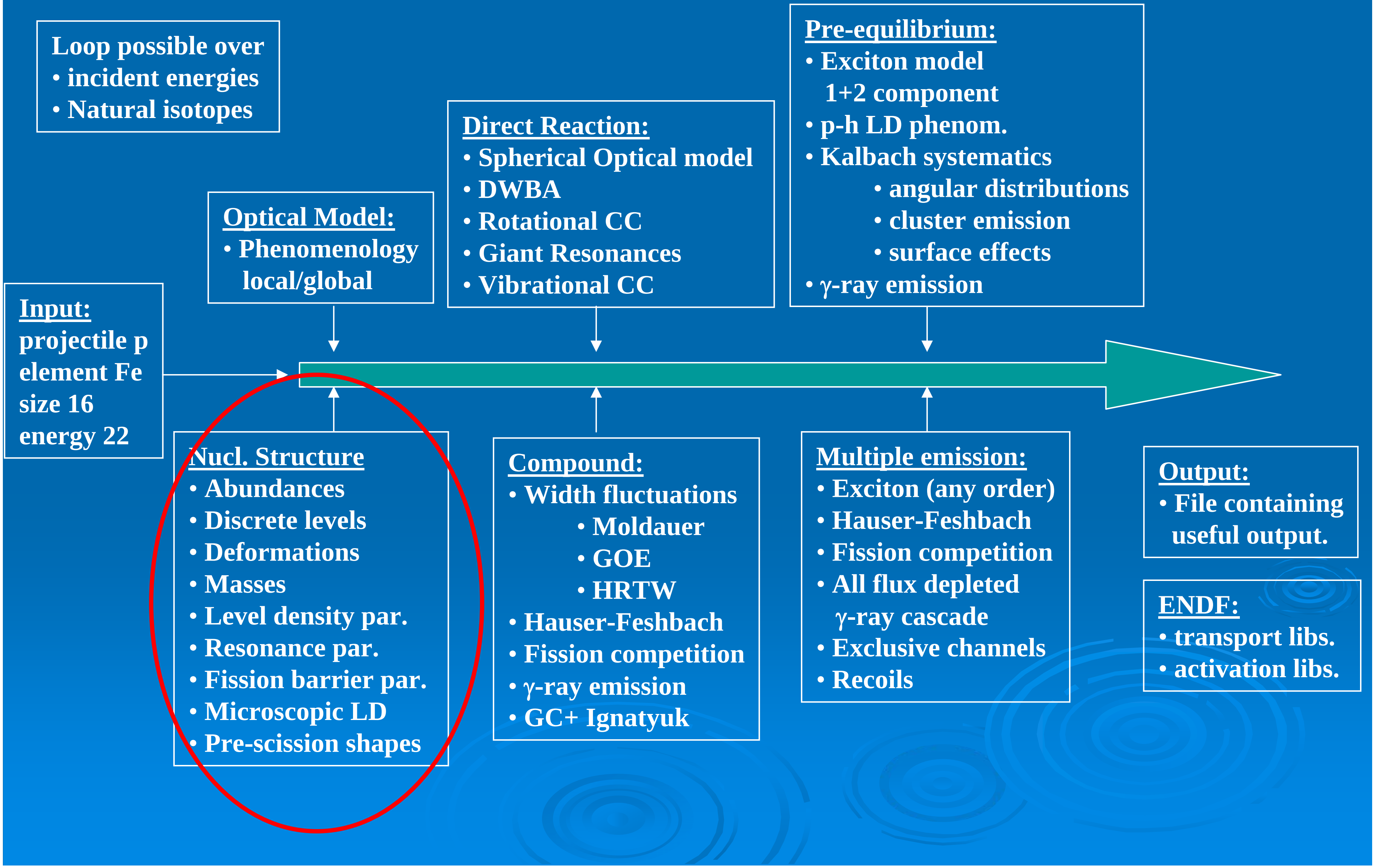
→ **Need to quantify shielding, activation, burn, and dosimetry at higher energy and intensities.**

'Incomplete' experiments → **nuclear theory with higher predictive power**
→ **reliable estimates of the quality of the nuclear theory**
→ **realistic margins for the observables**

Reason for improved theory:
Number of open channels significantly increased –experiments cannot cover the whole variety. Because of budget limitations, feed back (Validation) experiments are limited and an optimization must be achieved already at the level of the prototype.

Theoretical inputs to the reaction problem….

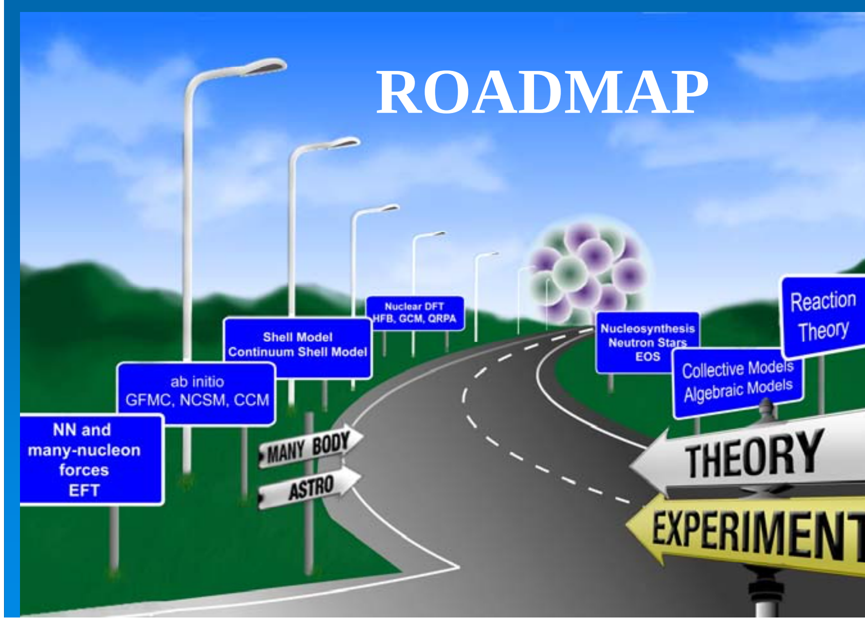
from TALYS – Calculational Scheme



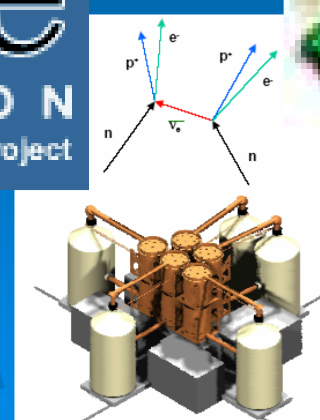
Key science drivers of rare isotopes

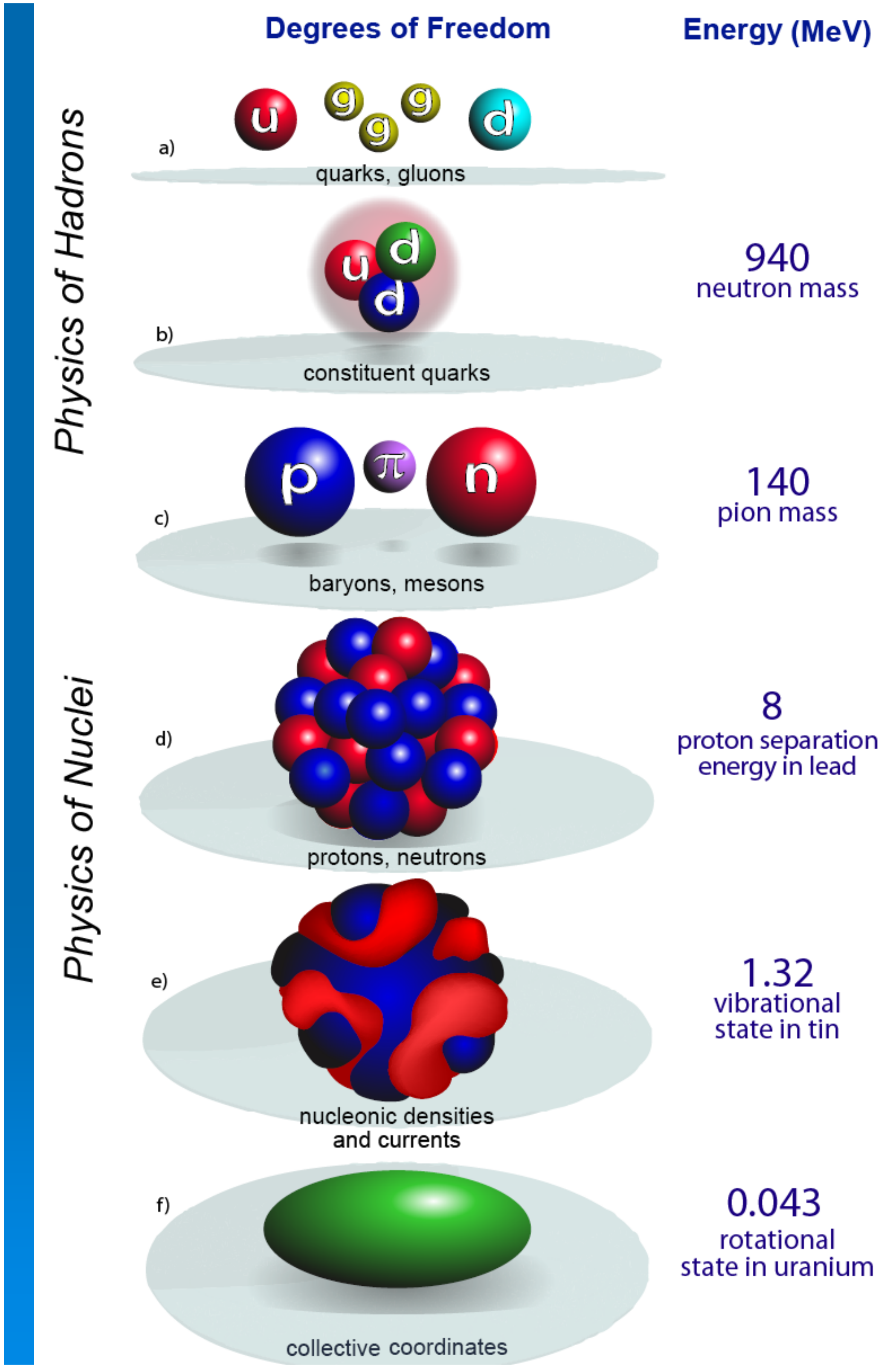
- **Test the predictive power of models by extending experiments to new regions of mass and proton-to-neutron ratio**
- **Identify new phenomena that will challenge existing many-body theory**

- **Create and study super heavy nuclei**
- **Characterize neutron skins and excitation modes**
- **Constrain r-process site and explosive nucleosynthesis**
- **Constrain nuclear equation of state (neutron star crusts)**
- **Societal Applications: Energy, Security**
- **Beyond 'Standard Model': ββ0ν decay; Dark Matter, EDM…**



