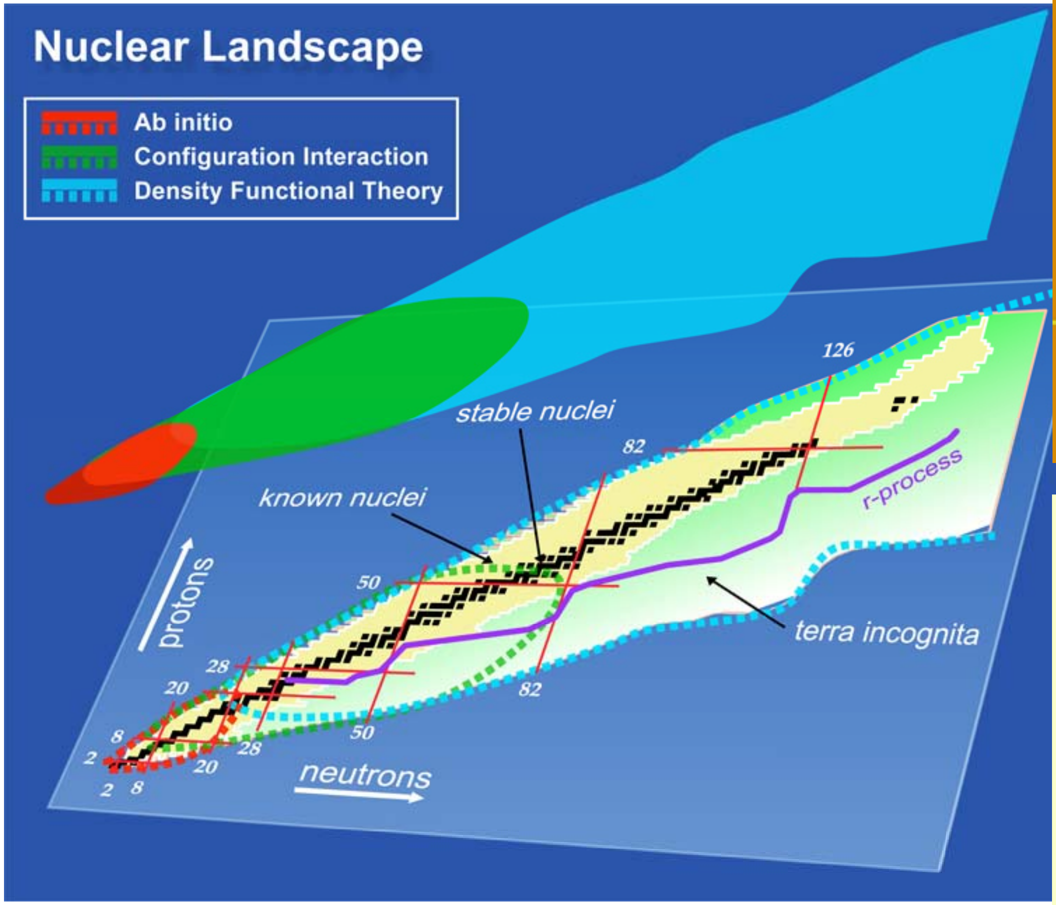
Computing Atomic Nuclei

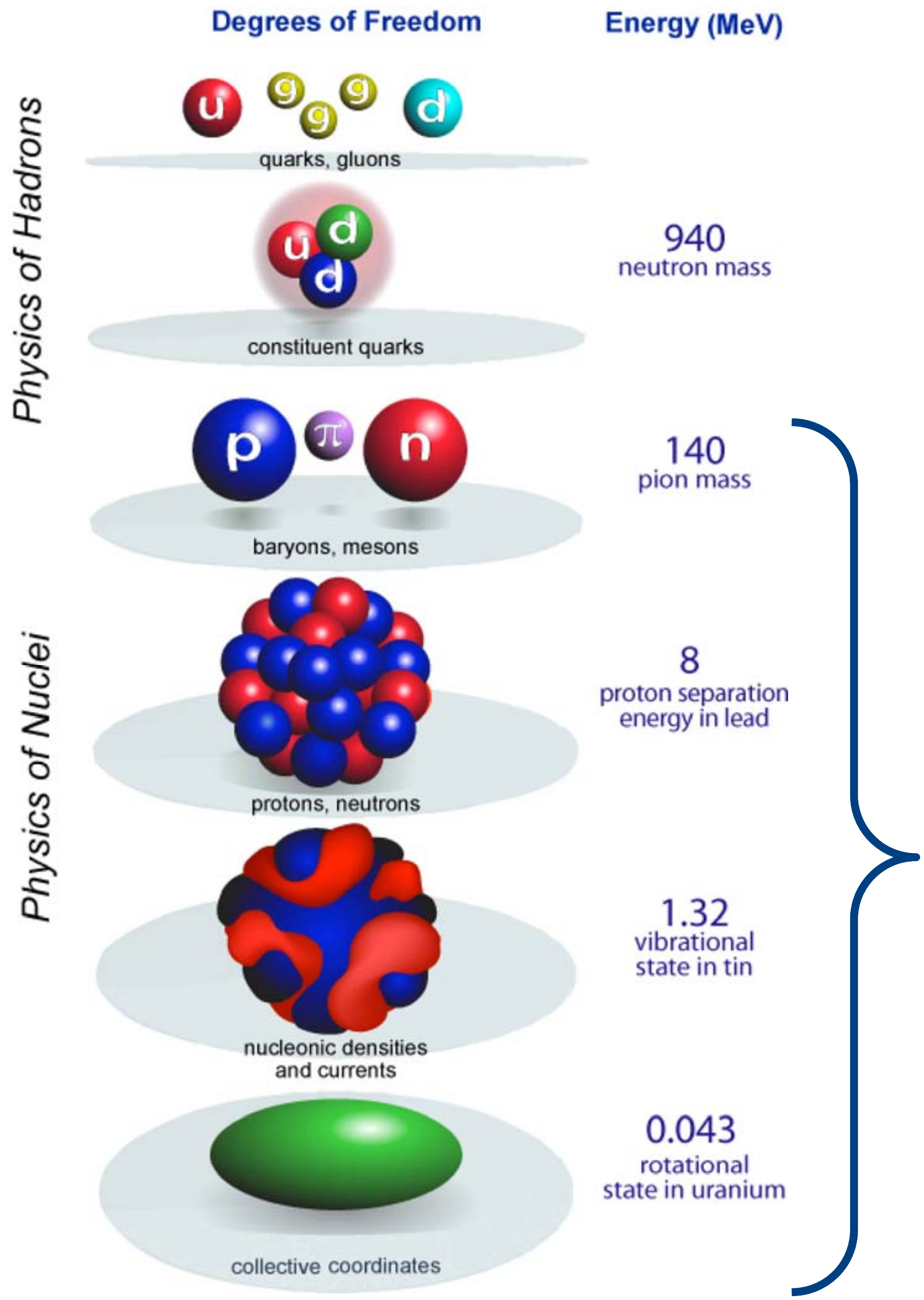
Witold Nazarewicz (UTK/ORNL)

National Nuclear Physics Summer School, June 29, 2009



- Introduction
    - Territory, Principles
- Progress report
- Computing
    - UNEDF
- Perspectives

Introduction



Nuclear Structure

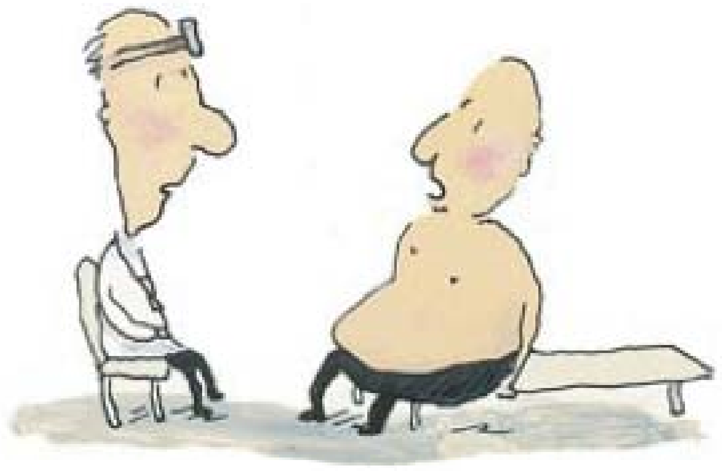
Weinberg's Laws of Progress in Theoretical Physics

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*)

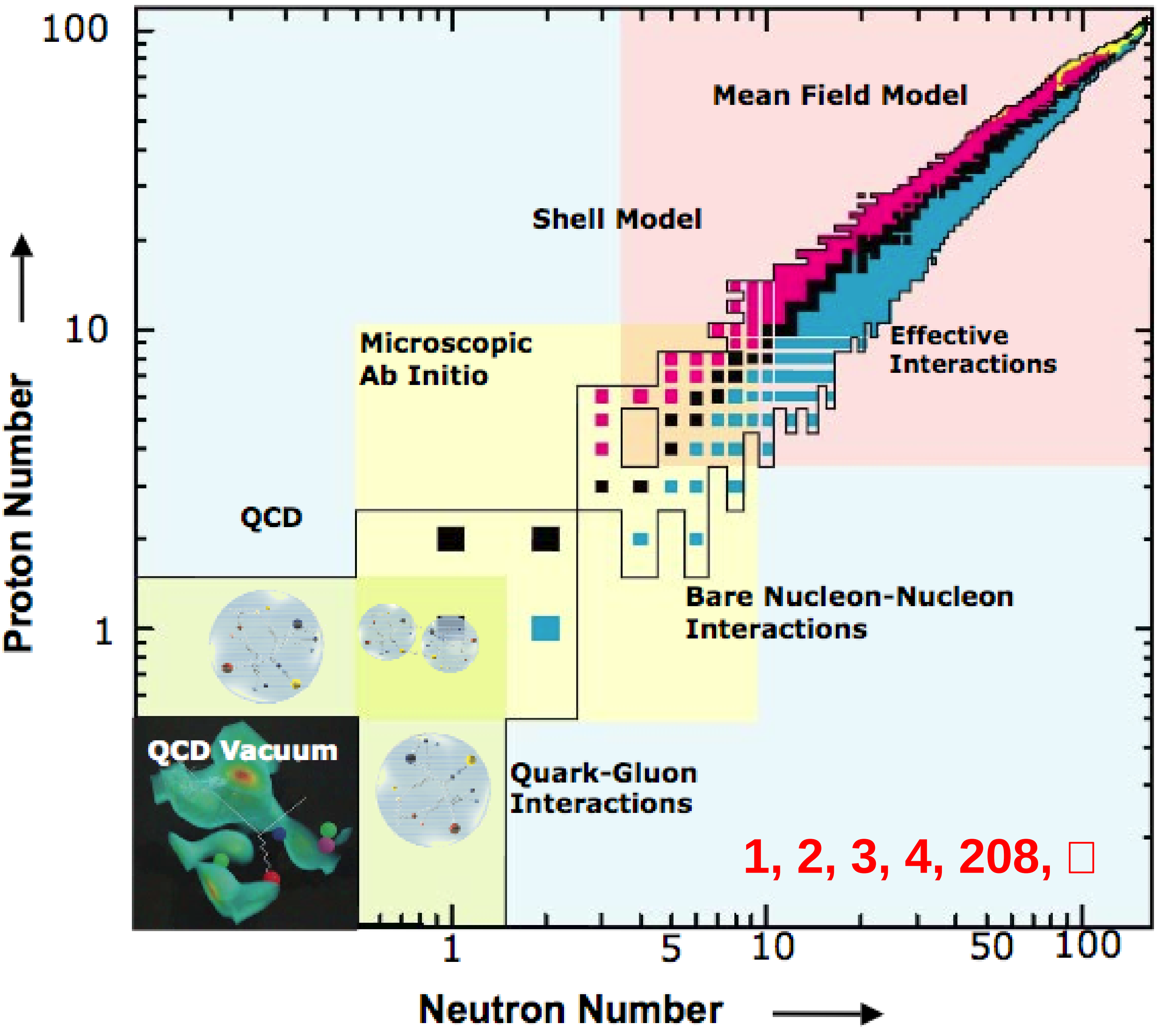
Second Law: "Do not trust arguments based on the lowest order of perturbation theory"

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.

Nuclear Structure Theory
Progress Report


100
10
1
Proton Number
Mean Field Model
Shell Model
Effective
Interactions
Microscopic
Ab Initio
QCD
Bare Nucleon-Nucleon
Interactions
QCD Vacuum
Quark-Gluon
Interactions
1
5
10
50
100
Neutron Number

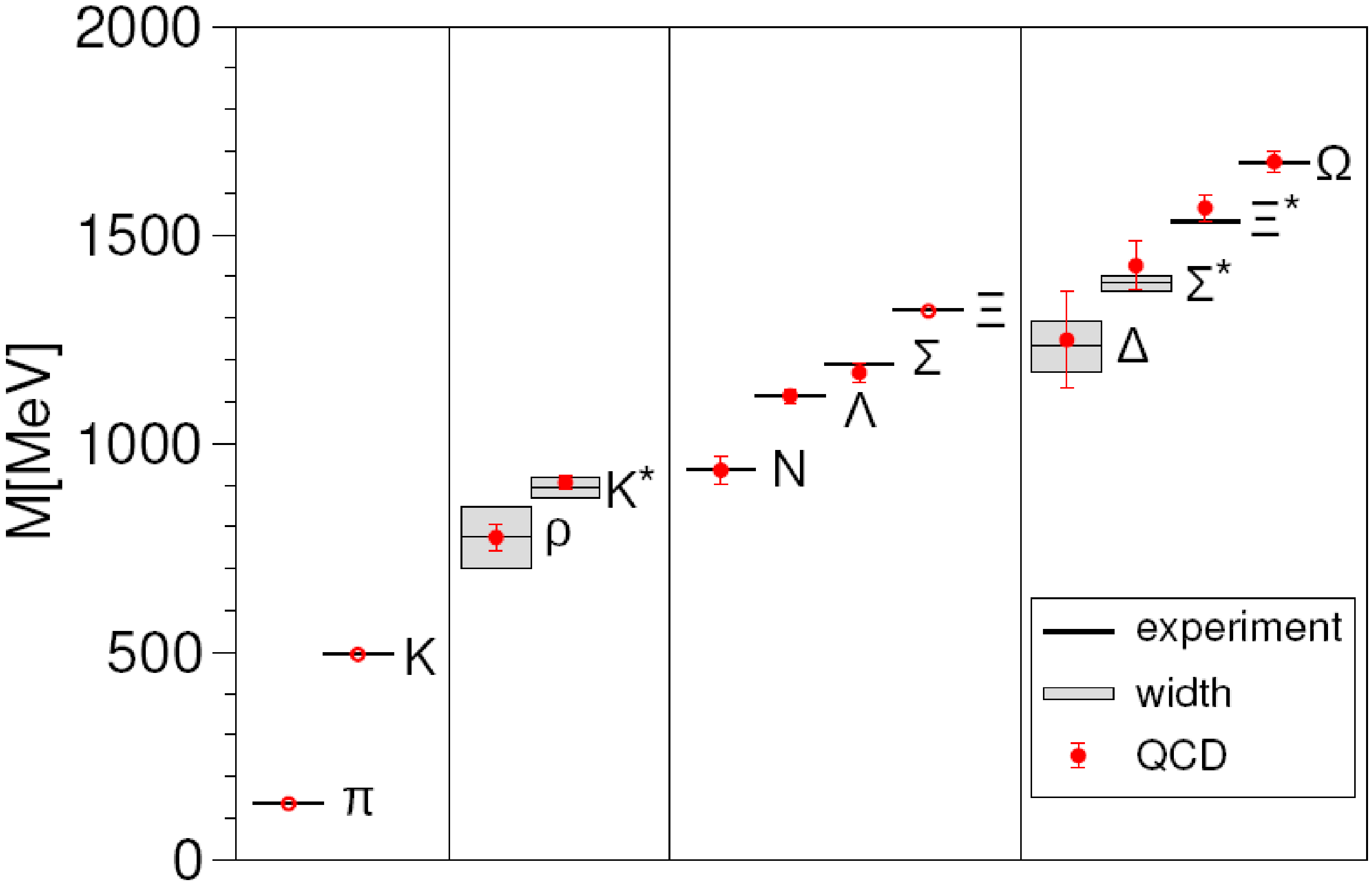
1, 2, 3, 4, 208, □

Low-lying Hadron Spectrum

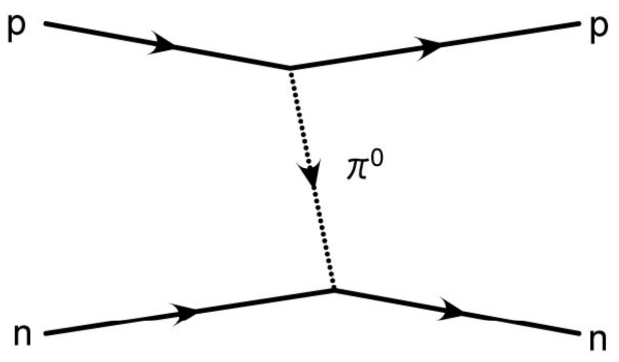
Dürr, Fodor, Lippert et al., BMW Collaboration

