Recent advances and new perspectives for the no core shell model

James P. Vary, Iowa State University

Michigan State University Workshop
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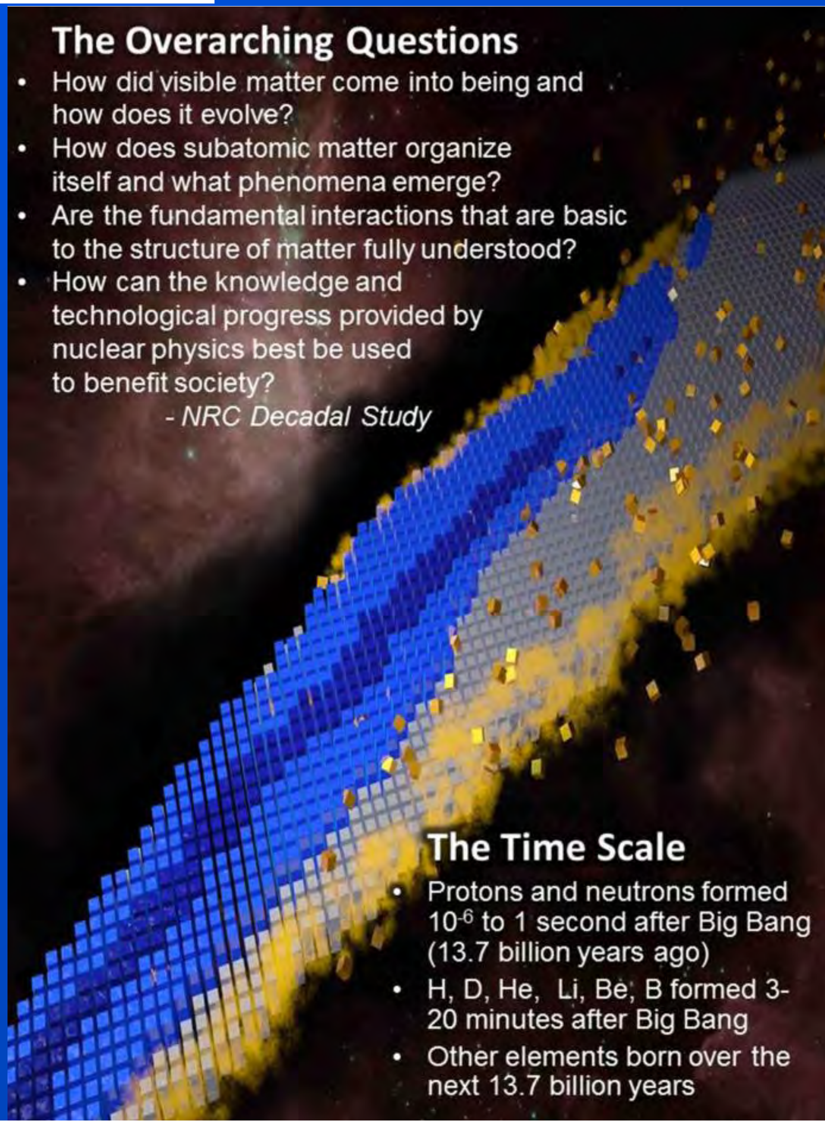
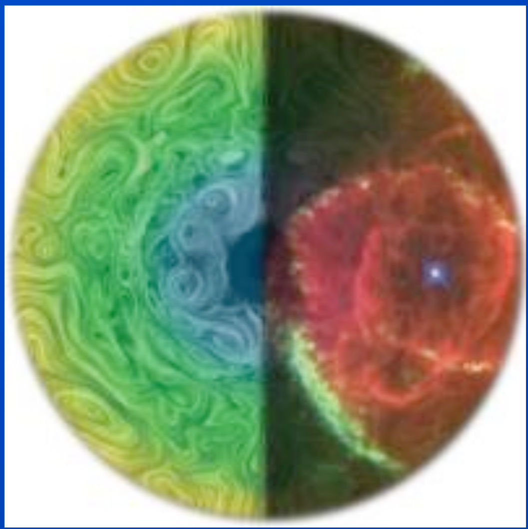
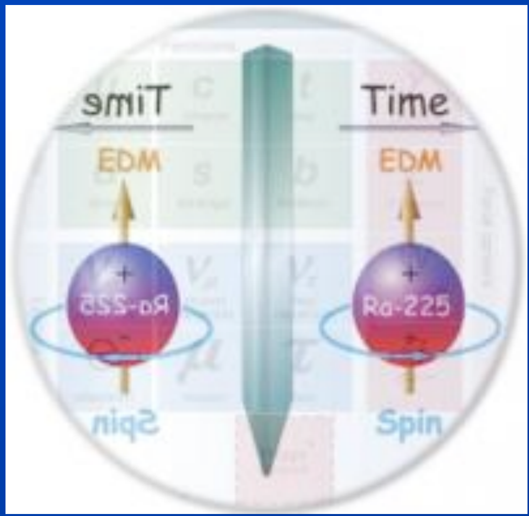
LENPIC