Xe
XENON
Dark Matter Project





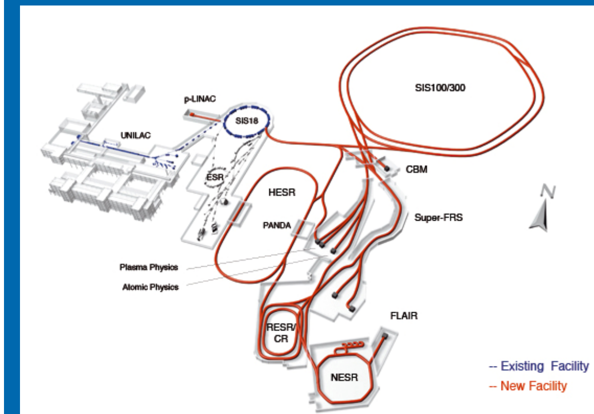
Nuclei are multiscale

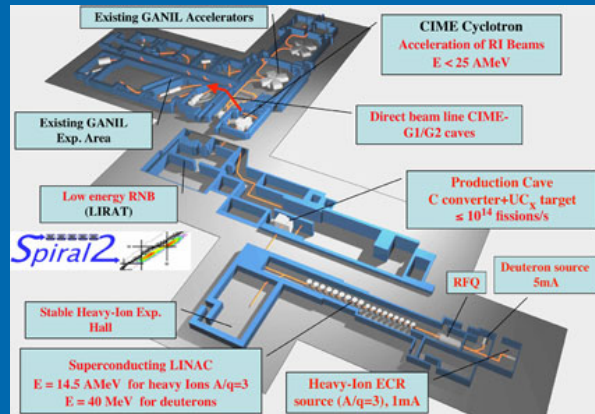
- QCD governs nucleons and their interactions: GeV
- Nuclear excitations: MeV
- Resonances in U: keV

Decay time scales vastly different
From 10^{-21} s to long-lived meta stable states

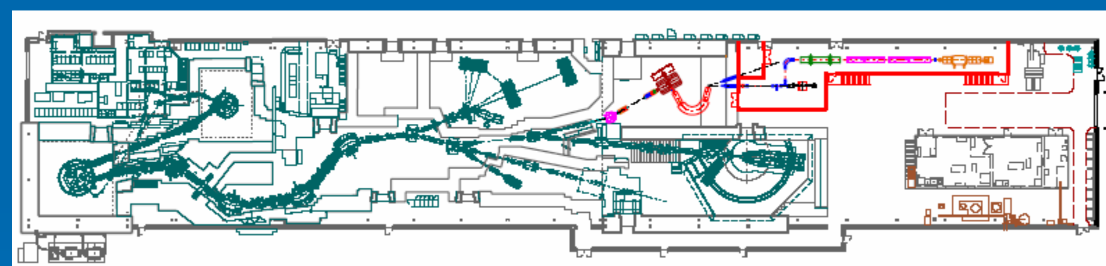
Huge variation in reaction rates

Present and next Generation Radioactive Ion Beam facilities (multi $100M investments world wide)

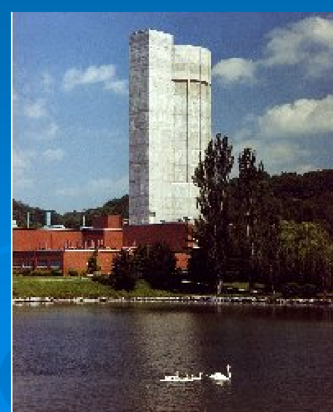




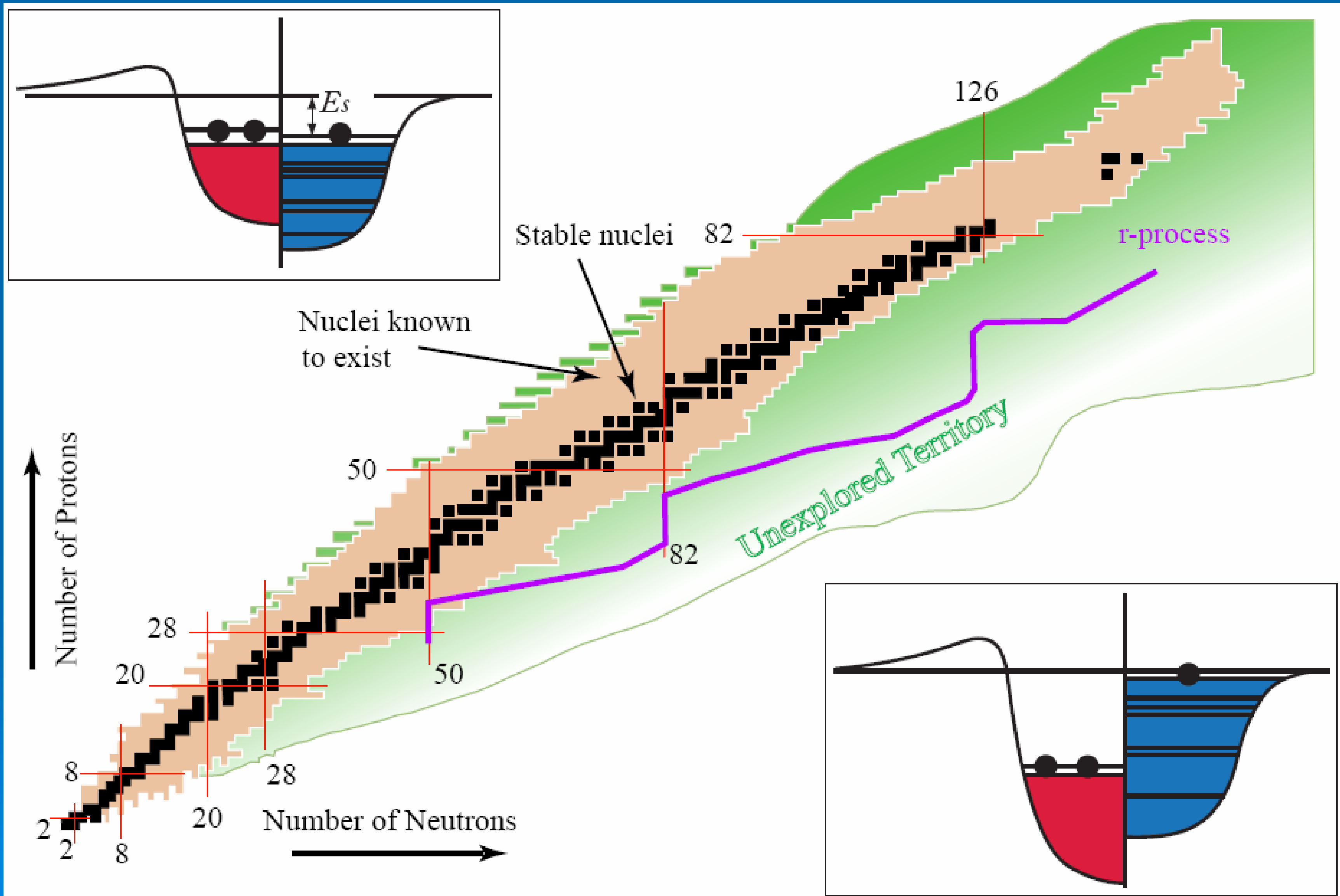
"[C]ountries throughout the world are aggressively pursuing rare-isotope science, often as their highest priority in nuclear science, attesting to the significance accorded internationally to this exciting area of research"
NAS RISAC Report



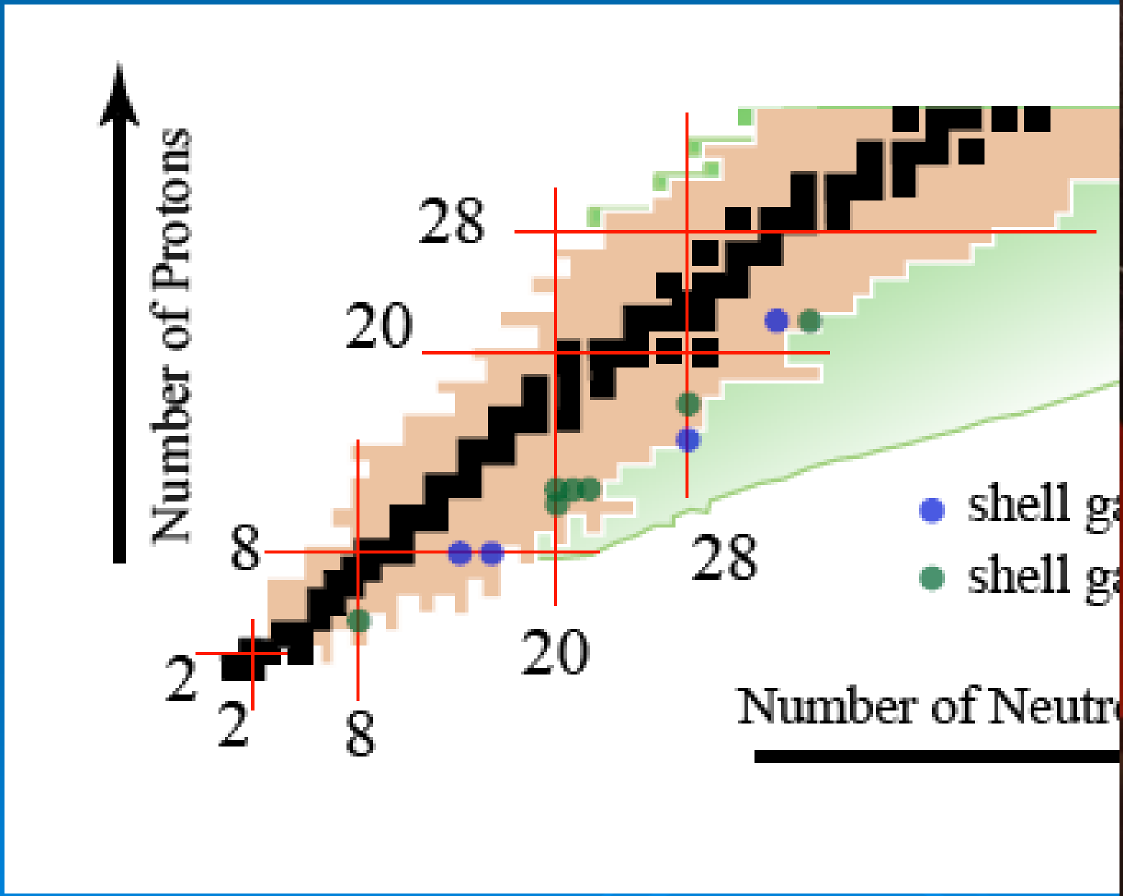
- Future U.S. FRIB based on a heavy-ion linac driver a high priority.
- Options in the interim?