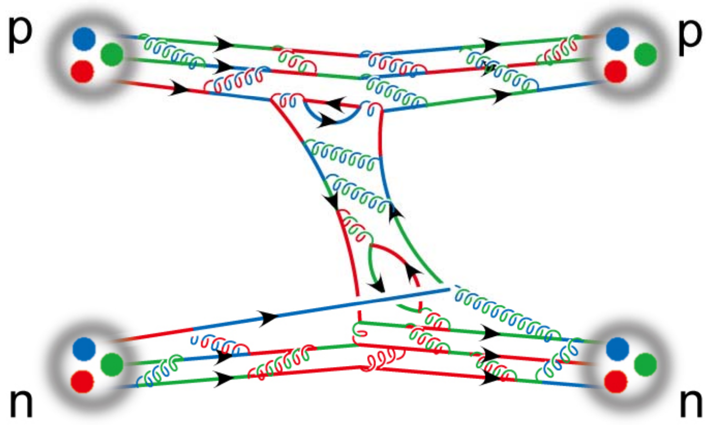
Science 322, 1224 November 2008

More than 99% of the mass of the visible universe is made up of protons and neutrons. Both particles are much heavier than their quark and gluon constituents, and the Standard Model of particle physics should explain this difference. We present a full ab initio calculation of the masses of protons, neutrons, and other light hadrons, using lattice quantum chromodynamics. Pion masses down to 190 mega–electron volts are used to extrapolate to the physical point, with lattice sizes of approximately four times the inverse pion mass. Three lattice spacings are used for a continuum extrapolation. Our results completely agree with experimental observations and represent a quantitative confirmation of this aspect of the Standard Model with fully controlled uncertainties

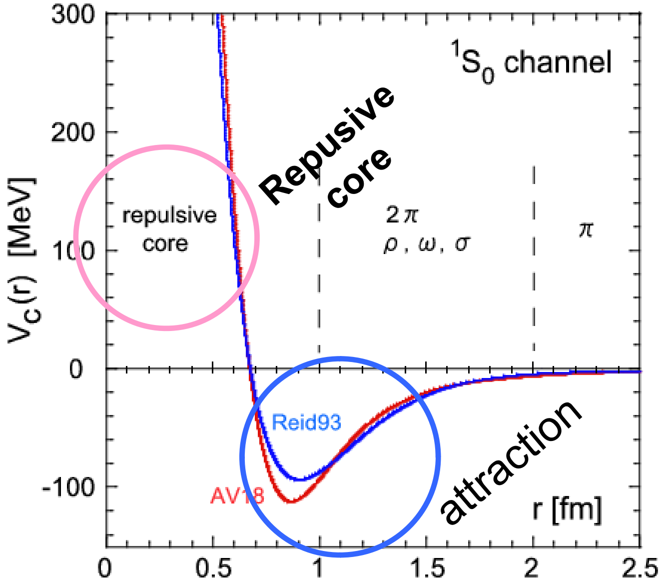


Lattice QCD calculation of nuclear force





Realistic nuclear force

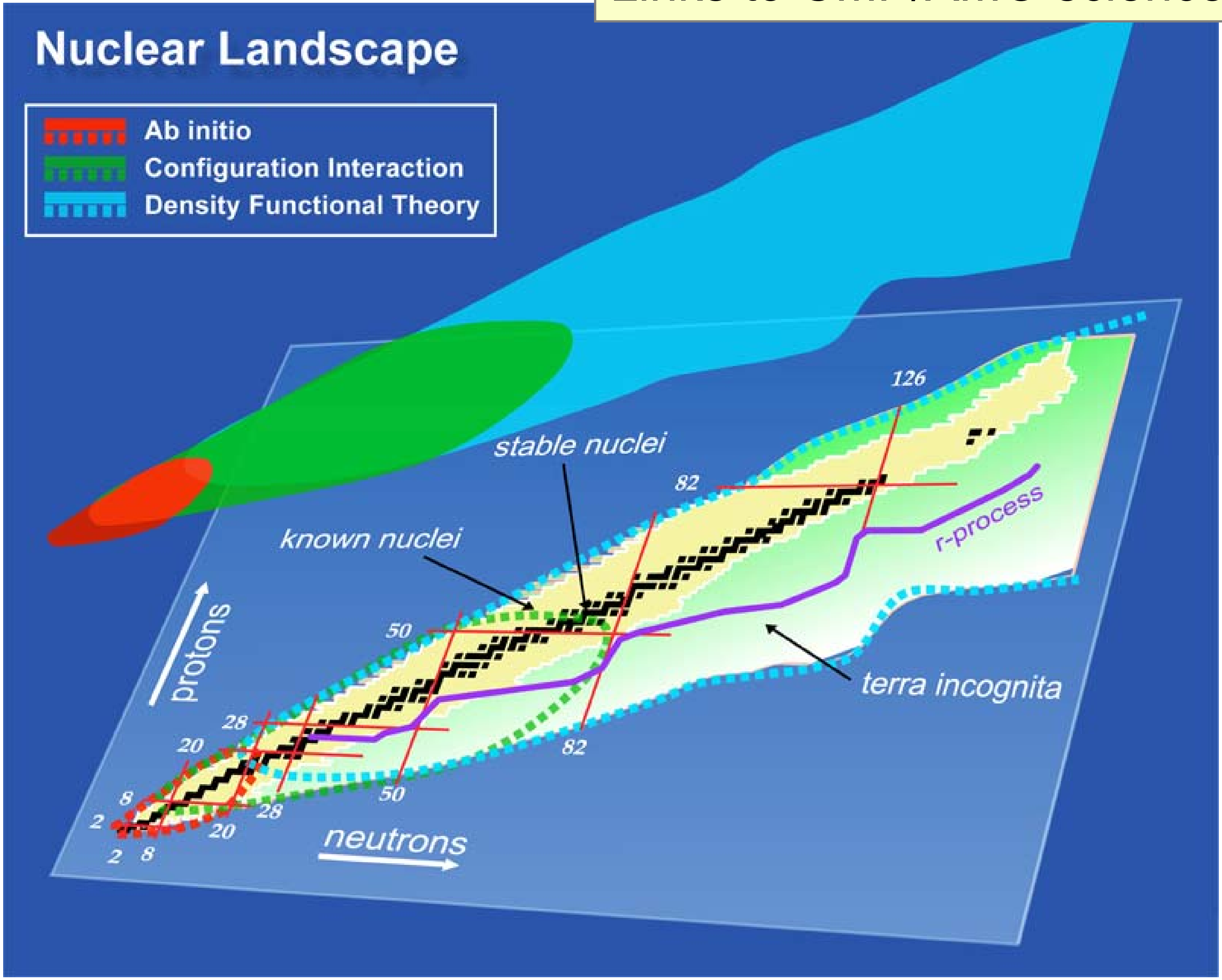


Reid93 is from
V.G.J.Stoks et al., PRC**49**, 2950 (1994).

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

N. Ishii, S. Aoki, T. Hatsuda, Phys. Rev. Lett. **99,** 022001 (2007)
Tensor force from LQCD: http://arxiv.org/pdf/0903.5497

Links to CMP/AMO science!!!

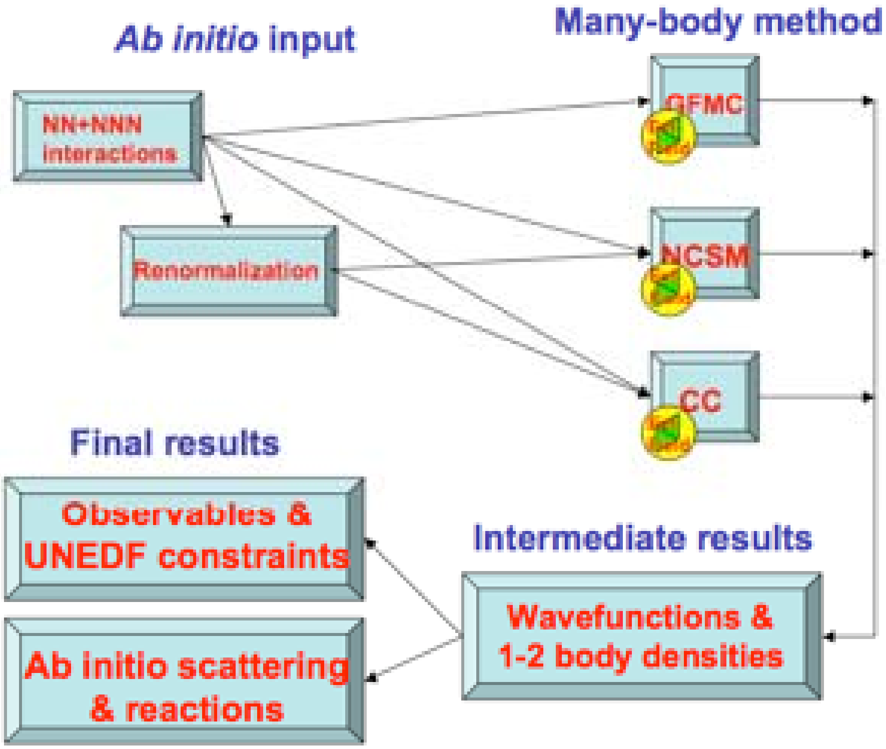


number of nuclei < number of processors!

Ab initio theory for light nuclei and nuclear matter

Ab initio: GFMC, NCSM, CCM

(nuclei, neutron droplets, nuclear matter)



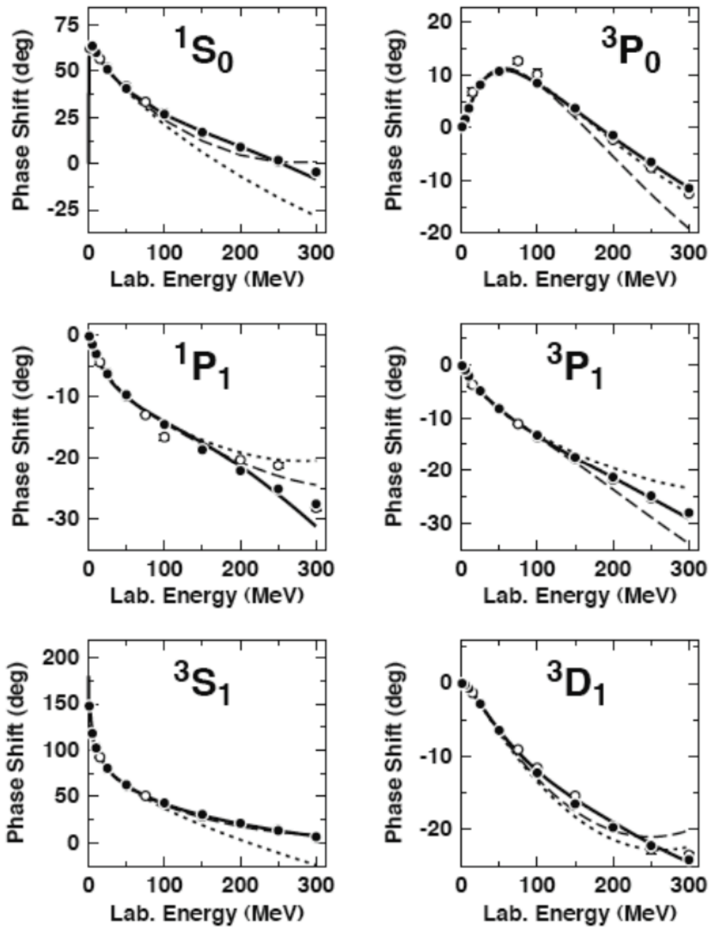
- Quantum Monte Carlo (GFMC) ^{12}C
- No-Core Shell Model ^{14}F
- Coupled-Cluster Techniques ^{56}Ni
- Faddeev-Yakubovsky
- Bloch-Horowitz
- …

Input:

- Excellent forces based on the phase shift analysis
- EFT based nonlocal chiral NN and NNN potentials

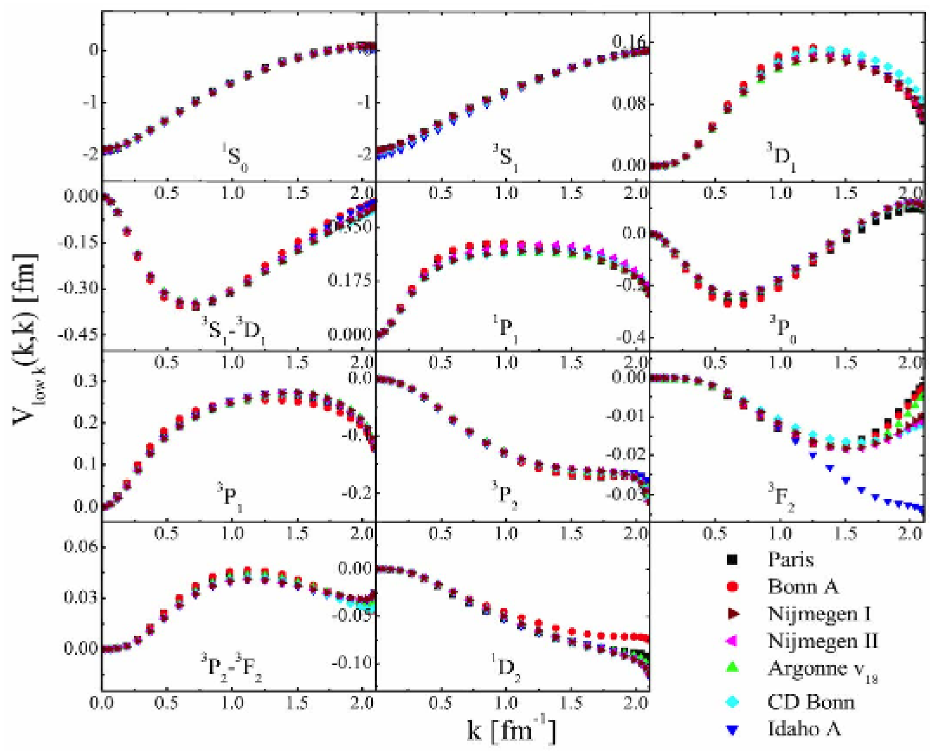
NN and NNN interactions

Effective-field theory (χPT) potentials



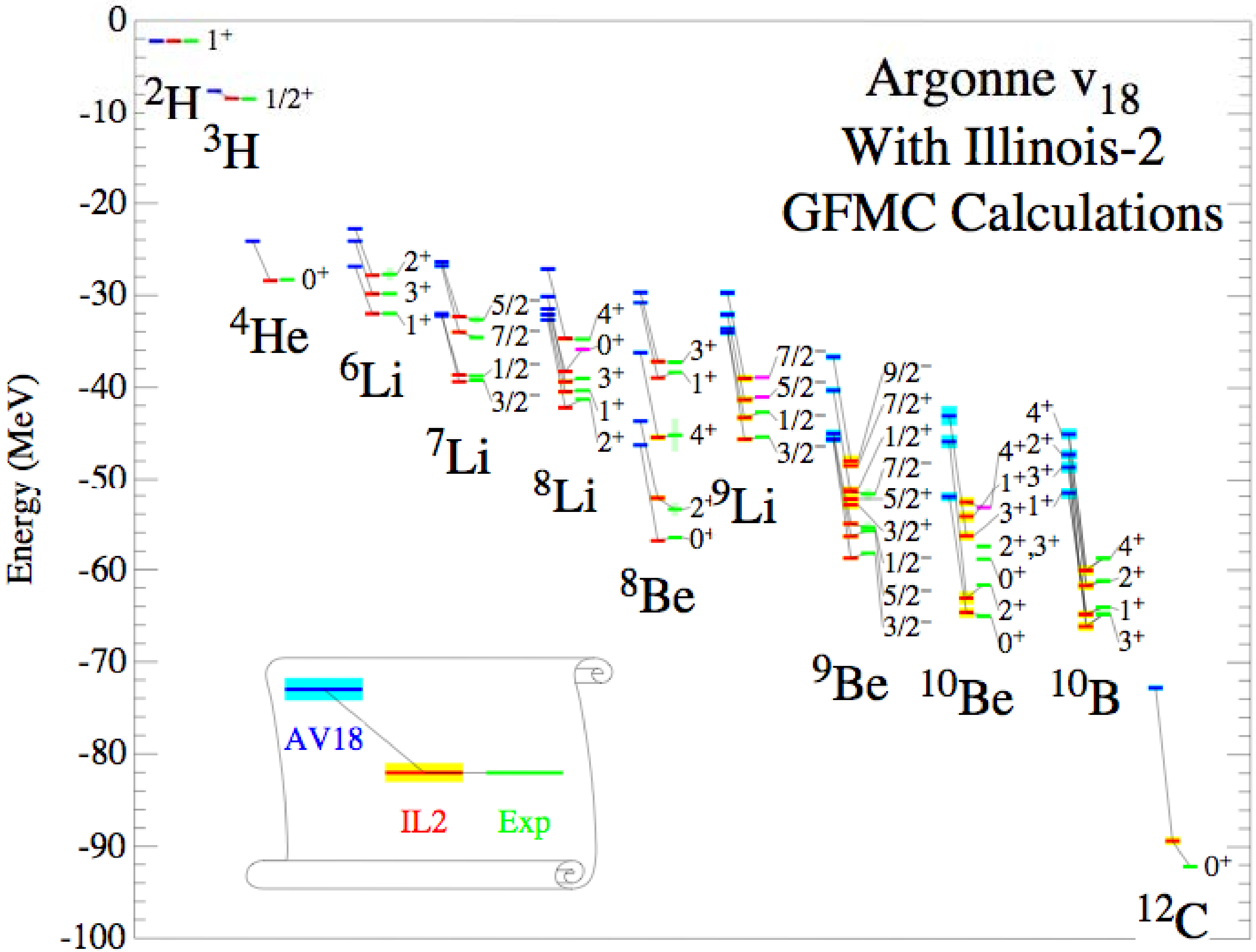
N^{3}LO: Entem et al., PRC68, 041001 (2003)
Epelbaum, Meissner, et al.