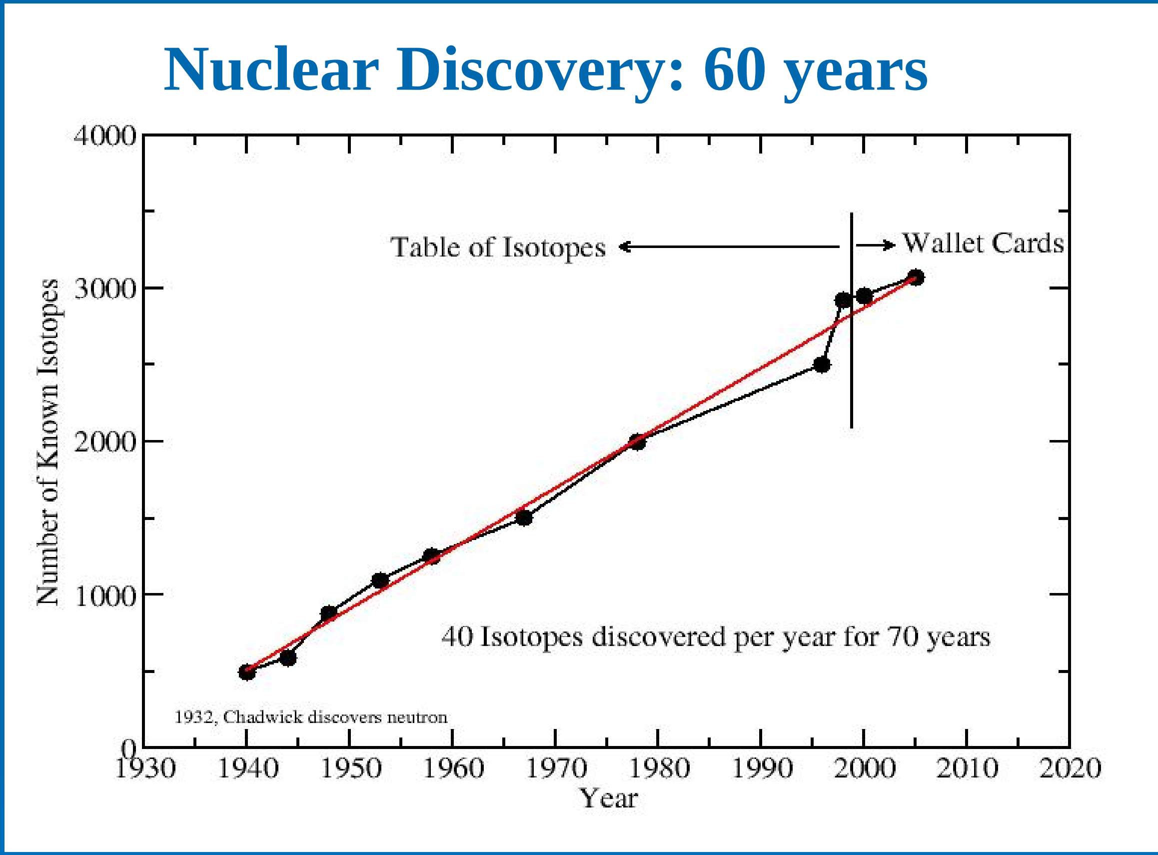
Landscape and consequences



Changing shell gaps: one of the challenges



Why do theory at all?



- Discovery of new nuclei a rather slow process
- Increasingly costly
- Probably will not reach ALL nuclei that are relevant even with FRIB
- Probably cannot measure all relevant nuclear properties
- Points to need for robust, predictive theory with quantifiable error bars

The challenge of theory for nuclei

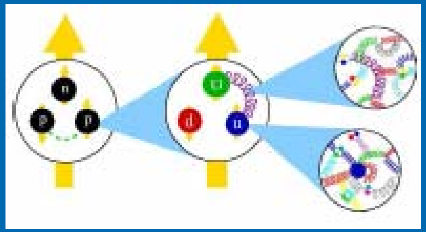
"The first, the basic approach, is to study the elementary particles, their properties and mutual interaction. Thus one hopes to obtain knowledge of the nuclear forces. If the forces are known, one should, in principle, be able to calculate deductively the properties of individual nuclei. Only after this has been accomplished can one say that one completely understands nuclear structure ….The other approach is that of the experimentalist and consists in obtaining by direct experimentation as many data as possible for individual nuclei. One hopes in this way to find regularities and correlations which give a clue to the structure of the nucleus….The shell model, although proposed by theoreticians, really corresponds to the experimentalist's approach."
–M. Goeppert-Mayer, Nobel Lecture

Two ways of doing business (I will focus primarily on the first):

- QCD → NN (and NNN) forces → calculate → predict → experiment
- Experiment → effective forces → calculate → predict
- Progress involves feedback…

Progress on the interaction: Effective Field Theory

Thus one hopes to obtain knowledge of the nuclear forces. If the forces are known… (MGM)



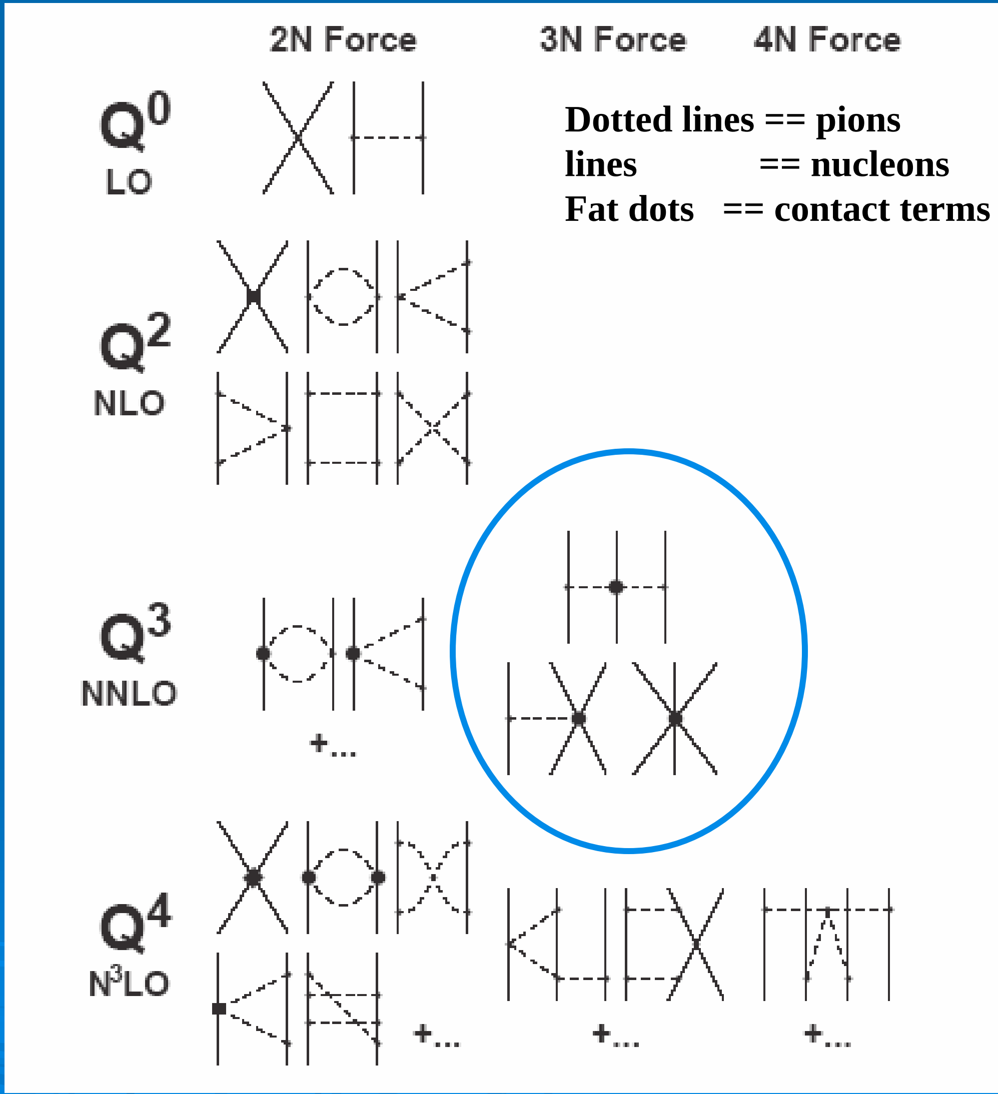
Effective Lagrangian → obeys QCD symmetries (spin, isospin, chiral symmetry breaking)

Lagrangian
→ infinite sum of Feynman diagrams.

Invoke power counting:
Expand in $O(Q/\Lambda_{QCD})$
Weinberg, Ordonez, Ray, van Kolck

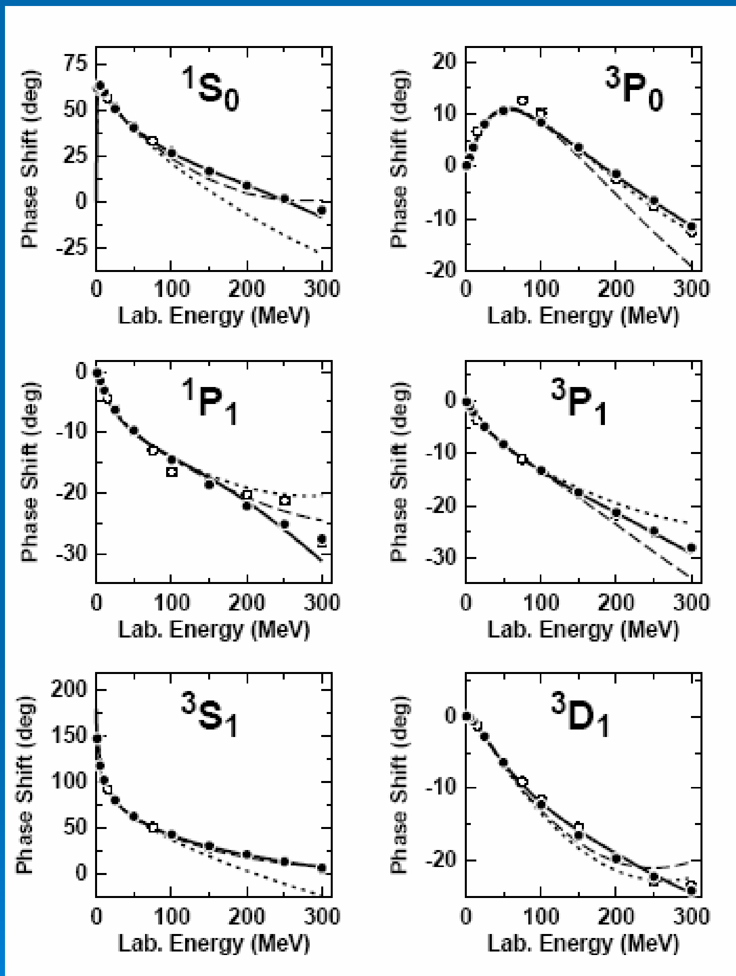
NN amplitude uniquely determined by two classes of contributions: contact terms and pion exchange diagrams.