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



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

- **Quality two- and three-nucleon interactions exist**
  - **Not uniquely defined (local, nonlocal)**
  - **Soft and hard-core**



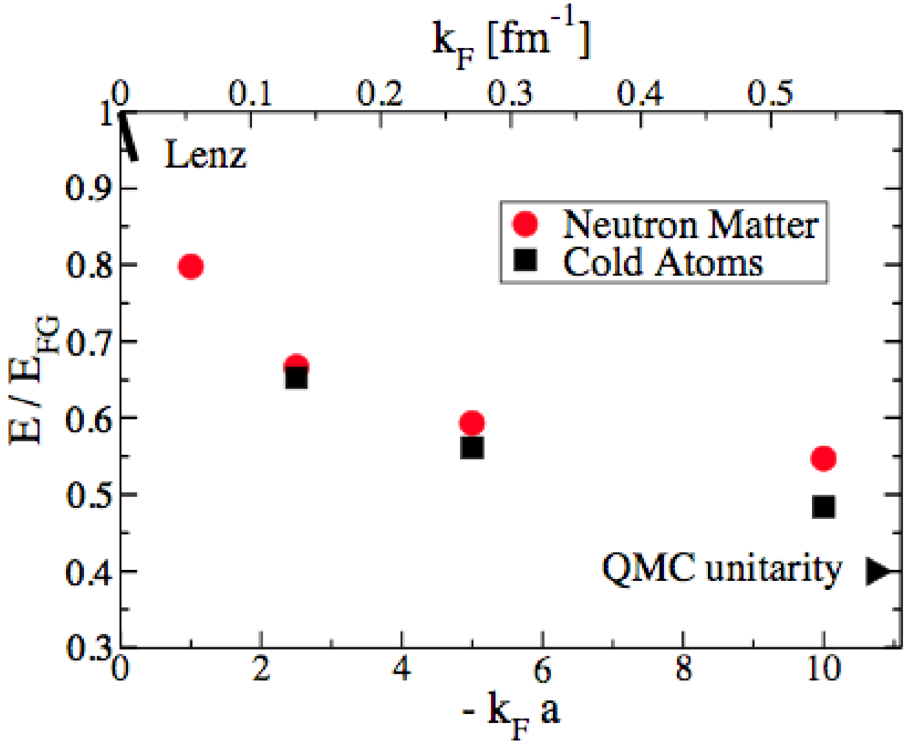
GFMC: S. Pieper, ANL

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

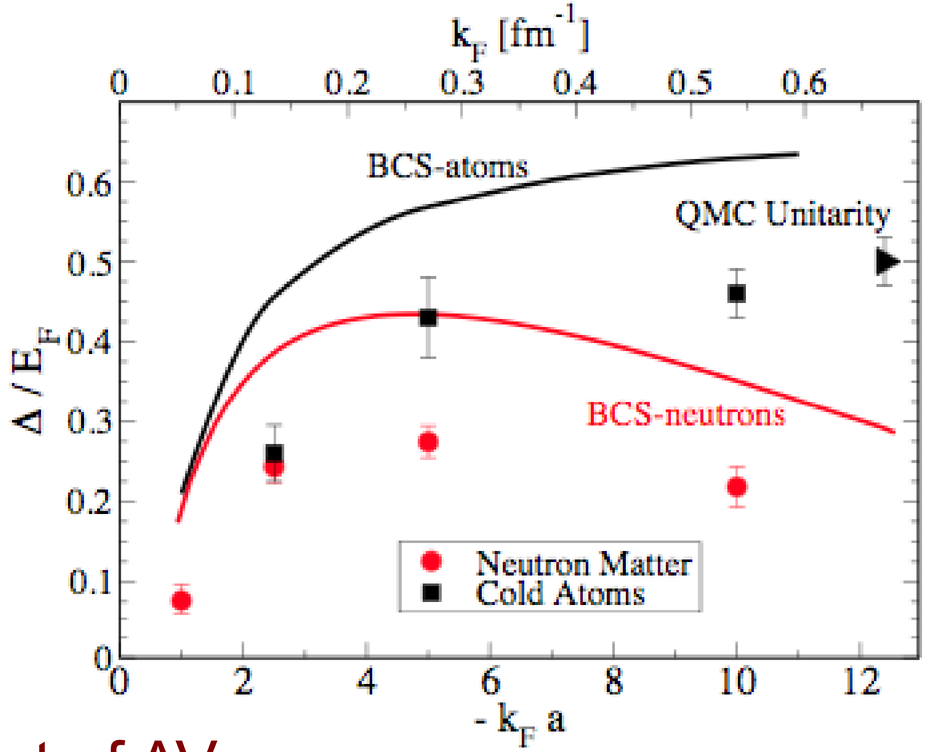
Strongly paired fermions: Cold atoms and neutron matter

a_n=-18.5 fm, r_e=2.7fm

Equation of State at Low Densities



pairing gap



s-wave part of AV_{18}

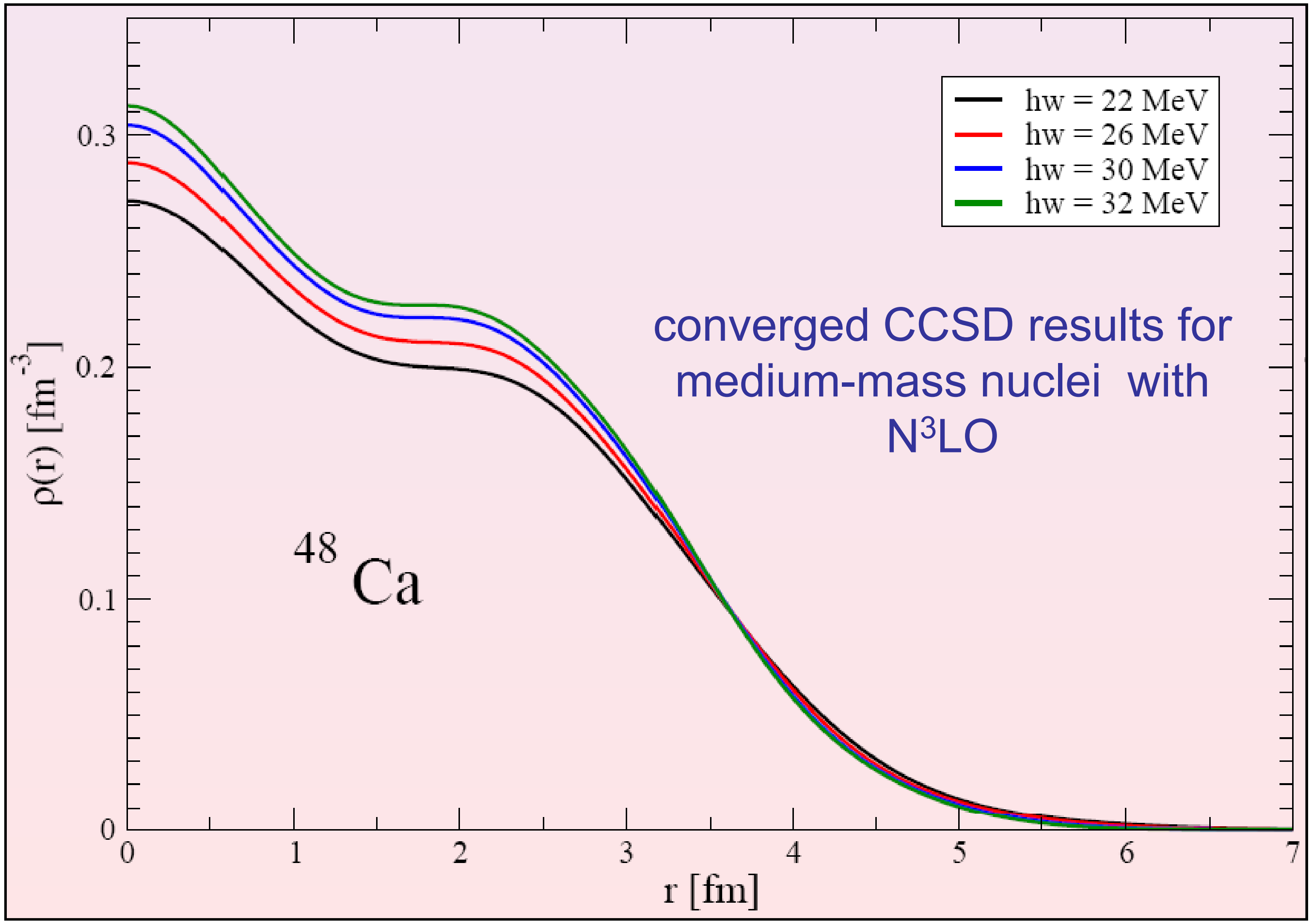
Gezerlis and Carlson, Phys. Rev. C 77, 032801(R) (2008)

Nuclear Coupled Cluster Theory

Size Extensive!

Medium-mass nuclei from chiral nucleon-nucleon interactions

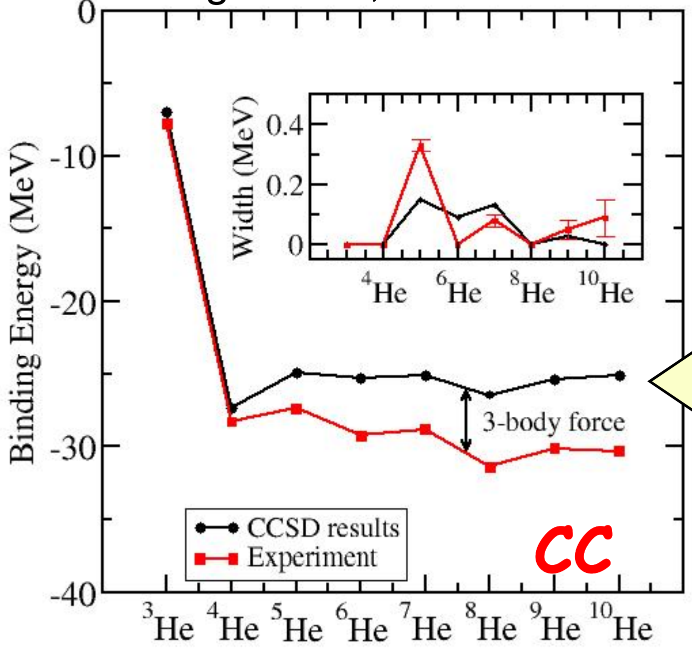
Hagen, Papenbrock, Dean, Hjorth-Jensen, Phys. Rev. Lett. 101, 092502 (2008)