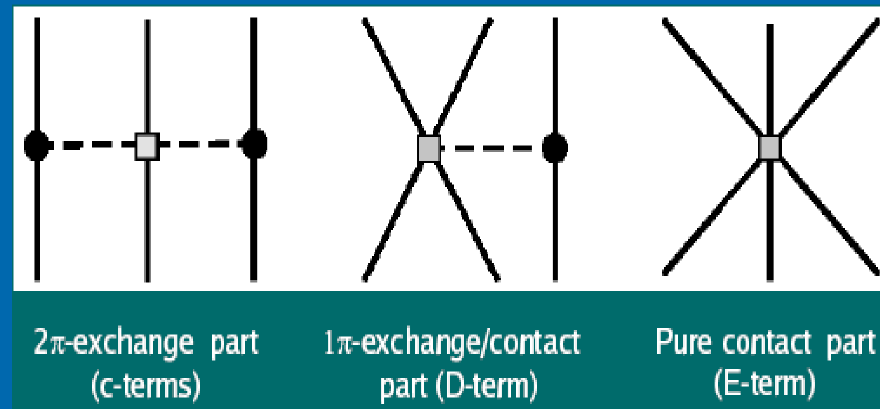
3-body (and higher) forces are inevitable.

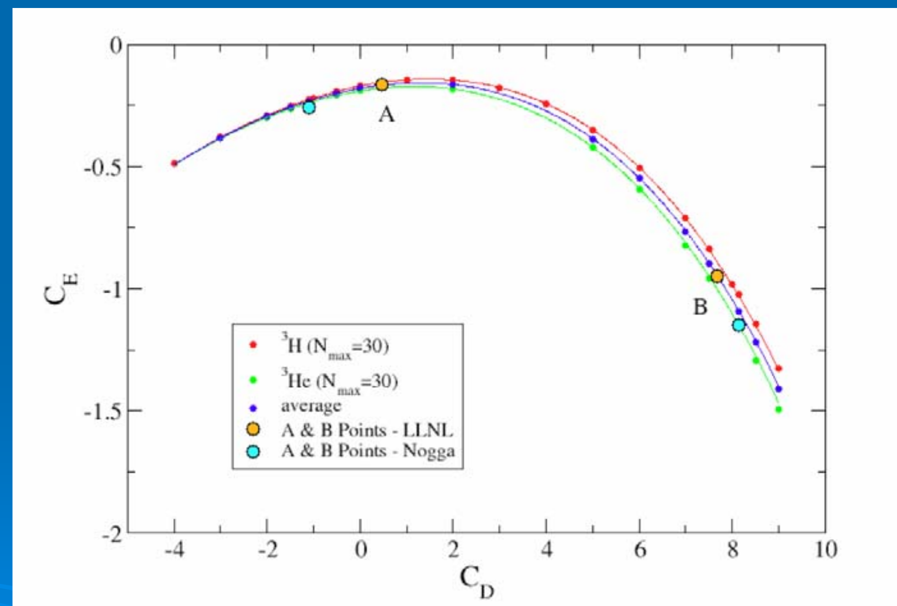


Effective field theory potentials bring a 3-body force

“…the force should be chosen on the basis of NN experiments (and possibly subsidiary experimental evidence…) (Bethe)







dashed → NLO
dot → N^2LO
solid → N^3LO

Challenge: Deliver the best NN and NNN interactions with their roots in QCD (eventually from LQCD, see Ishii, Aoki and Hatsuda, arXiv:nucl-th/0611096); Bedaque

From the interaction to solving the nuclear many-body problem

Begin with a NN (+3N) Hamiltonian

$$H = -\frac{\hbar}{2}\sum_{i=1}^{A}\frac{\nabla_i^2}{m_i} + \frac{1}{2}\sum_{i<j} V_{2N}\left(\vec{r}_i,\vec{r}_j\right) + \frac{1}{6}\sum_{i<j<k} V_{3N}\left(\vec{r}_i,\vec{r}_j,\vec{r}_k\right) - T_{com}$$

Bare (GFMC)
(Local only, Av18 plus adjusted 3-body)
Exponential scaling

Basis expansion (explore forces)

Basis expansions:
- Determine the appropriate basis
- Generate H_{eff} in that basis
- Use many-body technique to solve problem

Nucleus	4 shells	7 shells
4He	4E4	9E6
8B	4E8	5E13
12C	6E11	4E19
16O	3E14	9E24

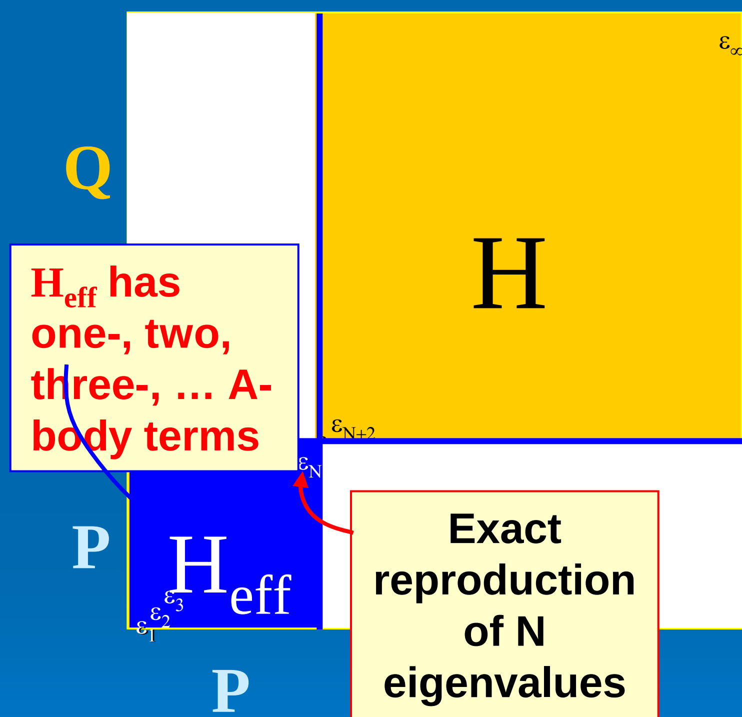
Oscillator single-particle basis states

Many-body basis states

Substantial progress in many-body developments
- GFMC; AFDMC
- No Core shell model (not a model)
- Coupled-cluster theory
- UCOM,…
- AFMC

Progress: Embracing renormalization

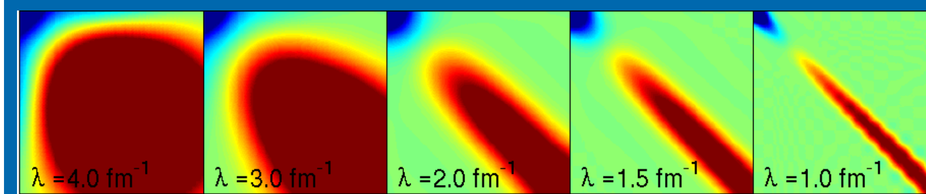
Project H into large basis;
Perform Lee-Suzuki (NCSM)
Use H_{eff} as 2-(+3) body interaction



Recovers Bare A-body in large space
Requires addition of 3-body force
for experimental binding (adjust to He-4)
Challenge: slow convergence

$$\frac{d}{d\Lambda}V^{\Lambda}_{\text{low }k}(k',k) = \frac{2}{\pi}\frac{V^{\Lambda}_{\text{low }k}(k',\Lambda)\,T^{\Lambda}(\Lambda,k;\Lambda^2)}{1-(k/\Lambda)^2}$$

- **Renormalize at a momentum cutoff Λ**
- **Project onto oscillator basis**
- **Preserves phase shifts to the cutoff**
- **“reasonable” convergence**



Challenges:
- **Does not recover bare result**
- **Requires 3-body force for experimental binding**
  …adjust to He-4
- **Λ-independence**

Schwenk, Bogner, Furnstahl,…

"…be able to calculate deductively the properties of individual nuclei"

- Computation absolutely essential
- "Moore's law" power law in raw computing power: 2 year doubling time.
- Petascale: 3 years
- Exascale: 10 years

- Challenge: develop algorithms that will effectively utilize both core speed and memory to attack nuclear problems.

- Measure of success: predictive nuclear theory in medium-mass nuclei (to mass 100).

Progress (example): Coupled Cluster Calculations in ^{16}O

$$|\Psi\rangle = \exp(T)|\Phi\rangle$$

$$T = T_1 + T_2 + T_3 + \cdots$$

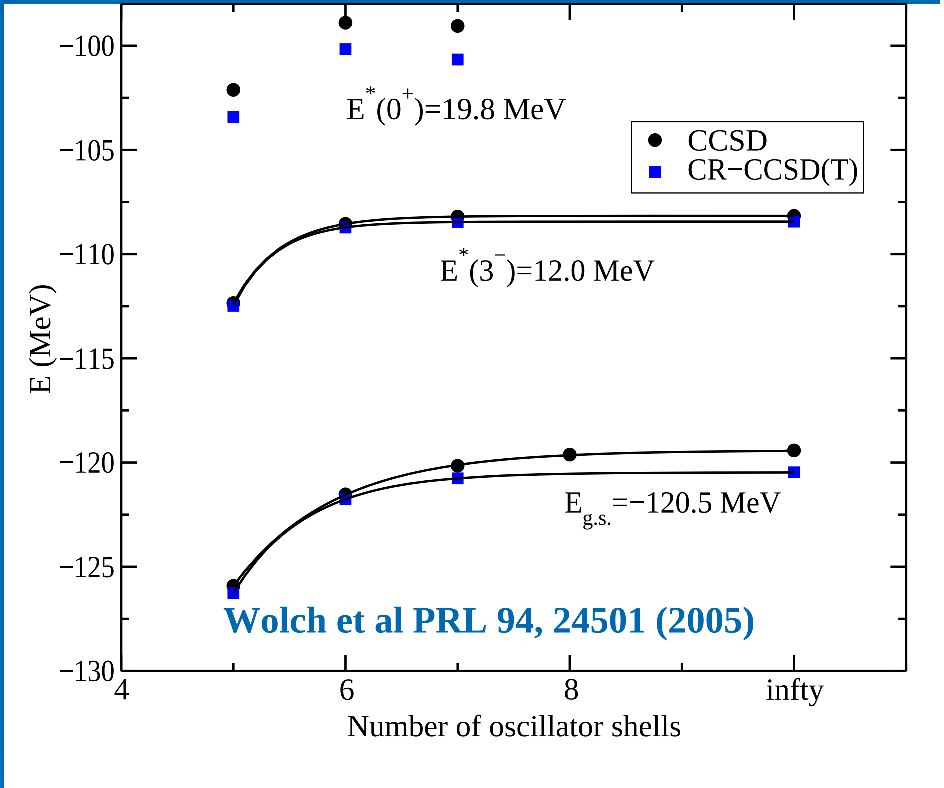
$$E = \langle\Phi|\overline{H}|\Phi\rangle = \langle\Phi|e^{-T} H e^{T}|\Phi\rangle$$

$$\langle\Phi_{ij\cdots}^{ab\cdots}|\overline{H}|\Phi\rangle = 0$$

$$R\overline{H}|\Phi\rangle = E^{*} R|\Phi\rangle$$

$R =$ excitation operator

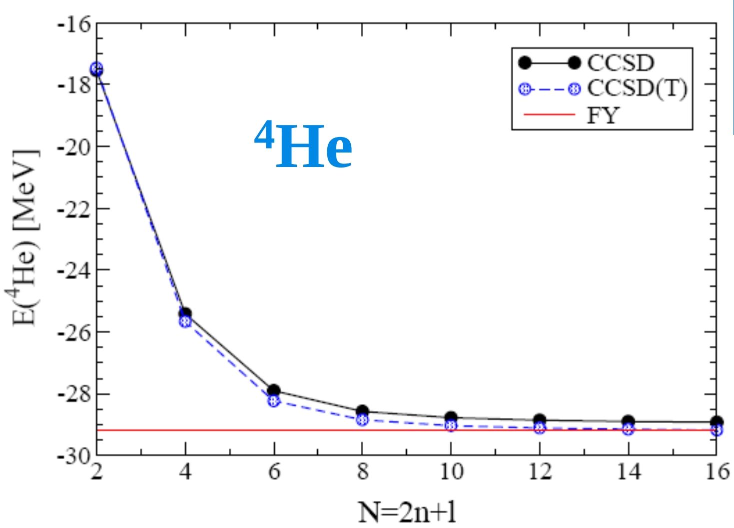
POLYNOMIAL SCALING!!