converged CCSD results for medium-mass nuclei with N^3LO

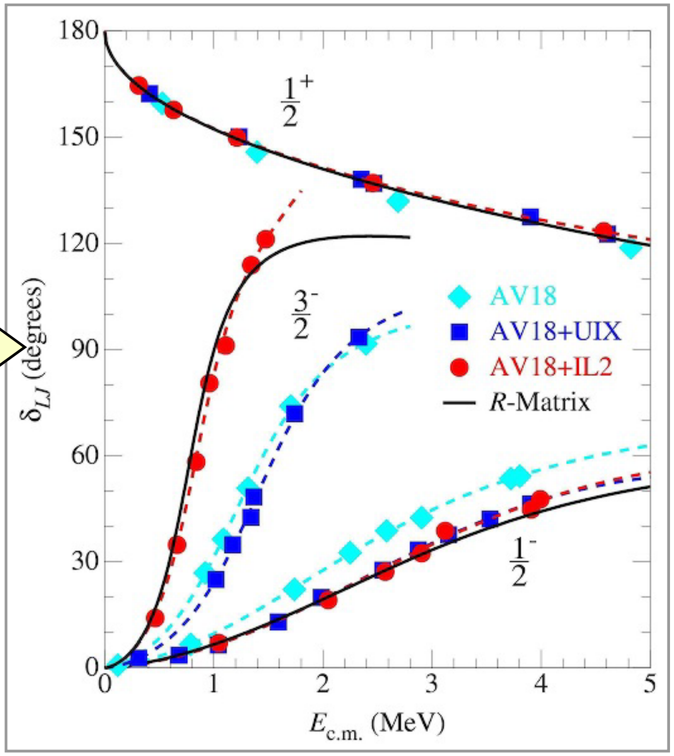
Ab initio: Reactions

Hagen et al, ORNL/UTK



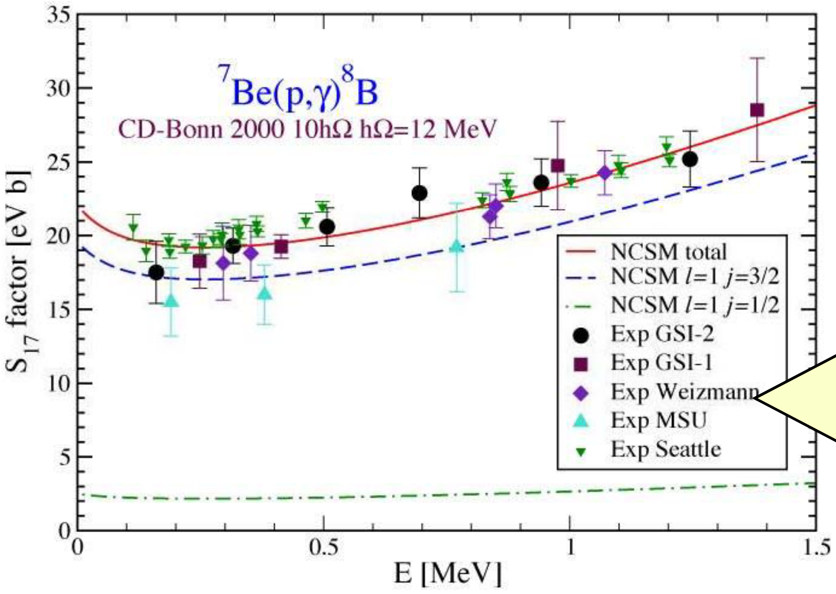
Coupled Clusters

Nollett et al, ANL



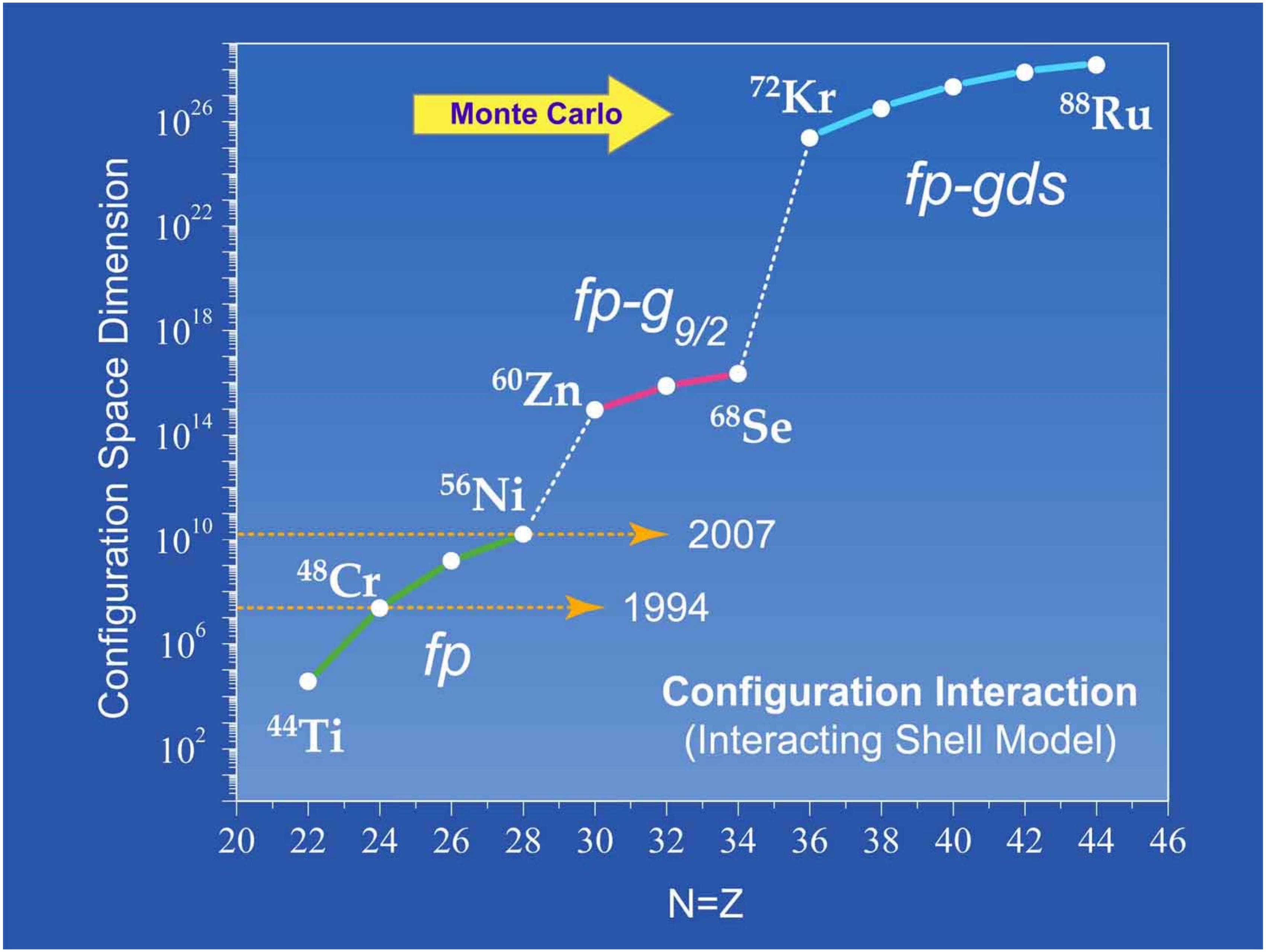
GFMC

Quaglioni & Navratil, LLNL 2008

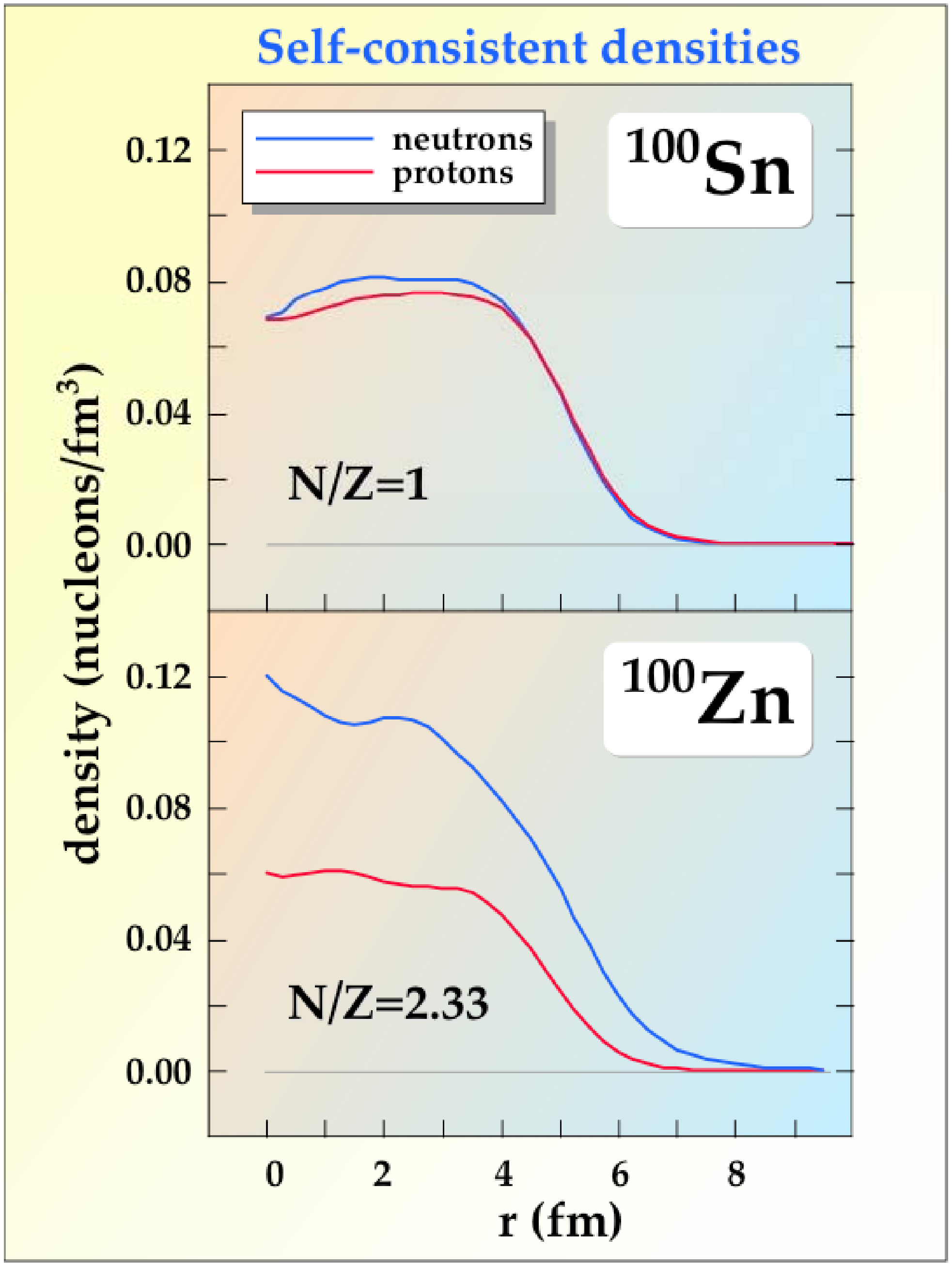


No Core Shell Model
+ Resonating Group
Method

^{11}Be: Phys. Rev. C 79, 044606 (2009)


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)
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

Mean-Field Theory ⇒ Density Functional Theory



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 0 n p

isovector (T=1) density 1 n p

+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)**

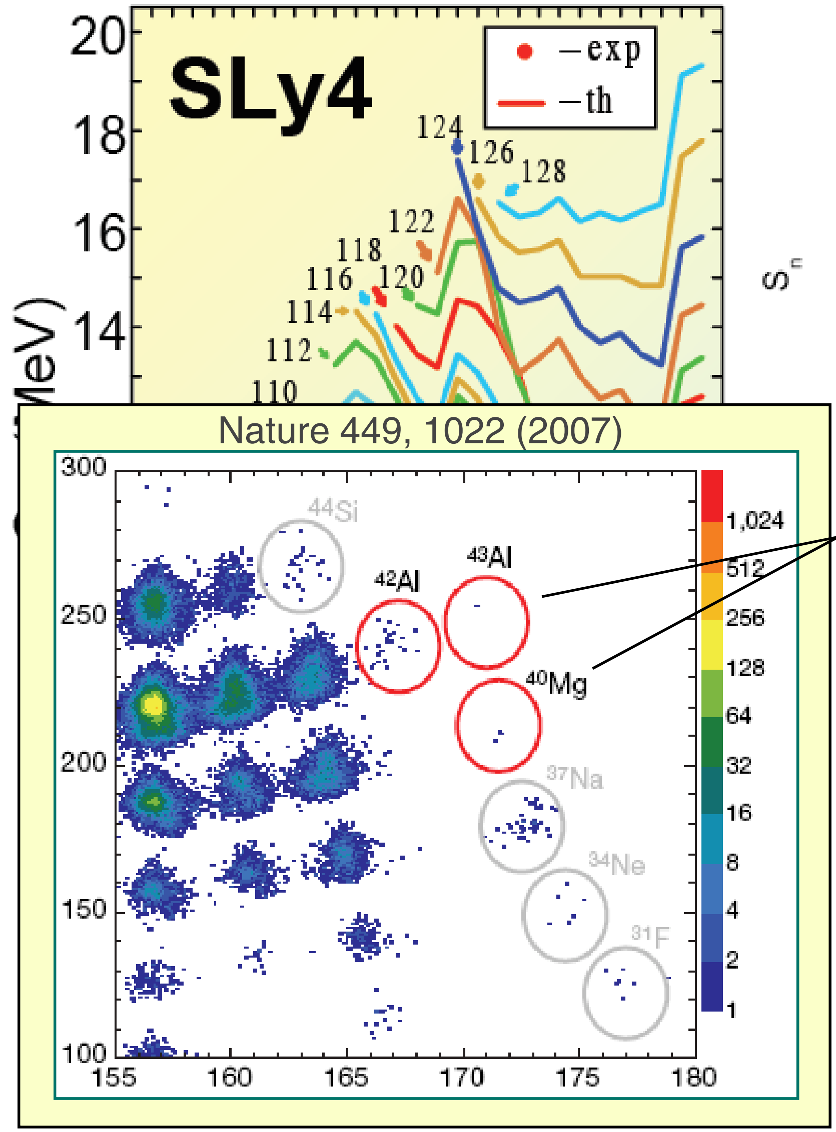
$$\mathcal{H}(r) = \frac{\hbar^2}{2m}\tau_0(r) + \sum_{t=0,1}\left(\chi_t(r) + \breve{\chi}_t(r)\right)$$

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)

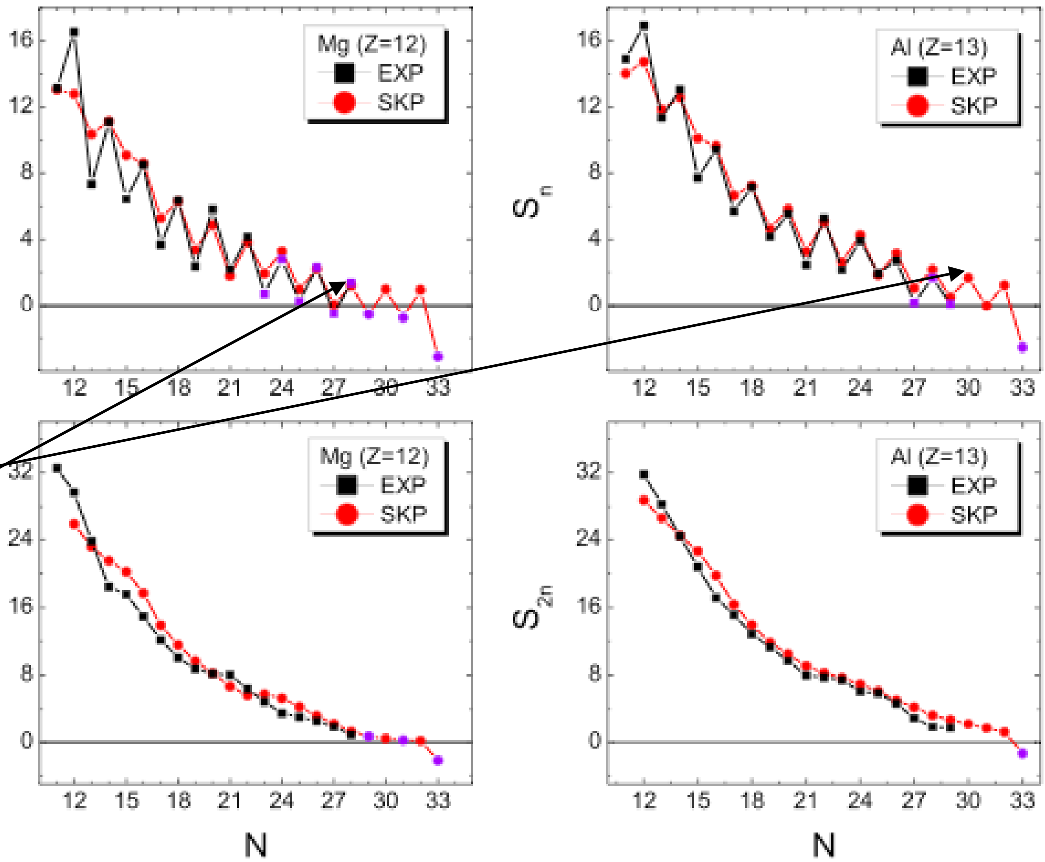
Nuclear DFT: works well for BE differences

S. Cwiok, P.H. Heenen, WN
Nature, 433, 705 (2005)



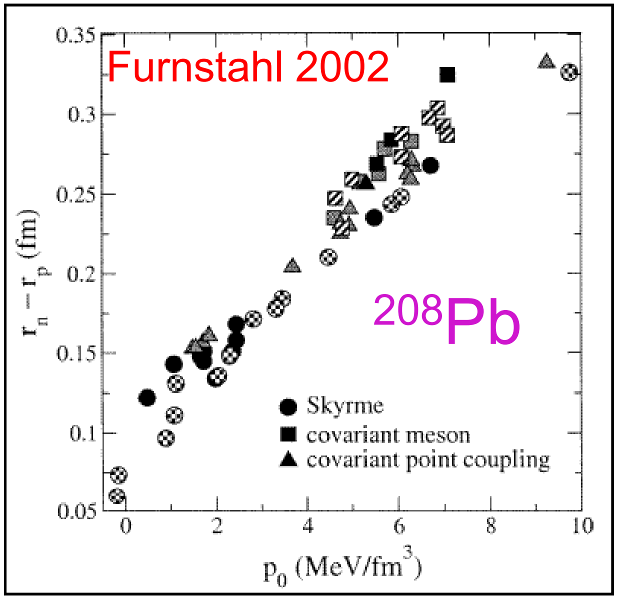
Nature 449, 1022 (2007)

Stoitsov et al., 2008



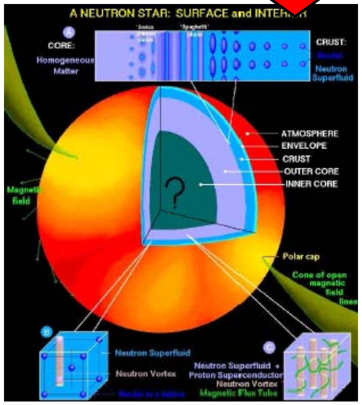
Neutron-rich matter and neutron skins

skin



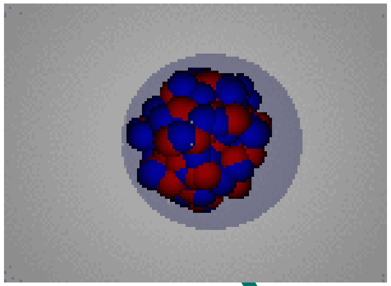
pressure $\dfrac{\partial \varepsilon}{\partial \rho}$