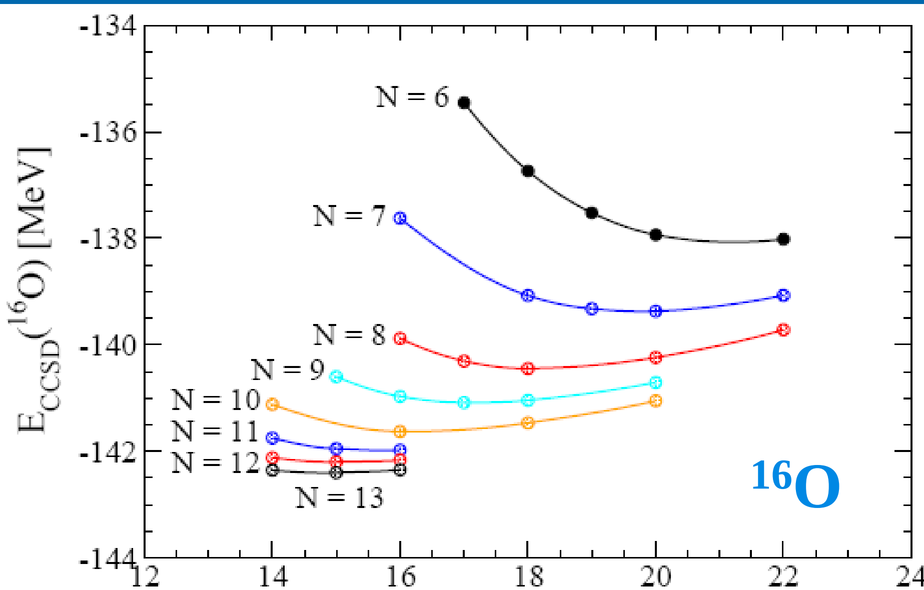


Note, converged spectrum but 3^- is 6 MeV high.

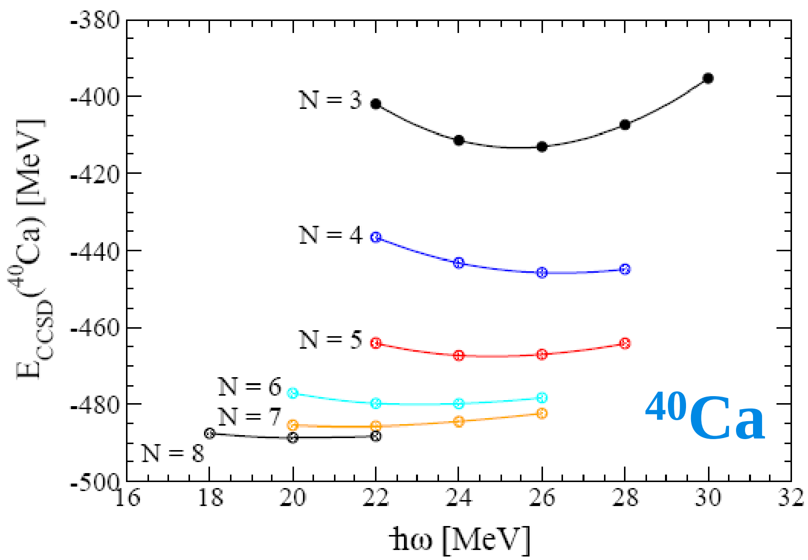
Challenge: how does the 3-body force affect these states?

Ab initio in medium mass nuclei





Hagen et al., arXiv:0707.1516

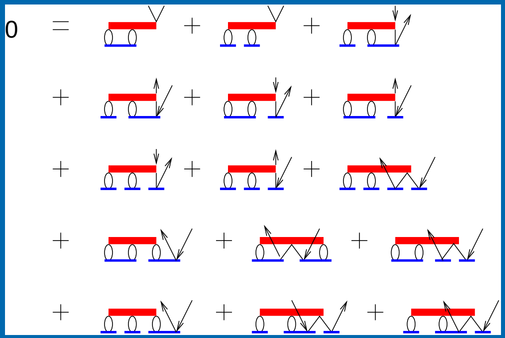


Error estimate: << 1% < 1% 1%

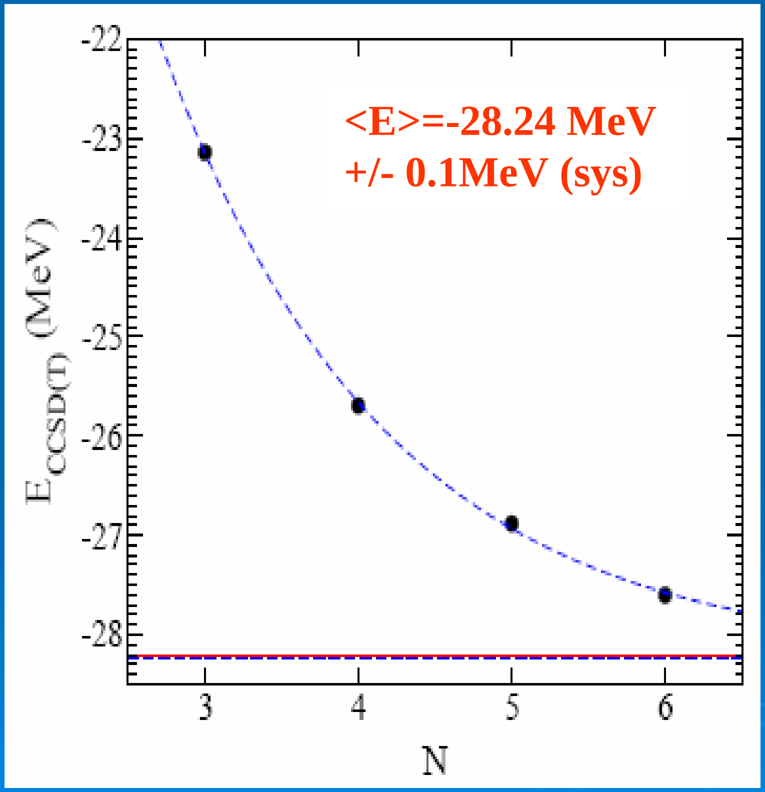
	^{4}He	^{16}O	^{40}Ca
E_0	-11.8	-60.2	-347.5
ΔE_{CCSD}	-17.1	-82.6	-143.7
$\Delta E_{CCSD(T)}$	-0.3	-5.4	-11.7
$E_{CCSD(T)}$	-29.2	-148.2	-502.9
exact (FY)	-29.19(5)		

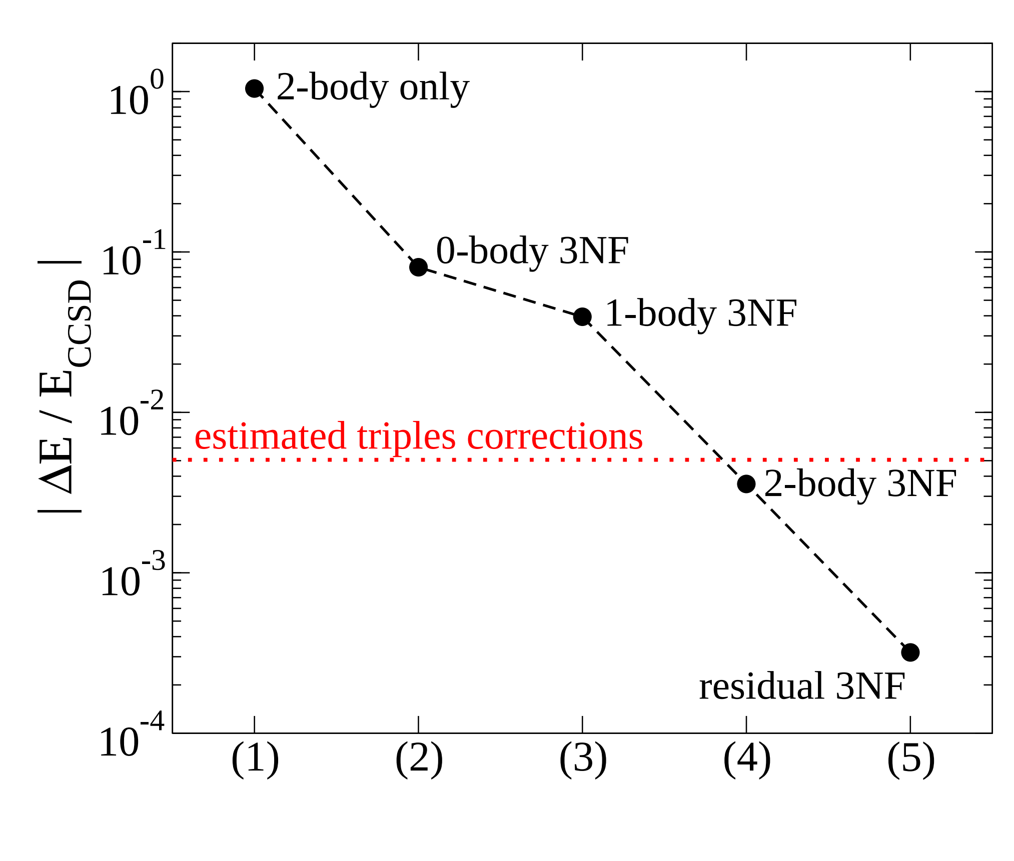
10^{63} many-body basis states

Progress: inclusion of full TNF in CCSD: F-Y comparisons in ^{4}He



Solution at CCSD and CCSD(T) levels involve roughly 67 more diagrams…..

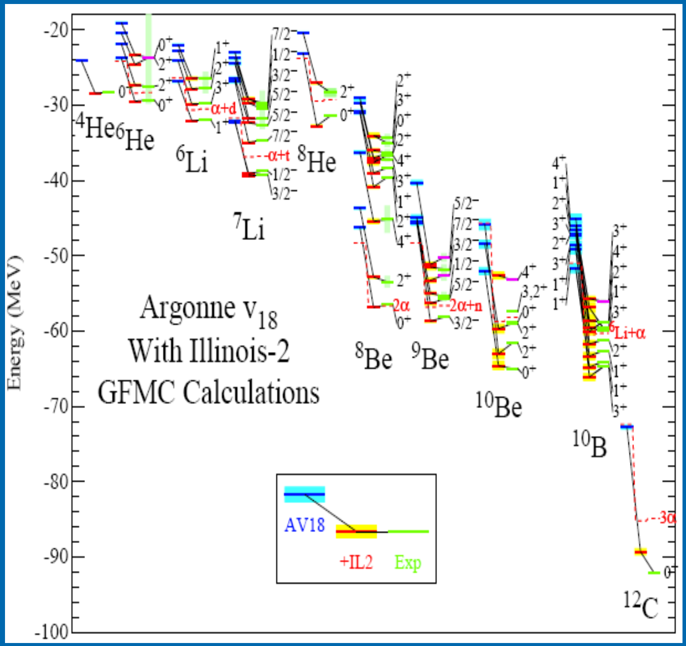




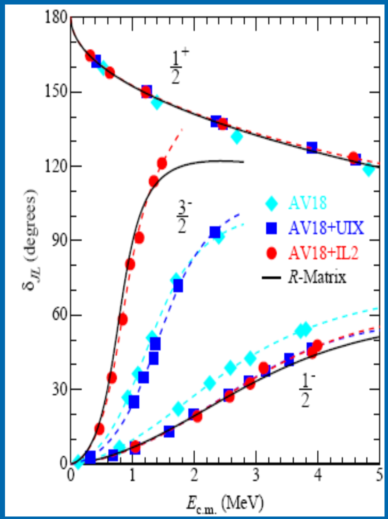
3-body force, or just its density dependent terms?

Hagen, Papenbrock, Dean, Schwenk, Nogga, Wloch, Piecuch arXiv:0704.3439

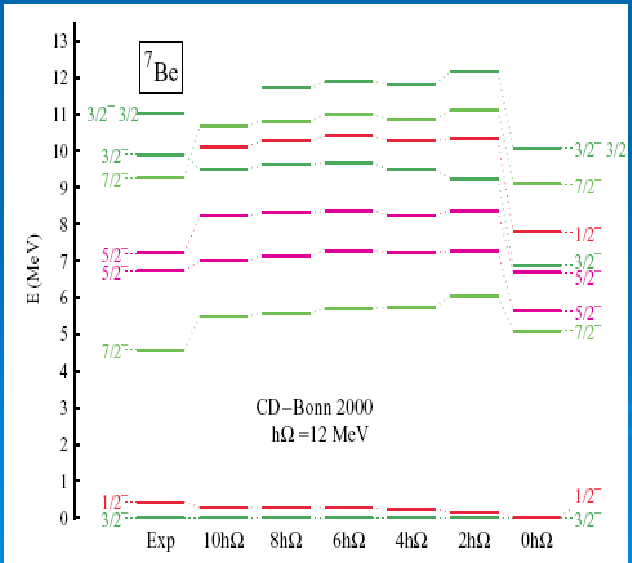
Progress: from structure to reactions in the same framework



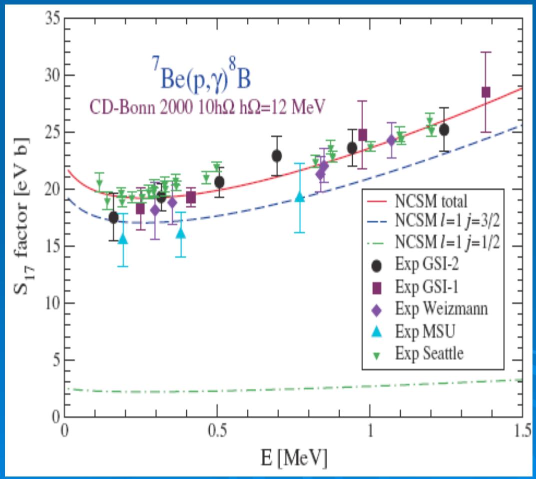
n-α scattering



Nollett et al, nucl-th/0612035



NCSM clusters

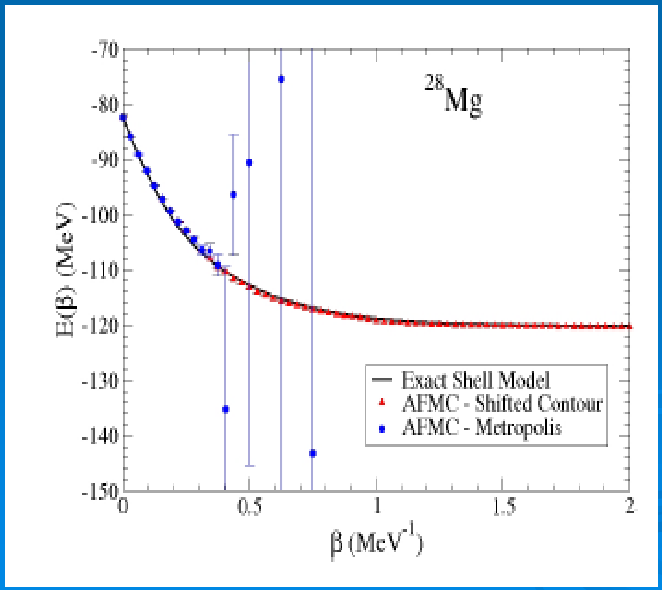


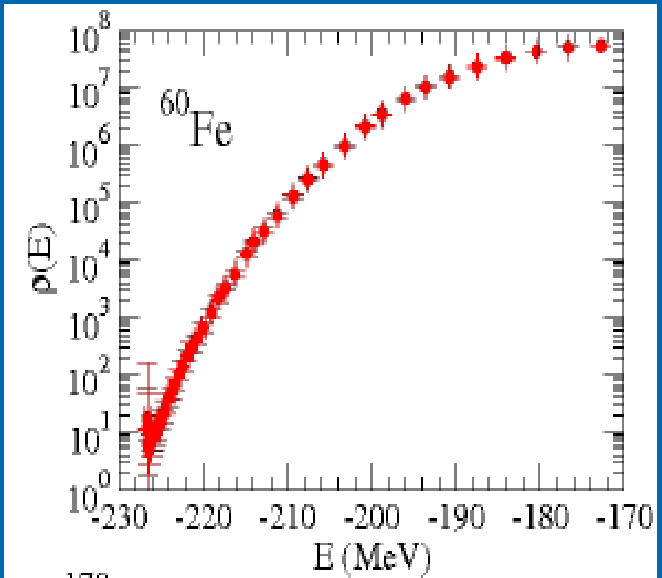
Navratil et al., PRC73, 065801 (2006)

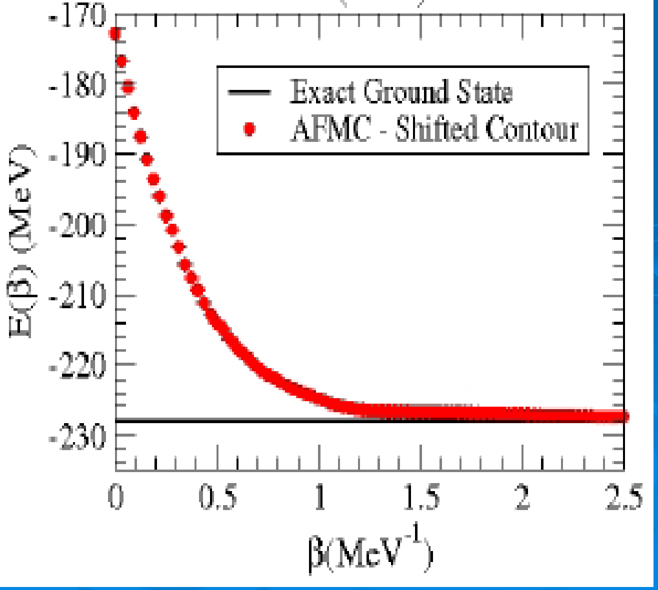
Progress: Level Densities with Auxiliary Field Monte Carlo

- Level densities are the most uncertain input to many reaction models
- AFMC has an MC sign problem
- Shift MC integration to the Hartree minimum of the fields
- Fully realistic shell model interactions
- Even and odd nuclei
- See also work by Alhassid, Langanke,…