Bulk neutron matter equation of state

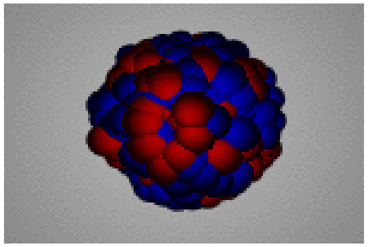


Constraints on the mass-vs-radius relationship of neutron stars

Pygmy dipole

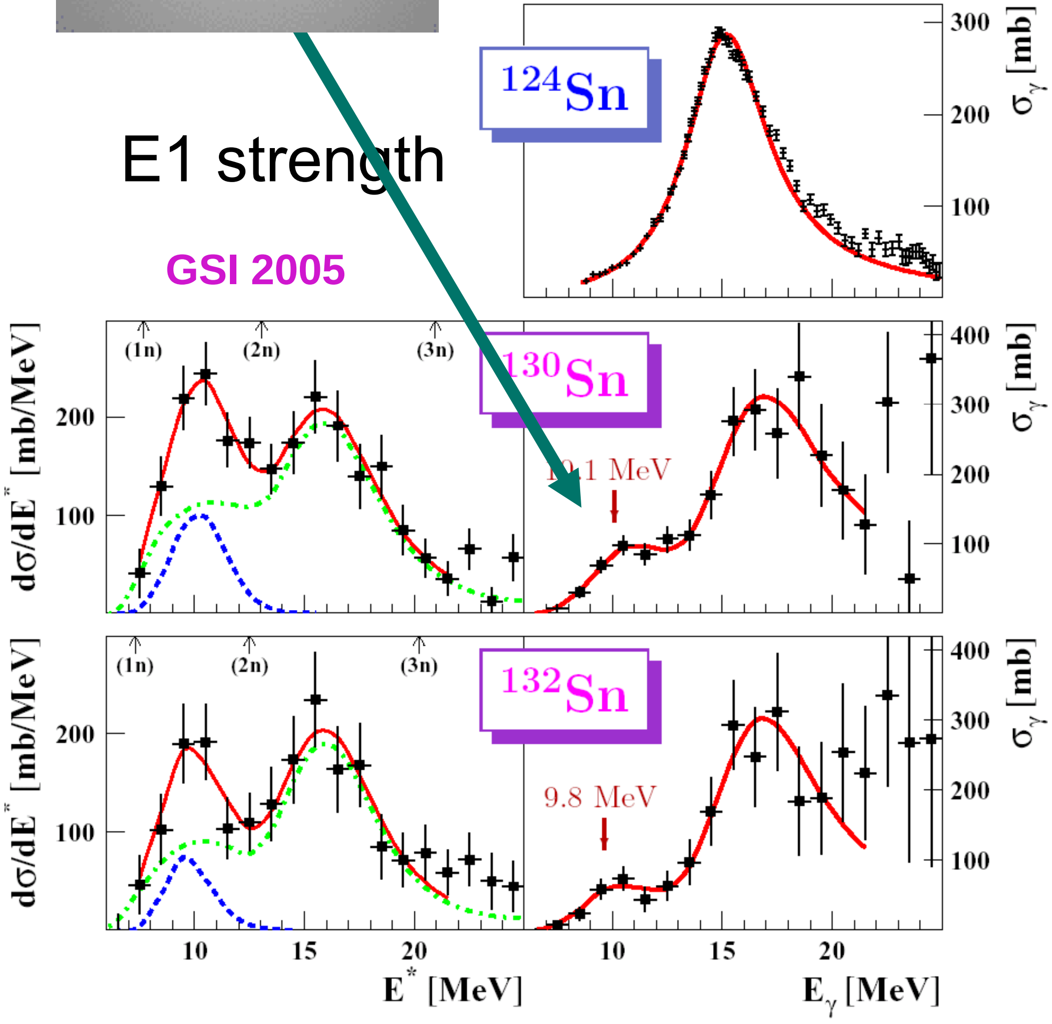


Giant dipole

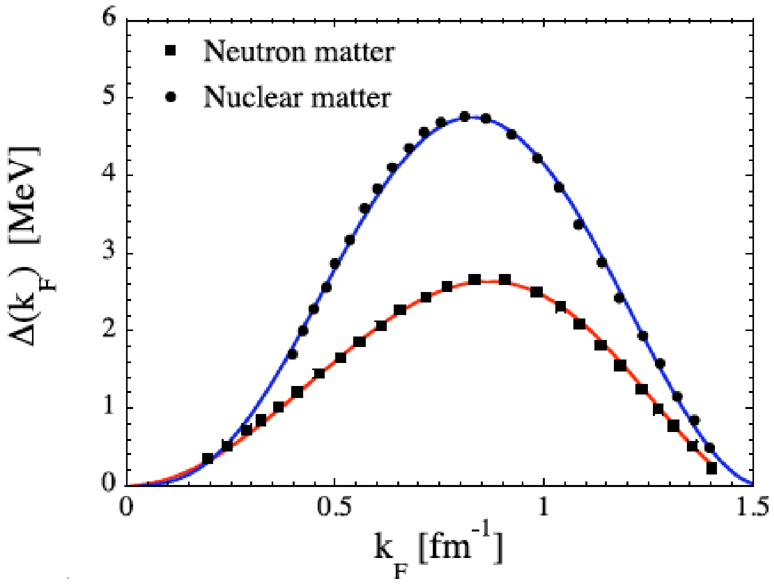


E1 strength

GSI 2005

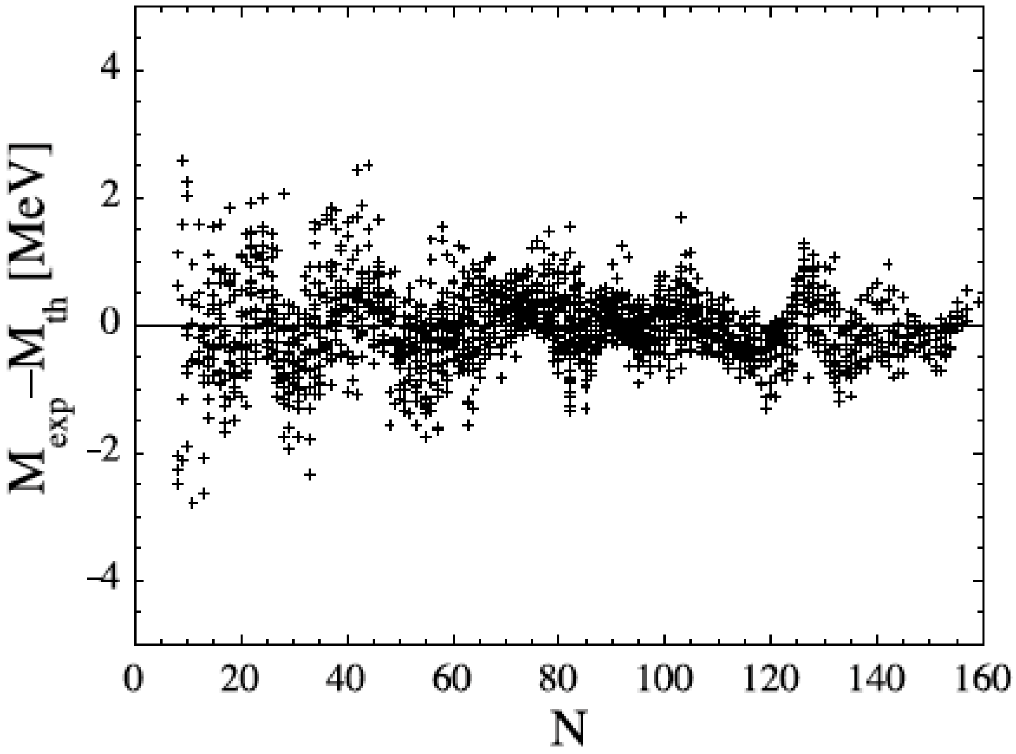


Microscopic mass table

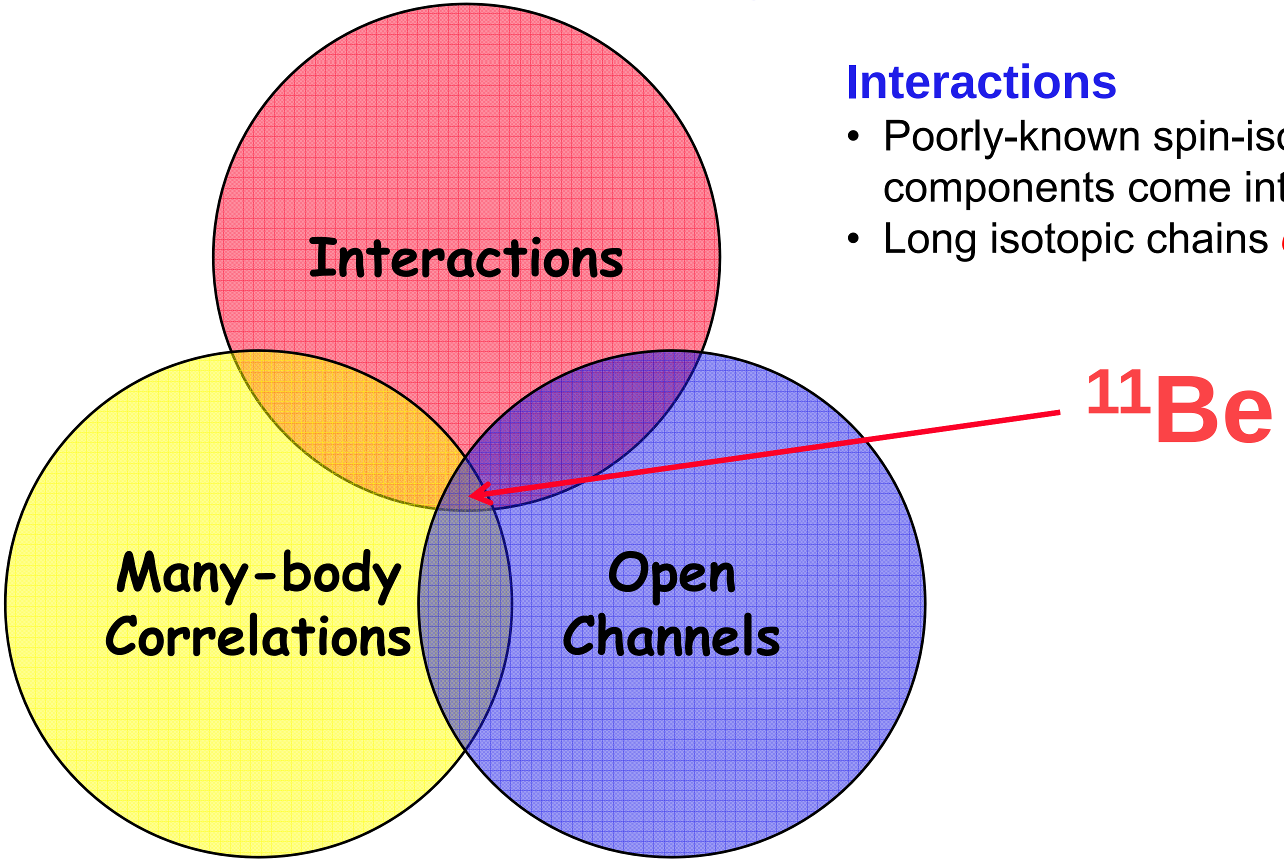


Goriely, Chamel, Pearson: HFB-17
Phys. Rev. Lett. 102, 152503 (2009)

$\delta m = 0.581$ MeV



A remark: physics of neutron-rich nuclei is demanding



Interactions

- Poorly-known spin-isospin components come into play
- Long isotopic chains ***crucial***

Configuration interaction

- Mean-field concept often ***questionable***
- Asymmetry of proton and neutron Fermi surfaces gives rise to new couplings
- New collective modes; polarization effects

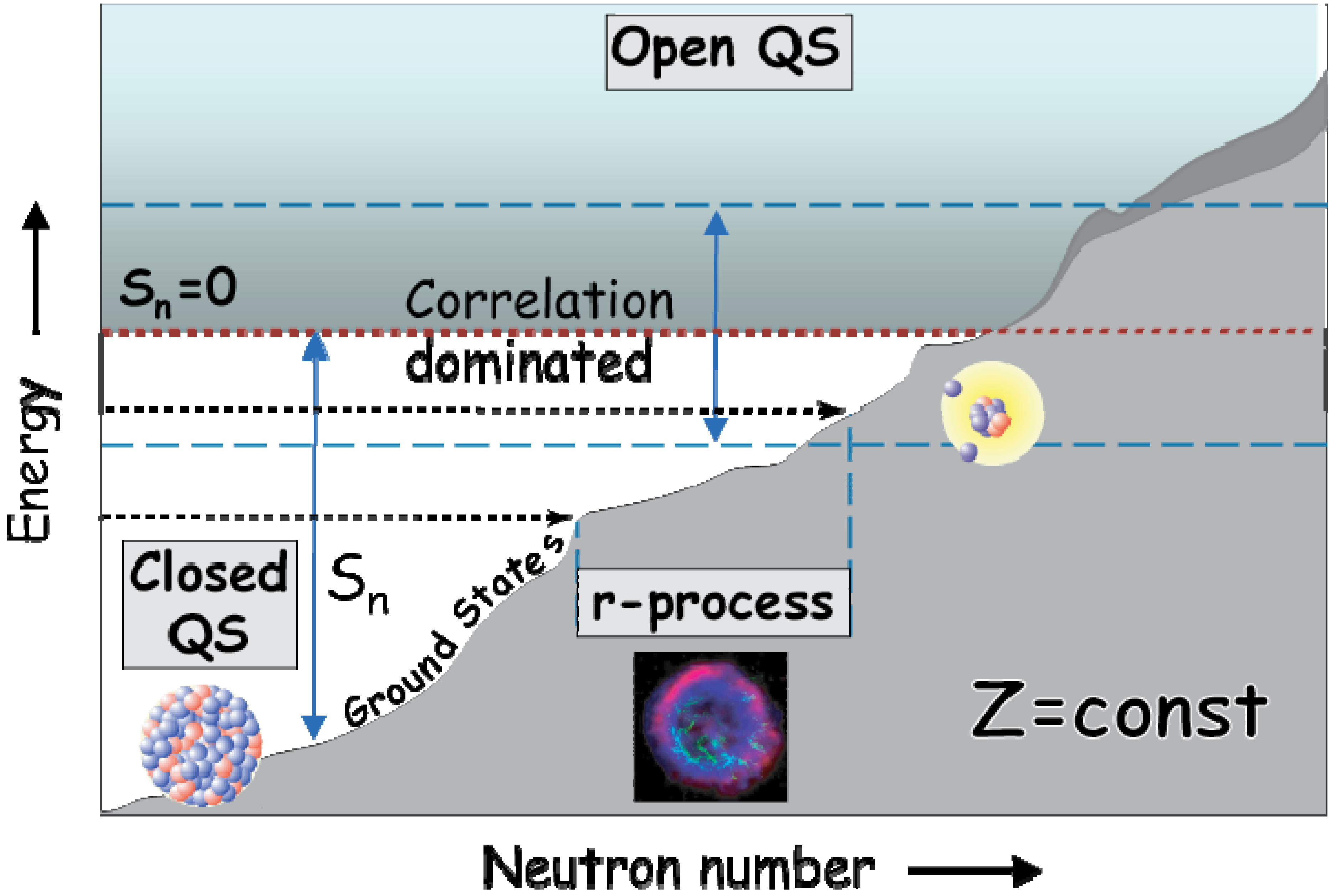
Open channels

- Nuclei are ***open quantum systems***
- Exotic nuclei have low-energy decay thresholds
- Coupling to the continuum important
  - Virtual scattering
  - Unbound states
  - Impact on in-medium Interactions

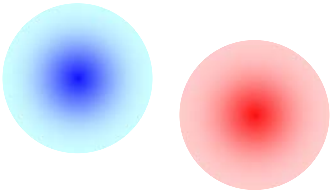
Wikipedia:

An open quantum system is a quantum system which is found to be in interaction with an external quantum system, the environment. The open quantum system can be viewed as a distinguished part of a larger closed quantum system, the other part being the environment.

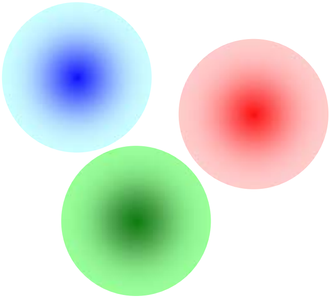
Prog. Part. Nucl. Phys. 59, 432 (2007)



Halos



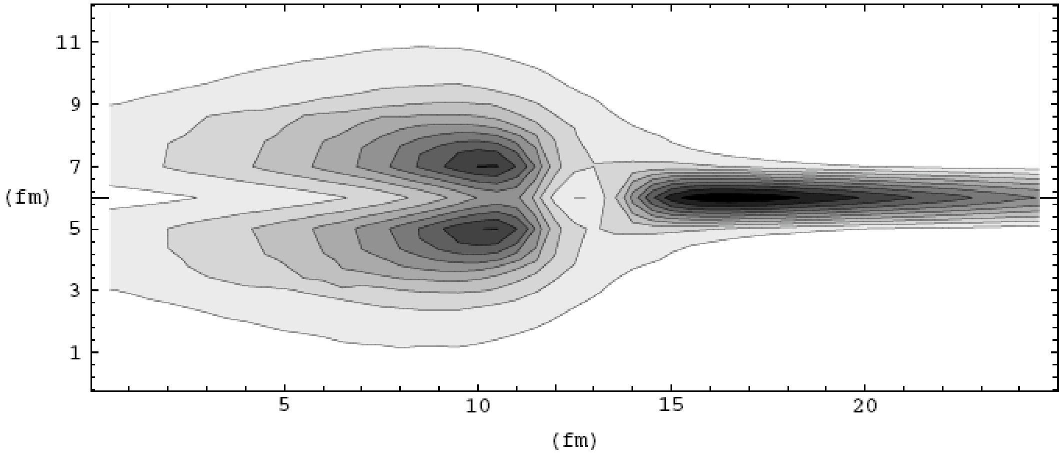
^2H (deuteron)
S_n=2.2 MeV, r_{np}=4 fm



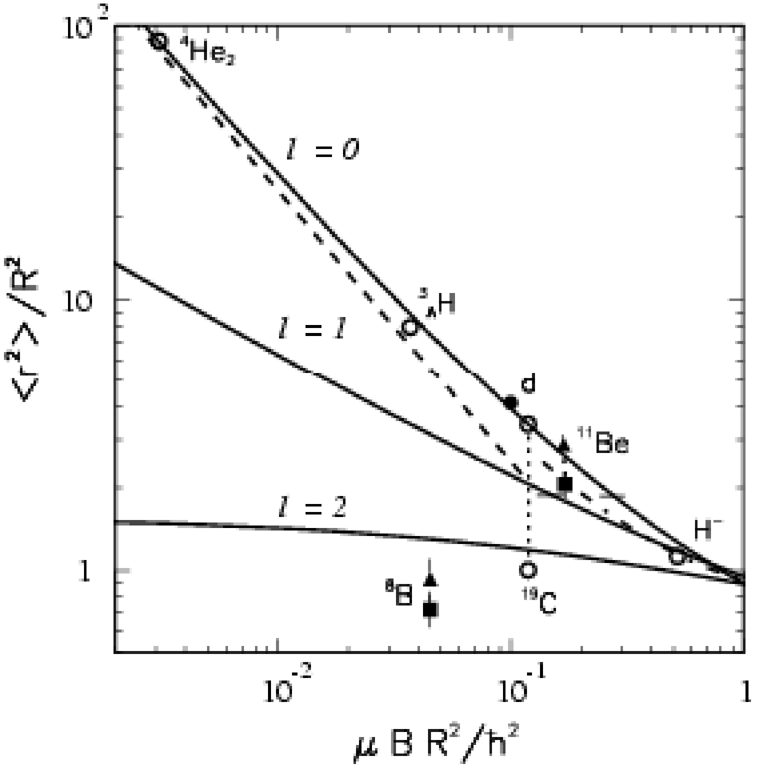
^3H_L (hypertriton)
S_Λ=0.08 MeV

Riisager, Fedorov, Jensen
Europhys. Lett. 49, 547 (2000)

$^4He_2$ (atomic helium dimer)
S=0.13 μeV, r=100 Å



Cobis,Jensen, Fedorov
J. Phys. G23, 401 (1997)



Rigged Hilbert Space: the natural framework to formulate quantum mechanics

In mathematics, a rigged Hilbert space (Gel'fand triple, nested Hilbert space, equipped Hilbert space) is a construction designed to link the distribution and square-integrable aspects of functional analysis. Such spaces were introduced to study spectral theory in the broad sense. They can bring together the 'bound state' (eigenvector) and 'continuous spectrum', in one place.

Mathematical foundations in the 1960s by Gel'fand et al. who combined Hilbert space with the theory of distributions. Hence, the RHS, rather than the Hilbert space alone, is the natural mathematical setting of Quantum Mechanics

I. M. Gel'fand and N. J. Vilenkin. Generalized Functions, vol. 4: Some Applications of Harmonic Analysis. Rigged Hilbert Spaces. Academic Press, New York, 1964.

$$\psi = \psi(r)e^{-iE_0t/\hbar - wt/2} = \psi(r)e^{-iEt/\hbar}$$

$$E = E_0 - i\frac{\Gamma}{2}; \quad \Gamma = \hbar w$$

J.J. Thompson, 1884
G. Gamow, 1928

relation between decay width and decay probability

IOP PUBLISHING JOURNAL OF PHYSICS G: NUCLEAR AND PARTICLE PHYSICS

J. Phys. G: Nucl. Part. Phys. **36** (2009) 013101 (40pp) doi:10.1088/0954-3899/36/1/013101

TOPICAL REVIEW

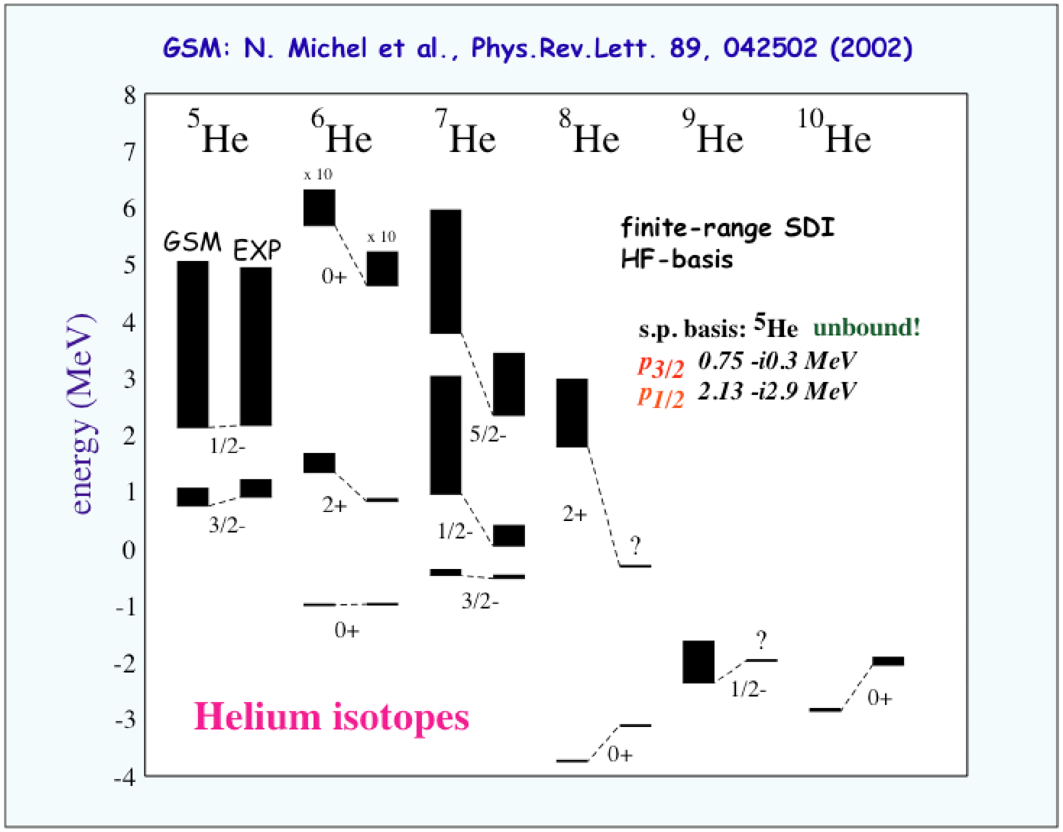
Shell model in the complex energy plane

N Michel[1,2], W Nazarewicz[3,4,5], M Płoszajczak[6] and T Vertse[7,8]