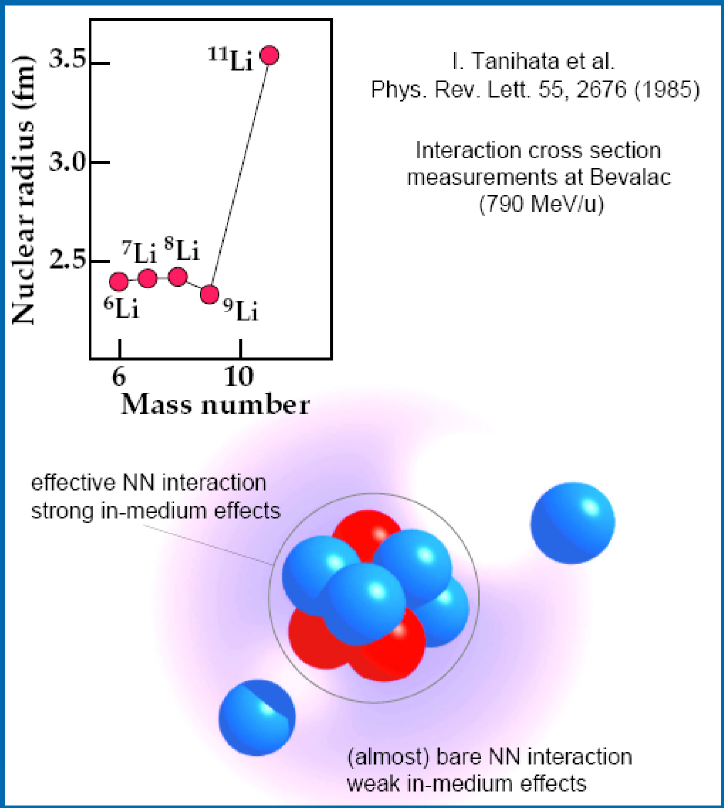
Stoicheva, Ormand, Neuhausser, Dean







Progress: understanding scale separation



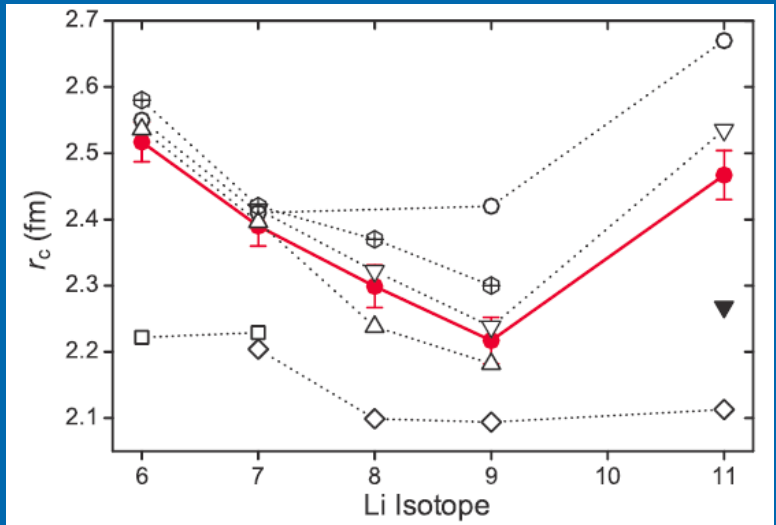
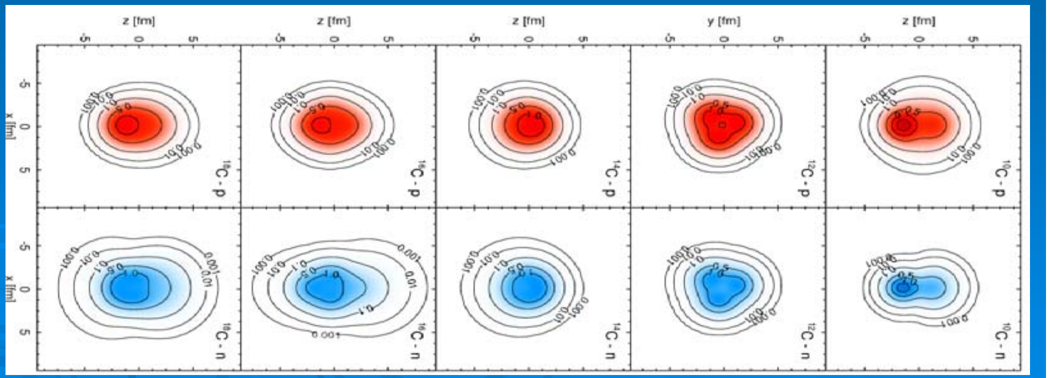


FIG. 2 (color online). Experimental charge radii of lithium isotopes (red, ●) compared with theoretical predictions: △: GFMC calculations [4,22], ▽: SVMC model [27,28] (▼: assuming a frozen ^{9}Li core), ⊕: FMD [26], ○: DCM [19], □ and ◇: *ab initio* NCSM [23,24].

R. Sanchez et al, PRL. 96 (2006) 33002.

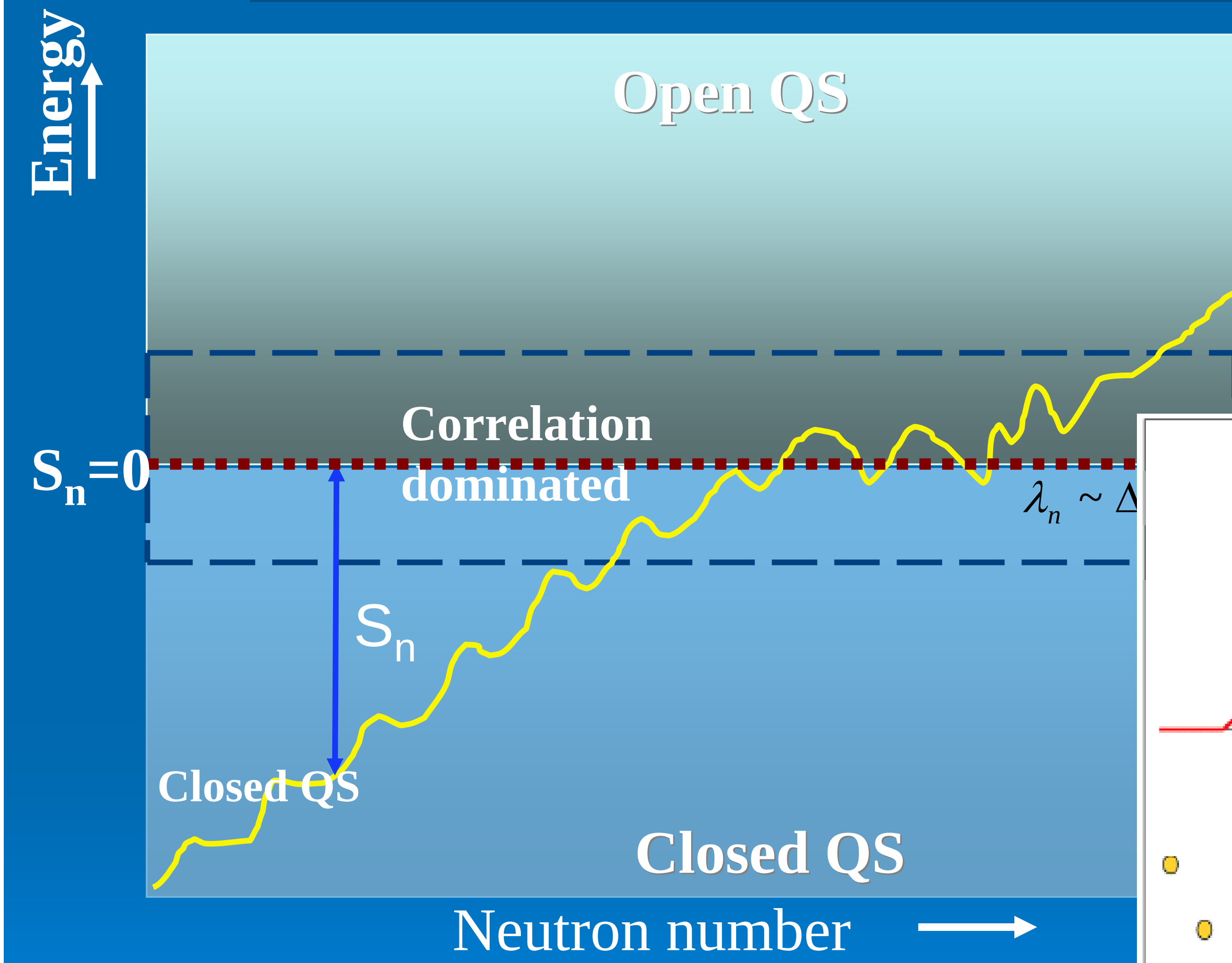
Decoupling of proton and neutron deformation in FMD calculations (Feldmeier et al)



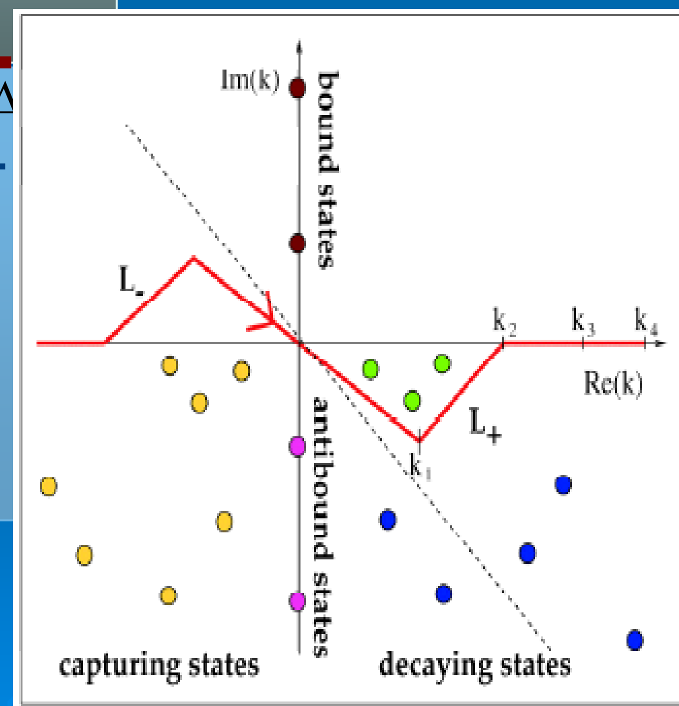
^{18}C ^{16}C ^{14}C ^{12}C ^{10}C

Challenge: the continuum

Progress: Coupling of nuclear structure and reaction theory (microscopic treatment of open channels)

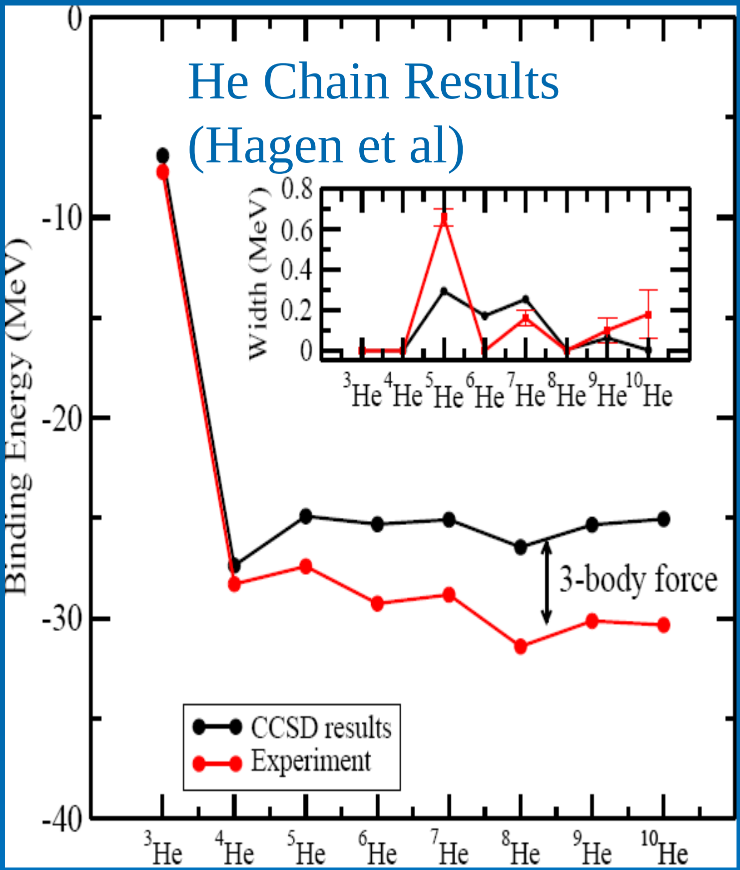


Important interdisciplinary aspects…(see recent ECT* workshop on subject)