Abstract

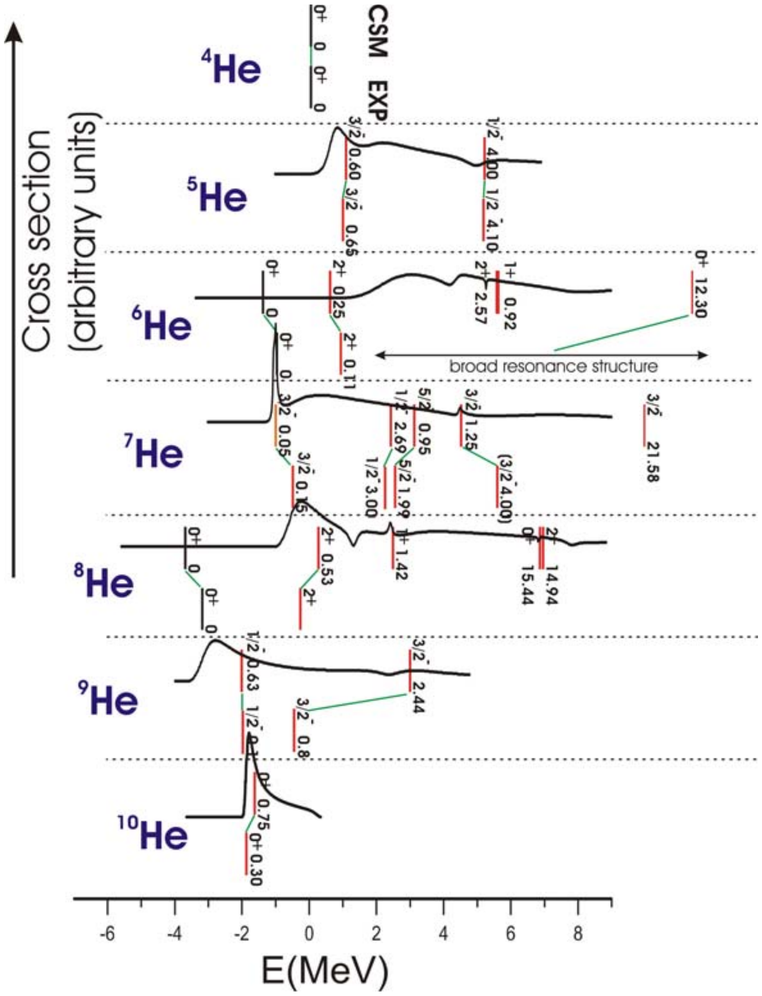
This work reviews foundations and applications of the complex-energy continuum shell model that provides a consistent many-body description of bound states, resonances and scattering states. The model can be considered a quasi-stationary open quantum system extension of the standard configuration interaction approach for well-bound (closed) systems.

Complex-energy Shell Model
Gamow Shell Model

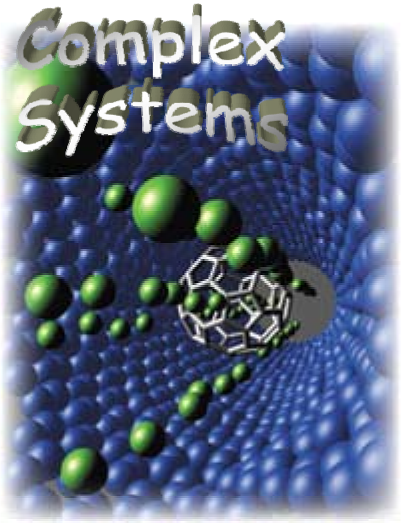

GSM: N. Michel et al., Phys.Rev.Lett. 89, 042502 (2002)

Real-energy Continuum Shell Model

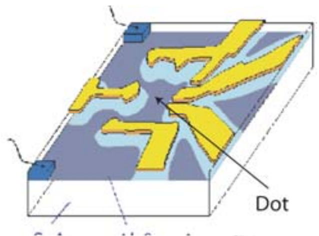
A. Volya and V. Zelevinsky,
Phys. Rev. C 67 (2003) 54322

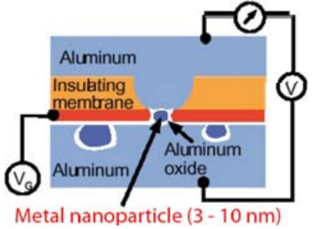


Connections to quantum many-body systems



- Understanding the transition from microscopic to mesoscopic to macroscopic
- Symmetry breaking and emergent phenomena
  - Pairing in finite systems
- Quantum chaos
- Open quantum systems
- Dynamical symmetries and collective dynamics



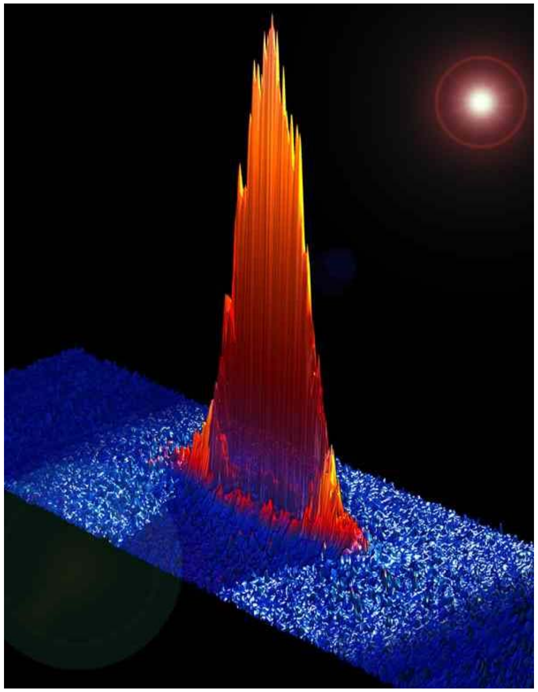


Dilute fermion matter:

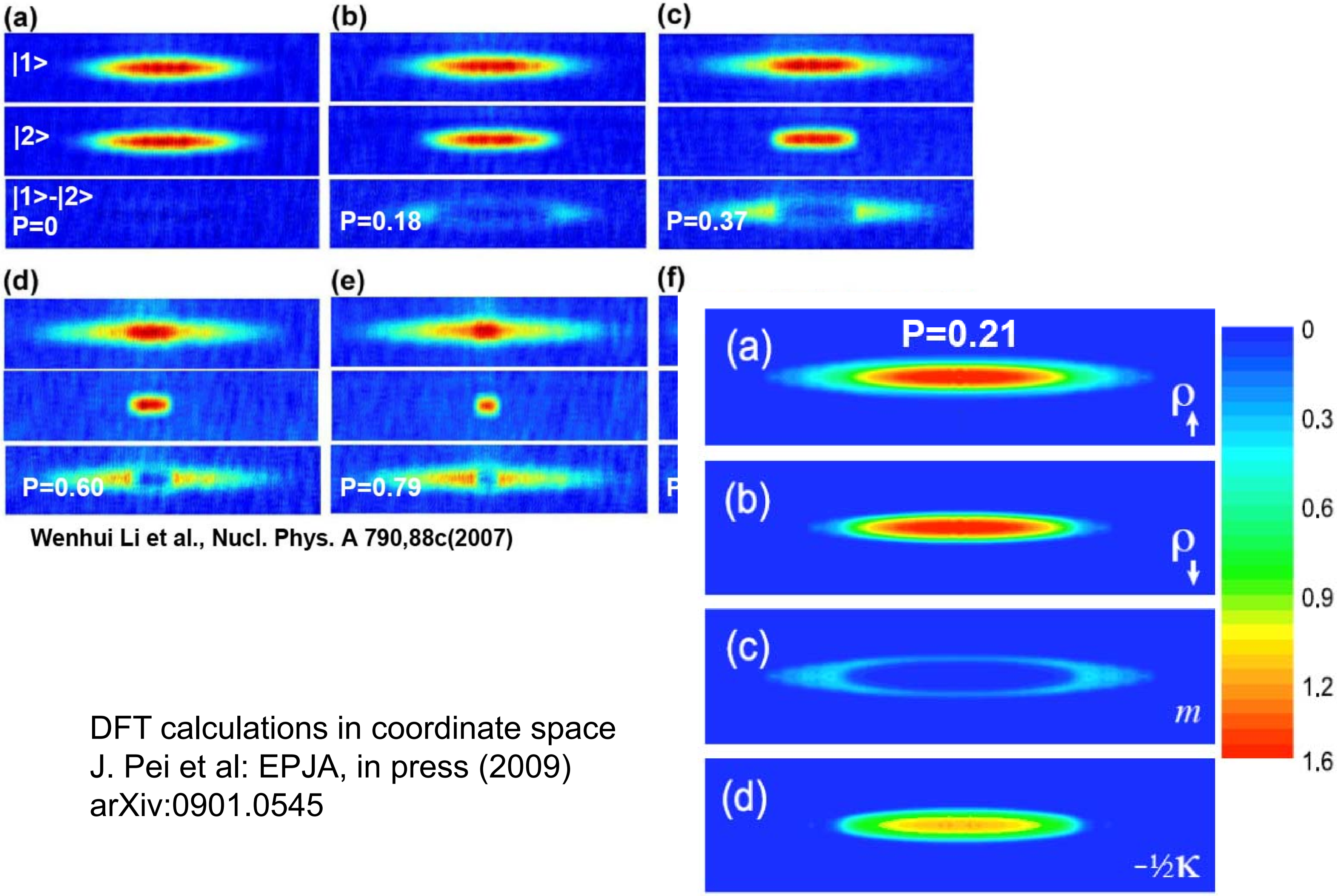
strongly correlated

very large scattering length (unitary limit)

- Low-density neutron matter
- Cold fermions in traps



Trapped ^{6}Li gas (Rice)



Wenhui Li et al., Nucl. Phys. A 790,88c(2007)

DFT calculations in coordinate space
J. Pei et al: EPJA, in press (2009)
arXiv:0901.0545

Computational Strategy

Connections to computational science

1Teraflop=10^{12} flops

1peta=10^{15} flops (next 2-3 years)

1exa=10^{18} flops (next 10 years)

Performance Development

Million-fold increase in computing and data capabilities (ORNL)

2004

Cray X1
3 TF

2005

Cray XT3
Single-core
26 TF

2006

Cray XT3
Dual-core
54 TF

2007

Cray XT4
119 TF

Cray XT4
Quad-core
166 TF
18 TB, 0.3 PB

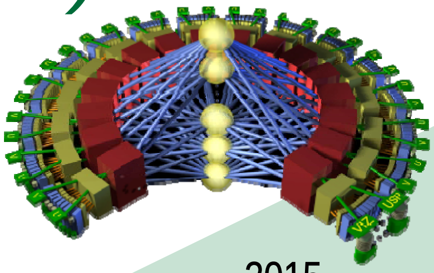
2008

Cray XT4
Quad-core
263 TF
62 TB, 1 PB

Cray “Baker”
8/12-core, dual-socket SMP
~1 PF
100 TB, 2.5 PB

2009

Cray “Baker”
8-core, dual-socket SMP
1.4 PF
300 TB, 10 PB



2011

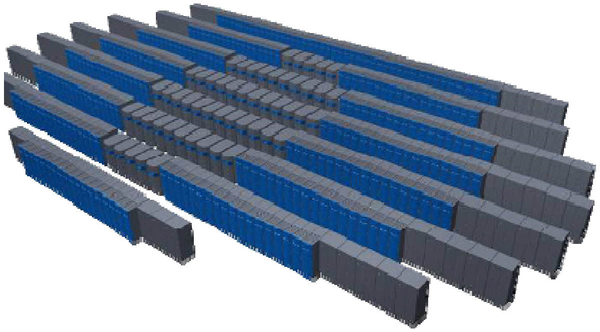
DARPA
HPCS
20 PF

2015

Future
system
100–250 PF

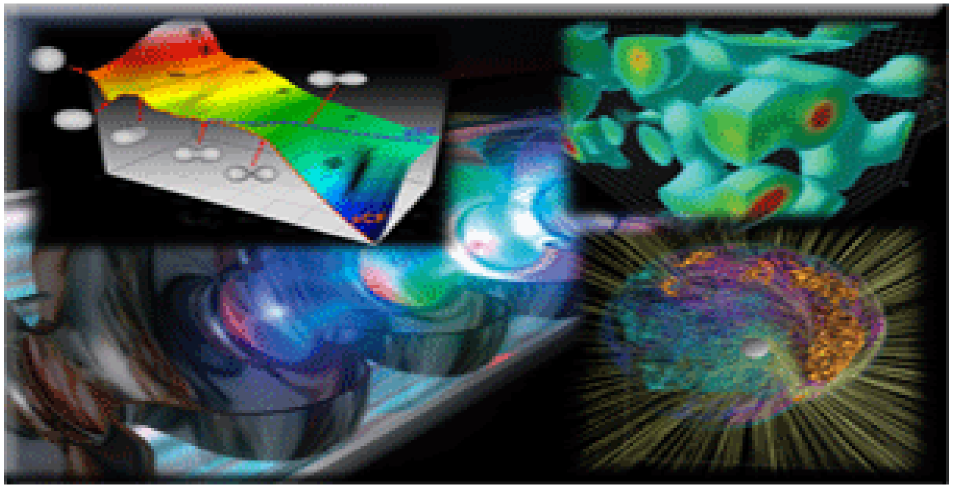
2018

Future
system
1000 PF
(1 EF)



Enabling science communities to address scientific grand challenges through extreme scale computational science

Workshop series:
- Climate Science
- High-Energy Physics
- Nuclear Physics
- Fusion Energy Sciences
- Nuclear Energy
- Biology
- Materials Science and Chemistry

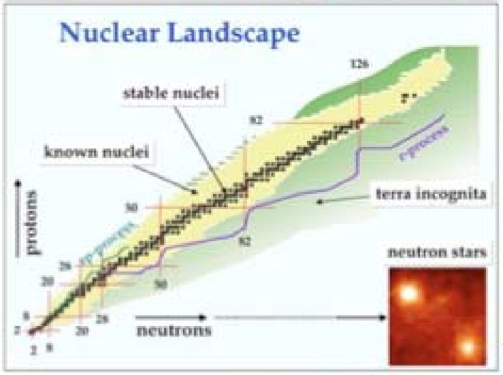


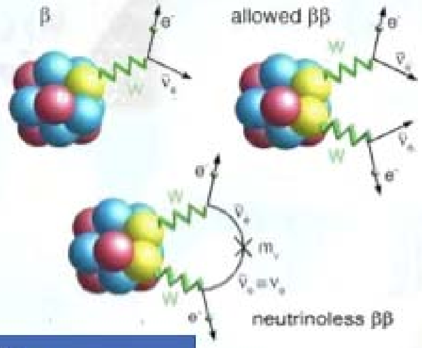
26-28 January 2009, Washington, DC
109 participants; DOE/NSF/NNSA reps

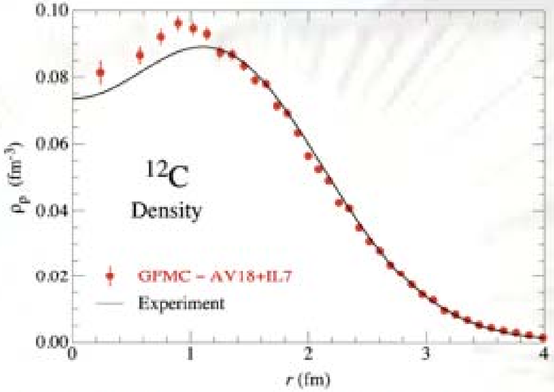
The Nuclear Physics Workshop defined Priority Research Directions in
- Nuclear Astrophysics
- Cold QCD and Nuclear Forces
- Nuclear Structure and Reactions
- Accelerator Physics
- Hot and Dense QCD

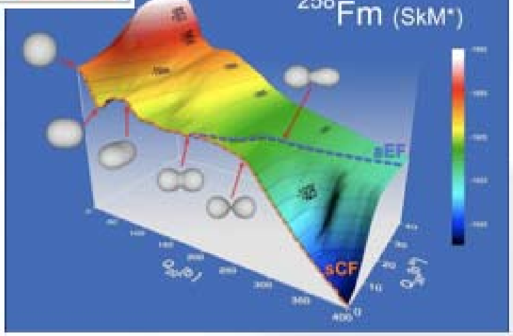
List of Priority Research Directions

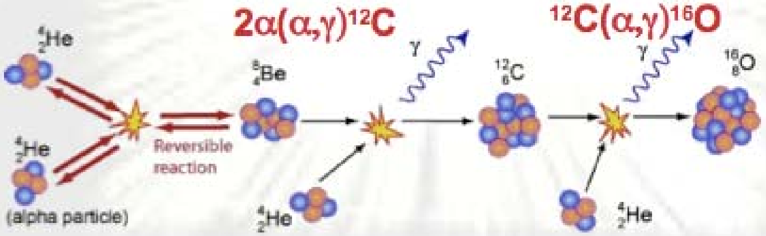
- **Physics of extreme neutron-rich nuclei and matter**
- **Microscopic description of nuclear fission**
- **Nuclei as neutrino physics laboratories**
- **Reactions that made us - triple α process and $^{12}C(\alpha,\gamma)^{16}O$**