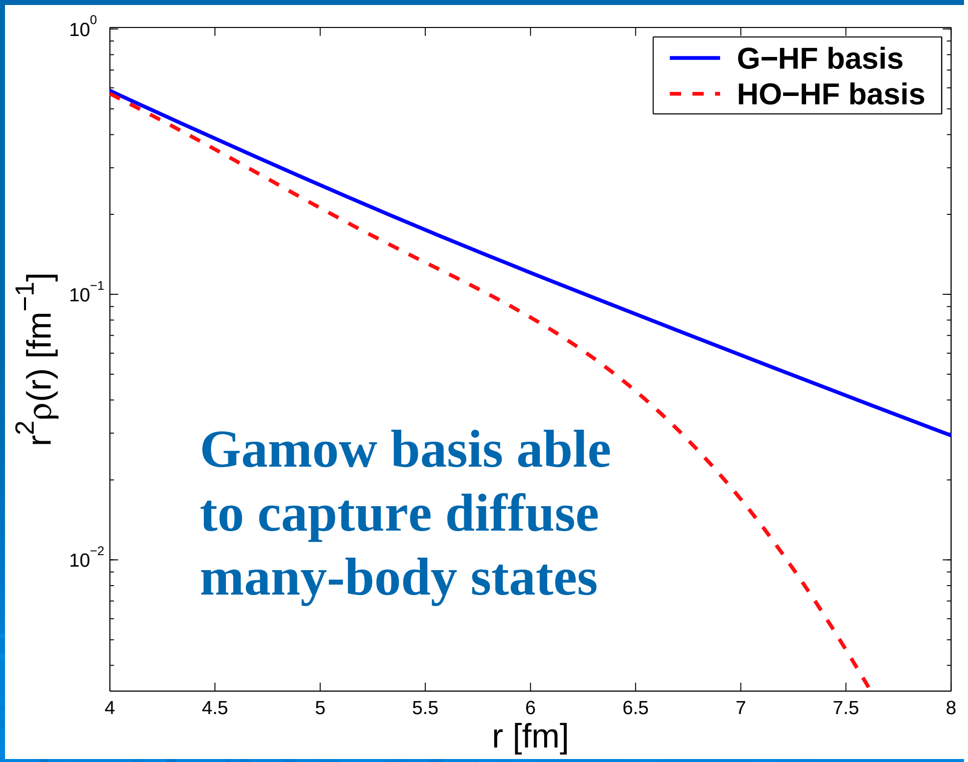
Introduction of
Continuum basis states (Gamow, Berggren)
→Continuum shell models
(many including: Michel, Rotureau, Volya, Ploszajczak, Liotta, Nazarewicz,…)

Progress: ab initio weakly bound and unbound nuclei



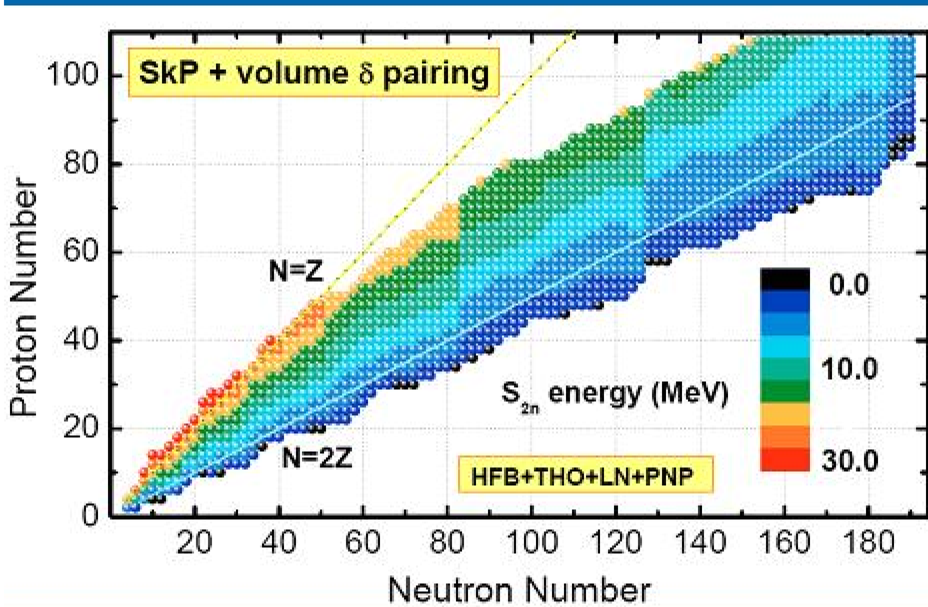
N^{3}LO V_{lowk} (λ=1.9 fm^{-1})

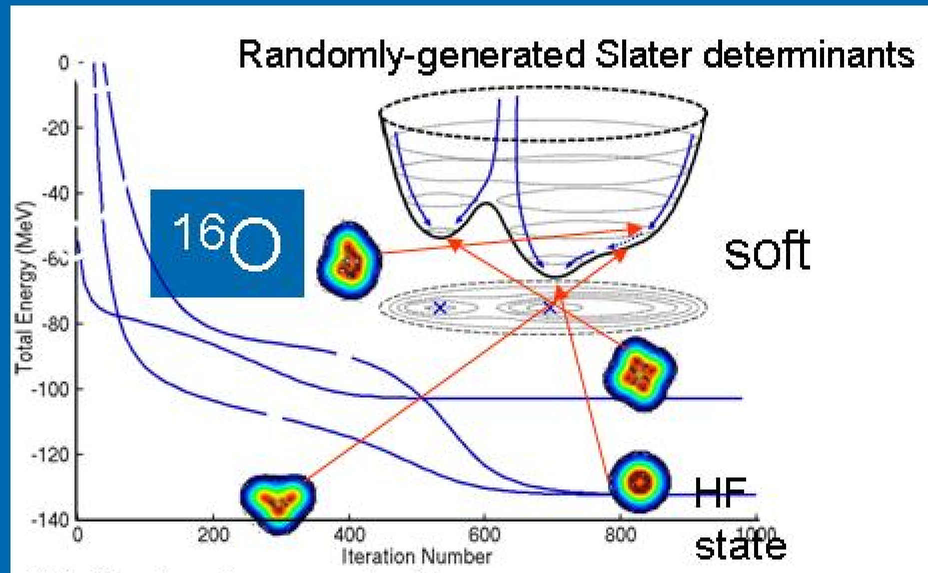
Single-particle basis includes bound, resonant, non-resonant continuum, and scattering states ENORMOUS SPACES….almost 1k orbitals. 10^{22} many-body basis states in ^{10}He



Challenge: include 3-body force

DFT: toward a universal energy density functional and beyond



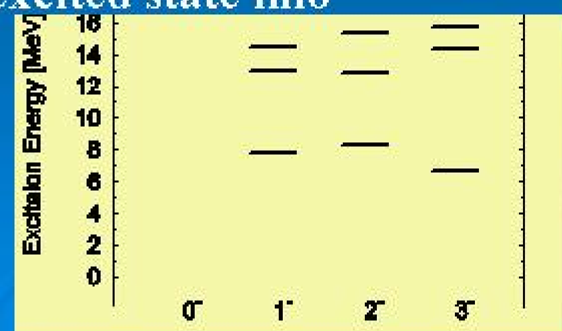


Nakatsukasa et al

Deformed Mass Table

- HFB mass formula: Δm~2MeV
- Good agreement for mass differences
- What about odd-A nuclei?
- Application of new forces to reactions

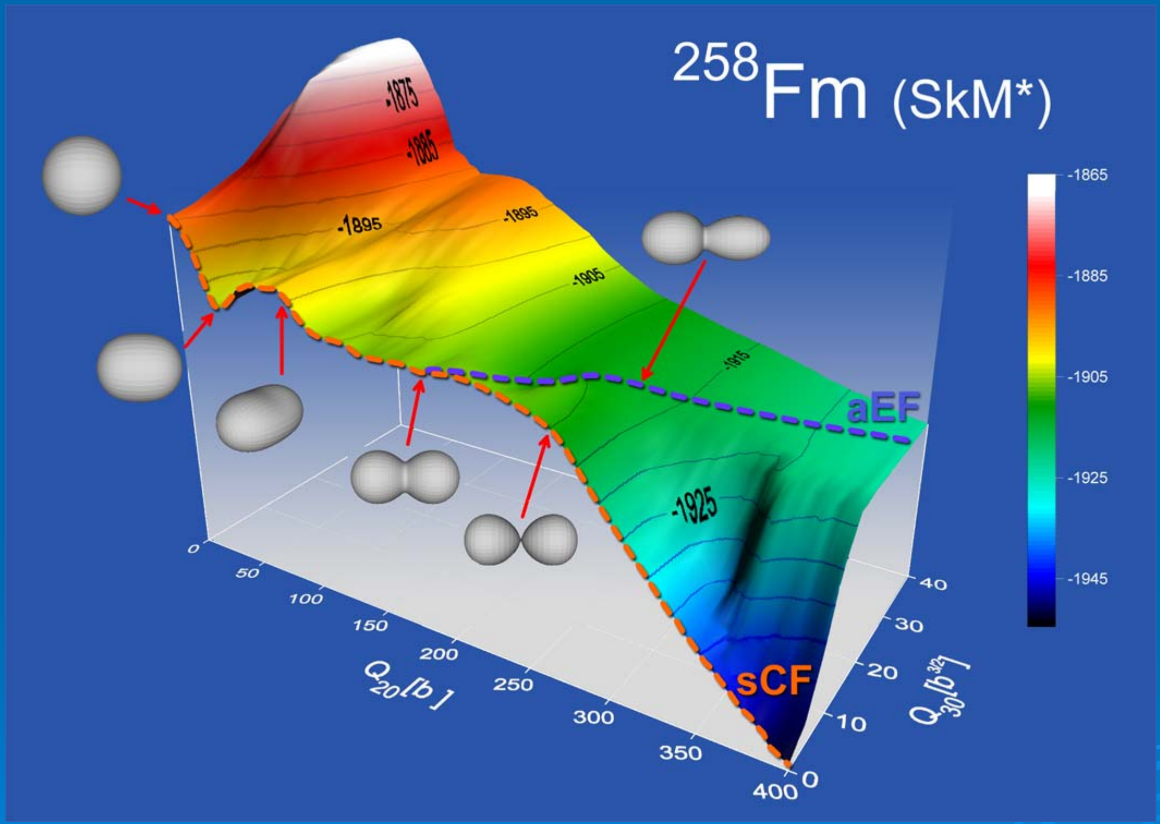
- Generate multiple Slater determinants
- Project
- Diagonalize norm matrix
- obtain excited state info



Compares nicely with expt.

Challenges:
- **Connection to QCD via EFT?**
- **300 keV accuracy with one density functional?**
- **Justify excited state DFT**

Can we utilize DFT functionals to improve a descriptions of fission?



From Andrzej Staszczak

Meeting the challenges

- Workforce issues:
  - Next generation expertise…
  - Training (NNSA Academic Alliance program)
- Increased base funding profile (???)
  - Articulate why we need more
  - Is timing an issue? (time critical)
  - What are the key problems?
- Initiatives (!)
  - America Competes Act
  - AFC/GNEP…
- Leveraging (!!)
  - Computing is a big deal
  - DOE/SC/NNSA SciDAC
  - NSF Computational program
- U.S. based FRIB would enhance all low-energy efforts

ASCR/NP/NNSA UNEDF

Universal Nuclear Energy Density Functional

Conclusions and perspectives

- The quantum many-body problem is everywhere; its solution is one of the great intellectual challenges of our day (major international efforts)
- Only touched on a few themes here
- Moving toward systematic theory with quantifiable error bars
  - PREDICTIVE theoretical capability in nuclei
    still requires further data on neutron rich nuclei
- Exciting physics in the neutron rich regime
  - Continuum physics (halos & skins, resonances)
  - Changes in shell structure
  - Astrophysical connections (e-capture, r-process…)
  - Simple patterns in complex nuclei
- Major benefit from computational sciences!!

- New data will help define Nuclear Energy Density Functional
- Various applications including reaction theory on heavy nuclei

- International collaborations essential