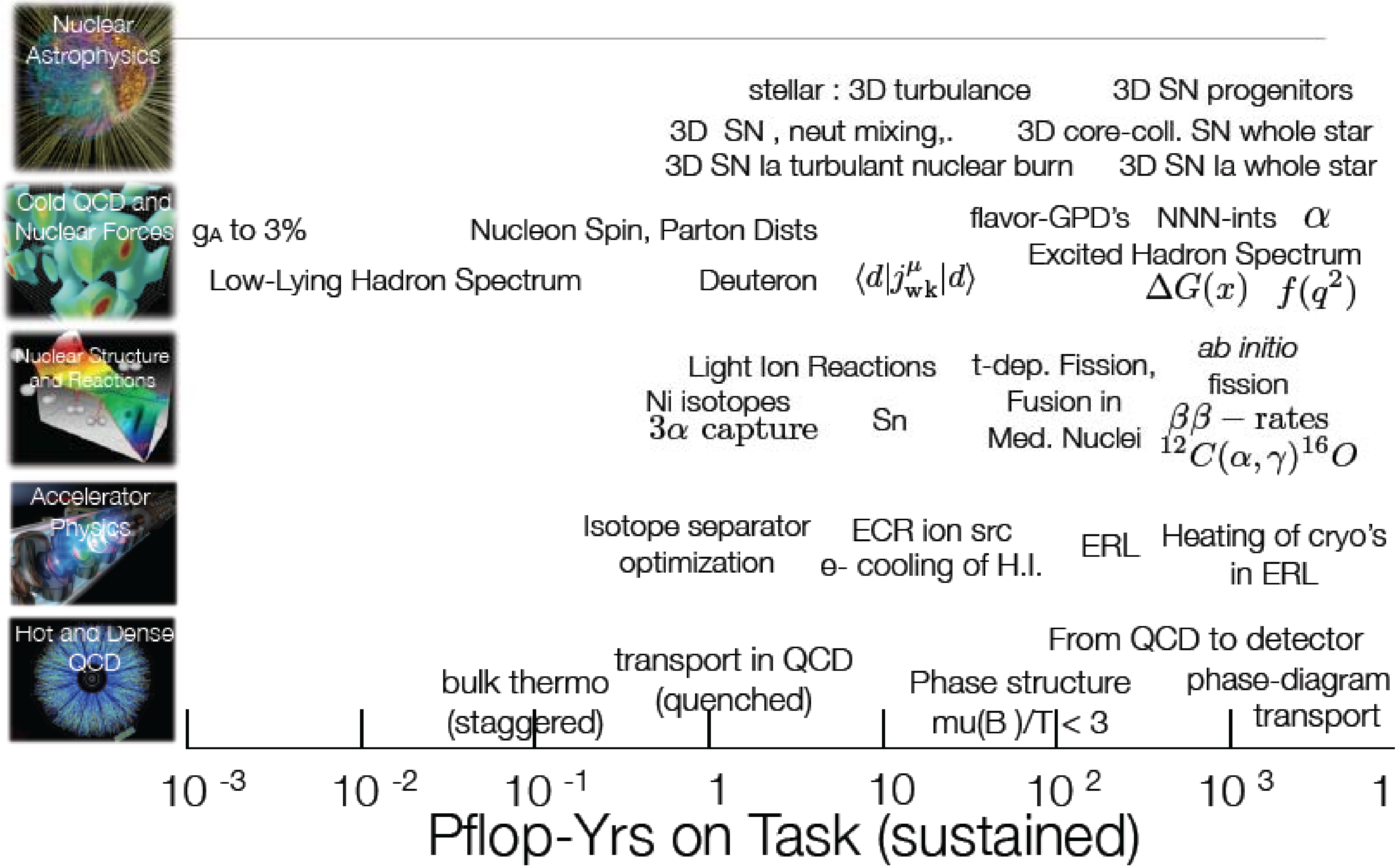








Nuclear Physics Requires Exascale Computing



Nuclear Astrophysics

stellar : 3D turbulance

3D SN progenitors

3D SN , neut mixing,.

3D core-coll. SN whole star

3D SN Ia turbulant nuclear burn

3D SN Ia whole star

Cold QCD and Nuclear Forces

g_A to 3%

Nucleon Spin, Parton Dists

flavor-GPD's NNN-ints α

Excited Hadron Spectrum

Low-Lying Hadron Spectrum

Deuteron

$\langle d|j^{\mu}_{\mathrm{wk}}|d\rangle$

$\Delta G(x)$ $f(q^2)$

Nuclear Structure and Reactions

Light Ion Reactions

t-dep. Fission, Fusion in Med. Nuclei

ab initio fission

Ni isotopes

3α capture

Sn

$\beta\beta$ − rates

${}^{12}C(\alpha,\gamma)^{16}O$

Accelerator Physics

Isotope separator optimization

ECR ion src

e- cooling of H.I.

ERL

Heating of cryo's in ERL

Hot and Dense QCD

From QCD to detector

bulk thermo (staggered)

transport in QCD (quenched)

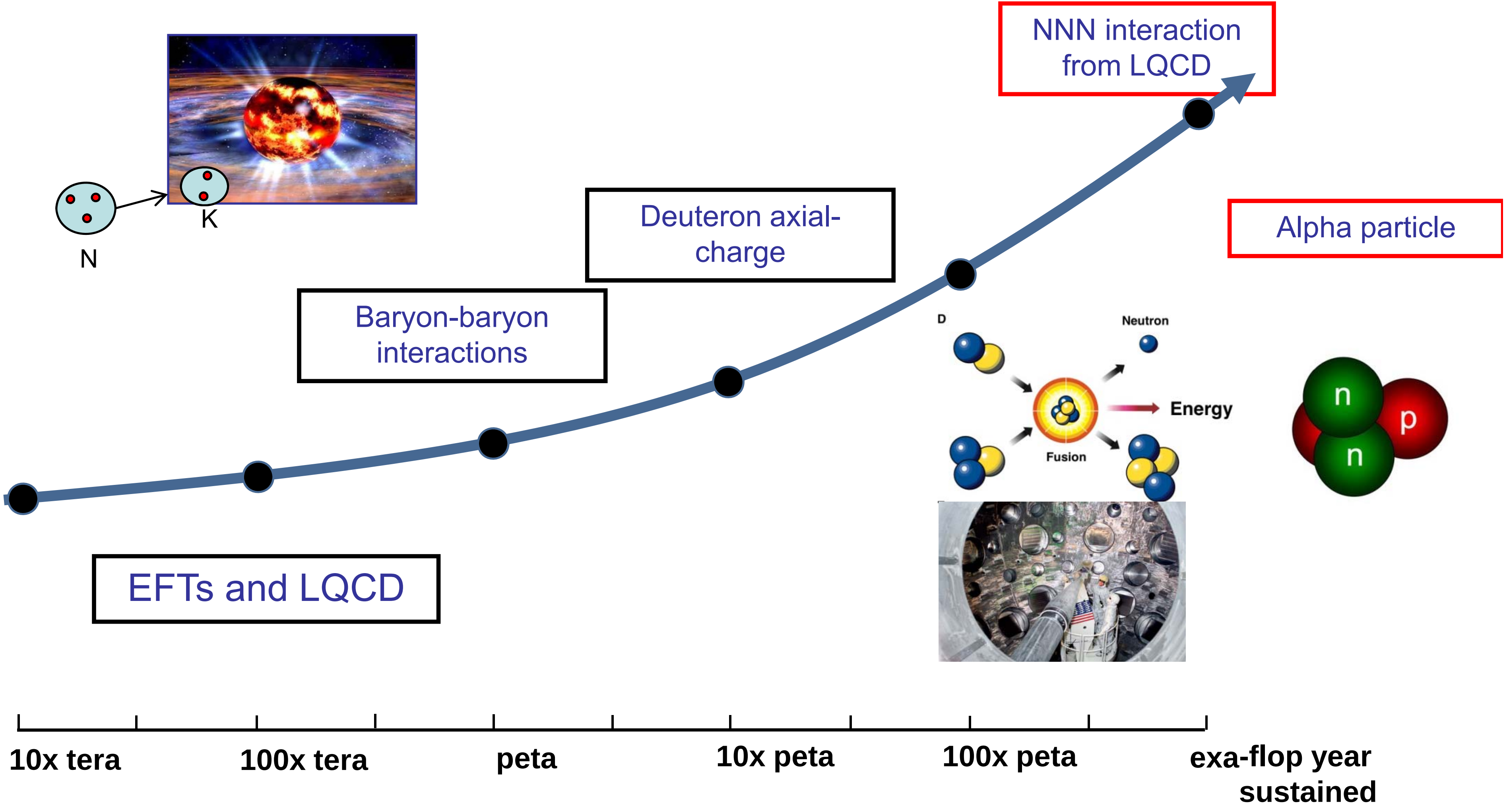
Phase structure mu(B)/T|< 3

phase-diagram transport

10^{-3} 10^{-2} 10^{-1} 1 10 10^{2} 10^{3} 1

Pflop-Yrs on Task (sustained)

The road to exascale for nuclear forces



EFTs and LQCD

Baryon-baryon interactions

Deuteron axial-charge

NNN interaction from LQCD

Alpha particle

SciDAC 2 Project: *Building a Universal Nuclear Energy Density Functional*

- Understand nuclear properties “for element formation, for properties of stars, and for present and future energy and defense applications”
- Scope is all nuclei, with particular interest in reliable calculations of unstable nuclei and in reactions
- Order of magnitude improvement over present capabilities
    - ➢ Precision calculations
- Connected to the best microscopic physics
- Maximum predictive power with well-quantified uncertainties

Universal Nuclear Energy Density Functional

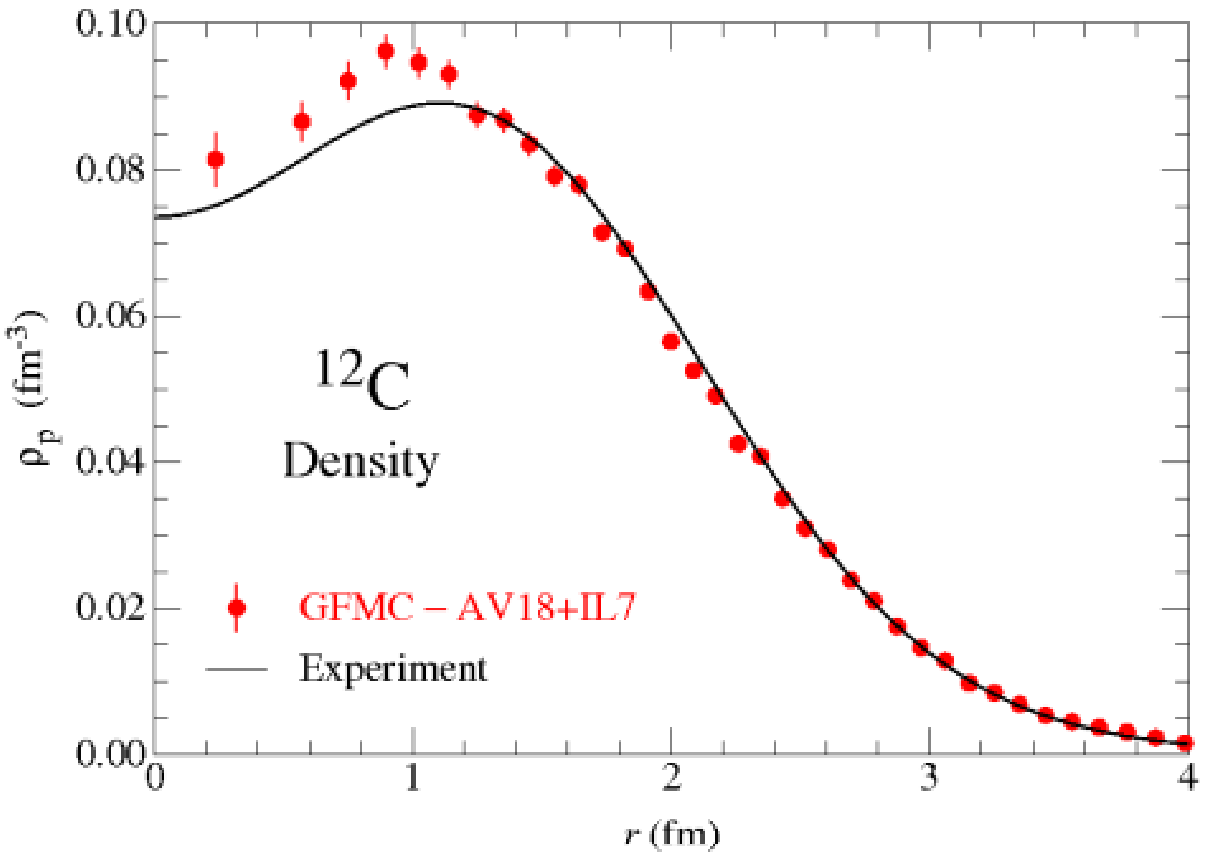
- Funded (on a competitive basis) by
  - Office of Science
  - ASCR
  - NNSA
- 15 institutions
- ~50 researchers
  - physics
  - computer science
  - applied mathematics
- foreign collaborators
- 5 years

  http://unedf.org/

[See http://www.scidacreview.org/0704/html/unedf.html by Bertsch, Dean, and Nazarewicz]

…unprecedented theoretical effort !

Ab-initio nuclear structure: towards $^{12}C(\alpha,\gamma)$



In January 2009: calculations of ^{12}C with a complete Hamiltonian (two- and three-nucleon potentials -- AV18+IL7) on 32,000 processors of the Argonne BGP. These are believed to be the best converged ab initio calculations of ^{12}C ever made. The result is quite good; 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. The figure compares the computed ^{12}C density with that extracted from electron-scattering experiments. Note the good reproduction of the dip at small radius.

Example: Large Scale Mass Table Calculations

Science scales with processors

M. Stoitsov

HFB+LN mass table, HFBTHO

Even-Even Nuclei

- The SkM* mass table contains 2525 even-even nuclei
- A single processor calculates each nucleus 3 times (prolate, oblate, spherical) and records all nuclear characteristics and candidates for blocked calculations in the neighbors
- Using 2,525 processors - about 4 CPU hours (1 CPU hour/configuration)

Jaguar Cray XT4 at ORNL

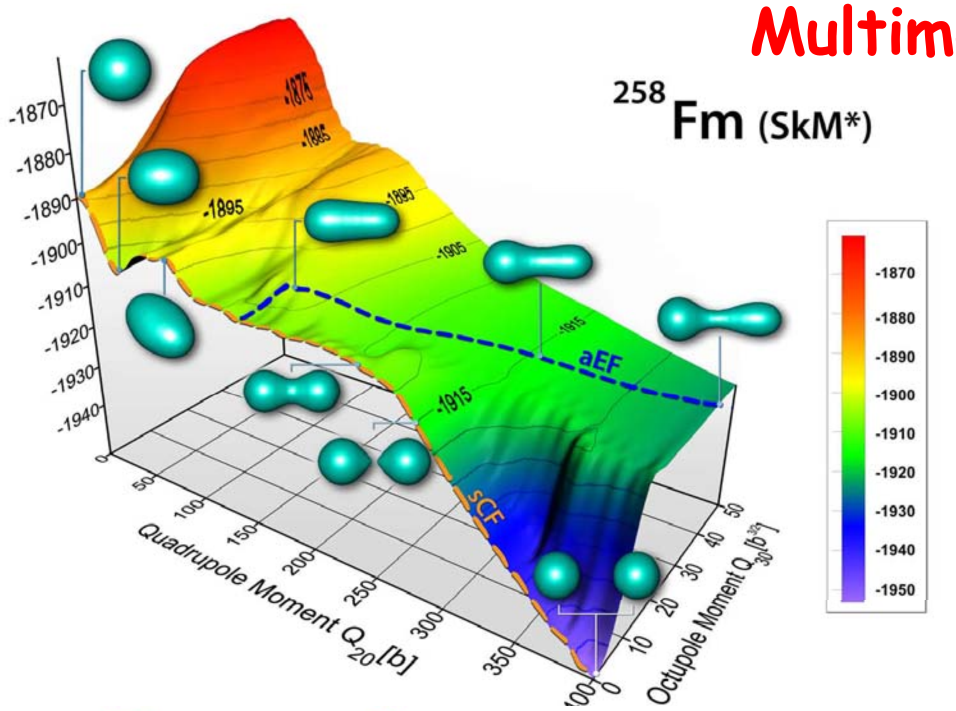
All Nuclei

- 9,210 nuclei
- 599,265 configurations
- Using 3,000 processors - about 25 CPU hours

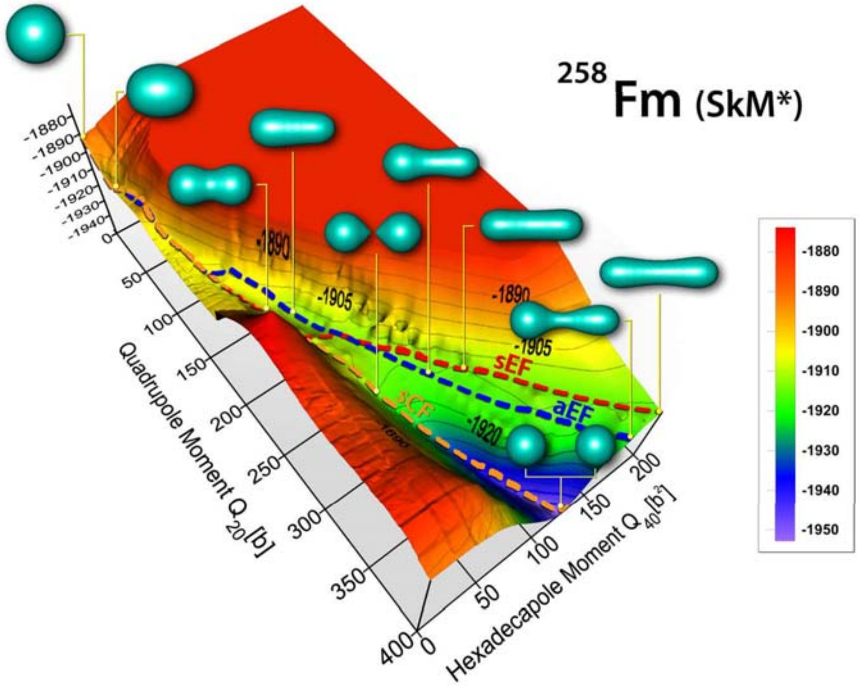
see MassExplorer.org

Multimodal fission in nuclear DFT

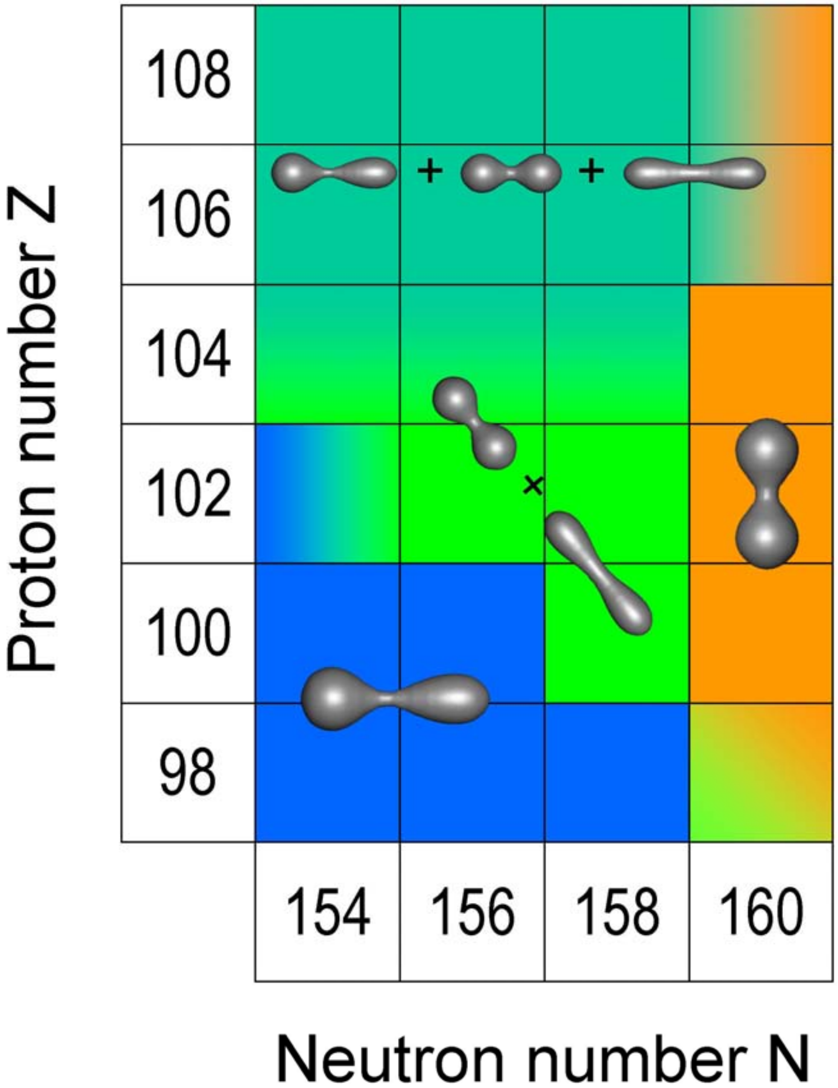
A. Staszczak, A.Baran,
J. Dobaczewski, W.N.



^{258}Fm (SkM*)

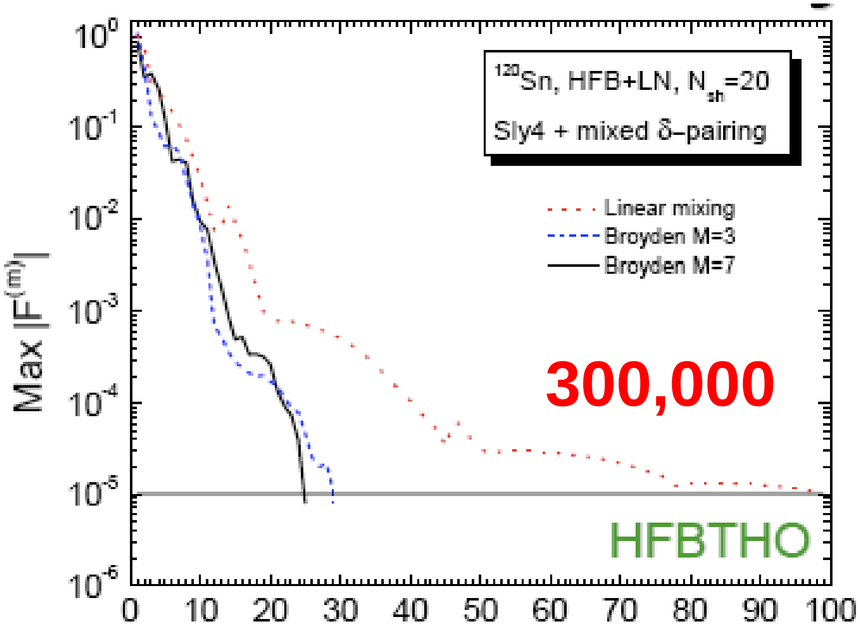


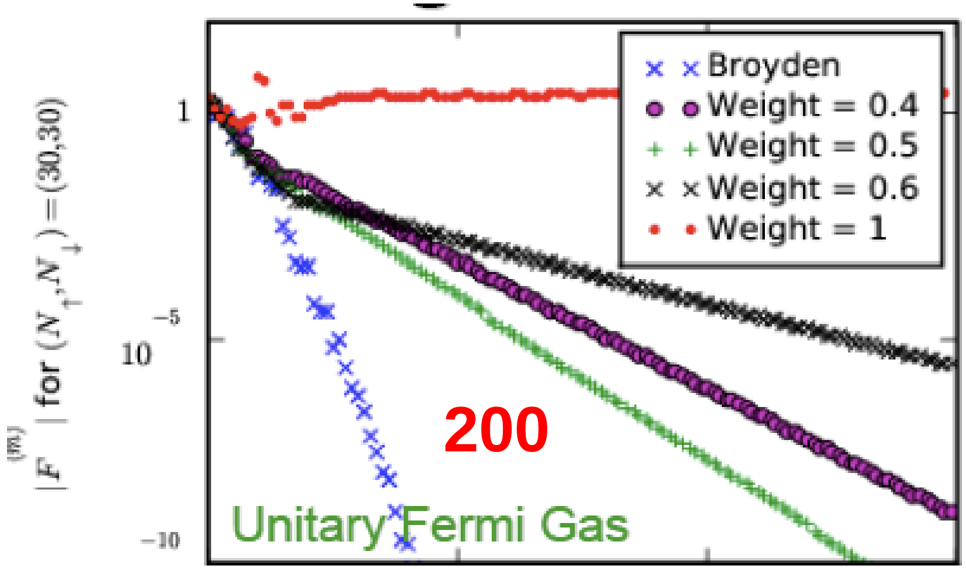
^{258}Fm (SkM*)

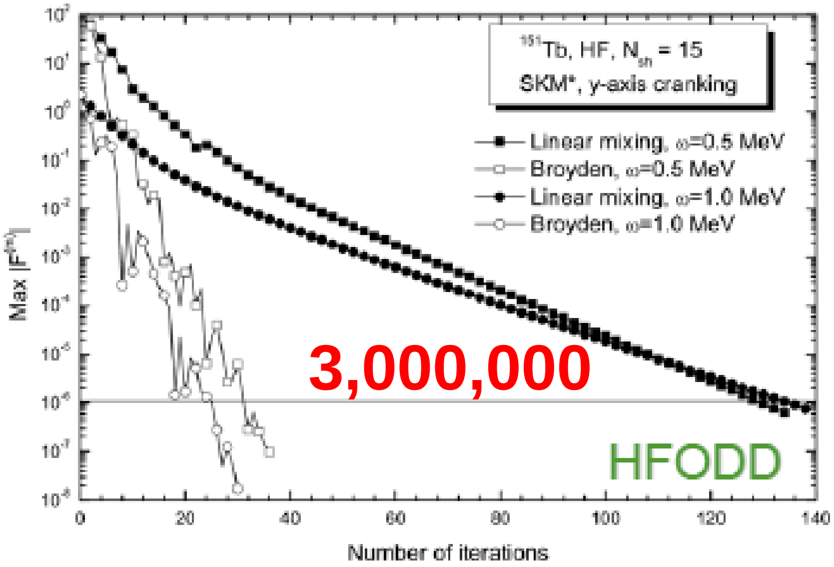


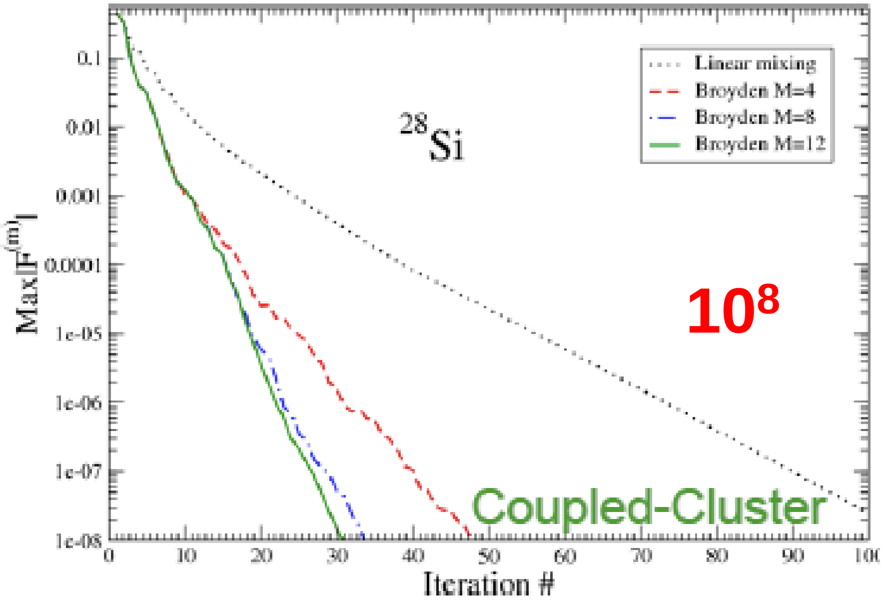
Broyden's Mixing Procedure: Phys. Rev. C 78, 014318 (2008)

A. Baran, A. Bulgac, M. McNeil Forbes, G. Hagen, W. Nazarewicz, N. Schunck and M.V. Stoitsov

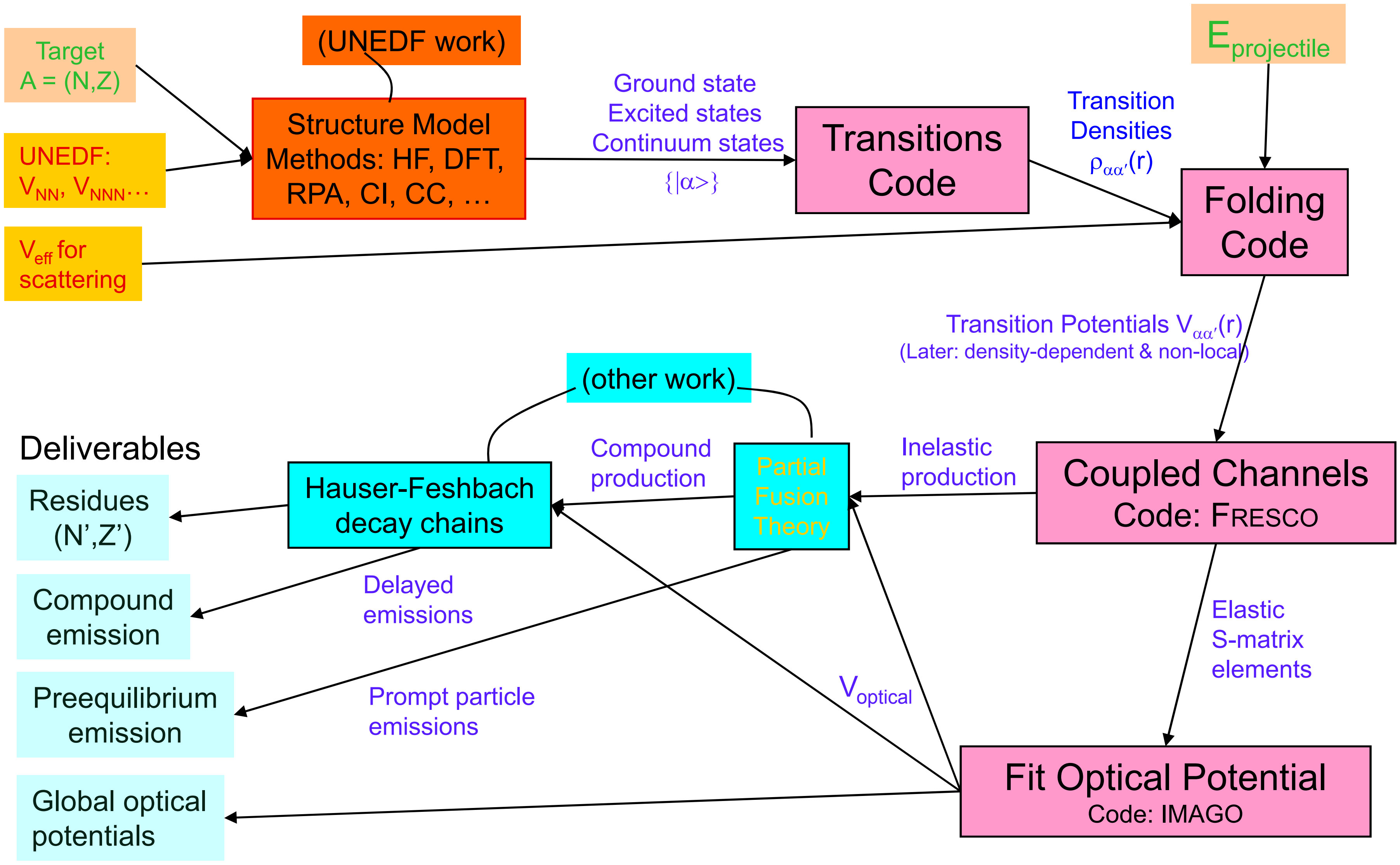








From Ian Thompson



Target
A = (N,Z)

UNEDF:
V_{NN}, V_{NNN}…

V_{eff} for scattering

(UNEDF work)

Structure Model Methods: HF, DFT, RPA, CI, CC, …

Ground state
Excited states
Continuum states
$\{|\alpha>\}$

Transitions Code

Transition Densities
$\rho_{\alpha\alpha'}(r)$

$E_{projectile}$

Folding Code

Transition Potentials $V_{\alpha\alpha'}(r)$
(Later: density-dependent & non-local)

Coupled Channels Code: FRESCO

Elastic S-matrix elements

Fit Optical Potential
Code: IMAGO

(other work)

Inelastic production

Partial Fusion Theory

Compound production

Hauser-Feshbach decay chains

$V_{optical}$

Delayed emissions

Prompt particle emissions

Deliverables

Residues (N',Z')

Compound emission

Preequilibrium emission

Global optical potentials

KEY:
Code Modules
UNEDF Ab-initio Input
User Inputs/Outputs
Exchanged Data
Future research

$\sigma(n+A\rightarrow X_i)$ at energy $E_{projectile}$
Computational Workflow

UNEDF Reaction work

Perspectives

Recent years: very successful period for theory of nuclei

- many new ideas leading to new understanding
- new theoretical frameworks
- exciting developments
- high-quality calculations

- The nucleon-based description works to <0.5 fm
- Effective Field Theory/Renormalization Group provides missing links
  Short-range repulsion: **a red herring!**
- Accurate ab-initio methods allow for interaction tests
- Worldwide attack on the nuclear energy density functional
- Quantitative microscopic nuclear structure
- Integrating nuclear structure and reactions
- High-performance computing continues to revolutionize microscopic nuclear many-body problem: impossible becomes possible
- Some of the most interesting physics outcomes will be at the interfaces:
  - QCD to forces to structure
  - structure and reactions with nuclear astrophysics

- **Exciting** science; old paradigms revisited
- **Interdisciplinary** (quantum many-body problem, cosmos,…)
- **Relevant** to society (energy, medicine, national security, …)

- Theory gives the mathematical formulation of our understanding and predictive ability
- New-generation computers provide unprecedented opportunities
- Large coherent international theory effort is needed to make a progress

Guided by data on short-lived nuclei, we are embarking on a comprehensive study of all nuclei based on the most accurate knowledge of the strong inter-nucleon interaction, the most reliable theoretical approaches, and the massive use of the computer power available at this moment in time. **The prospects look good.**

Thank You

Backup

(Nuclear) Many-Body Physics: “Old” vs. “New”

One Hamiltonian for all problems and energy/length scales	Infinite # of low-energy potentials; different resolutions $\Longrightarrow$ different dof’s and Hamiltonians
Find the “best” potential	There is no best potential $\Longrightarrow$ use a convenient one!
Two-body data may be sufficient; many-body forces as last resort	Many-body data needed and many-body forces inevitable
Avoid (hide) divergences	Exploit divergences (cutoff dependence as tool)
Choose diagrams by “art”	Power counting determines diagrams and truncation error

Short-range correlations: a red herring