Zach Kohley's Challenges earlier this week

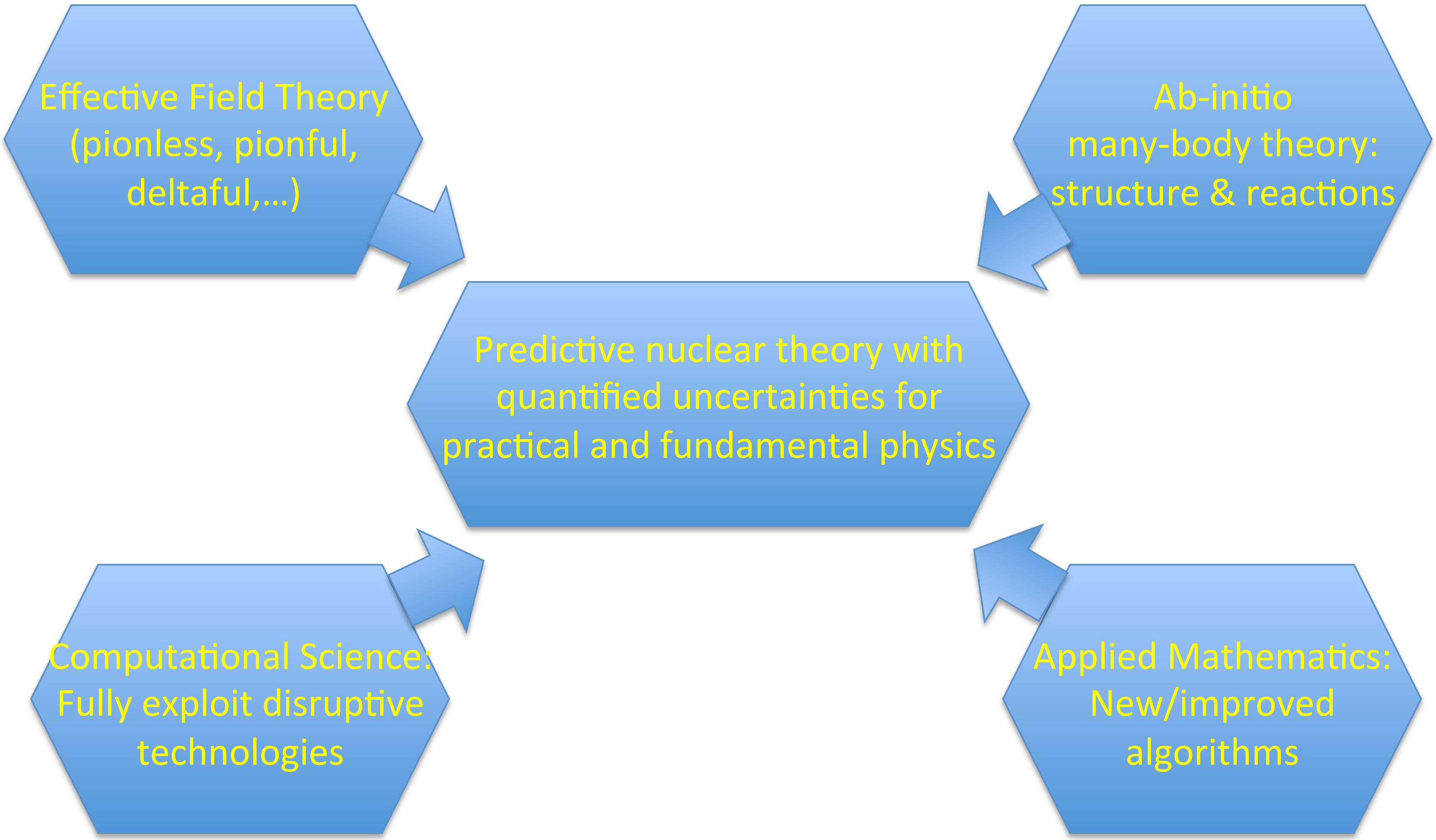
Discussion topics

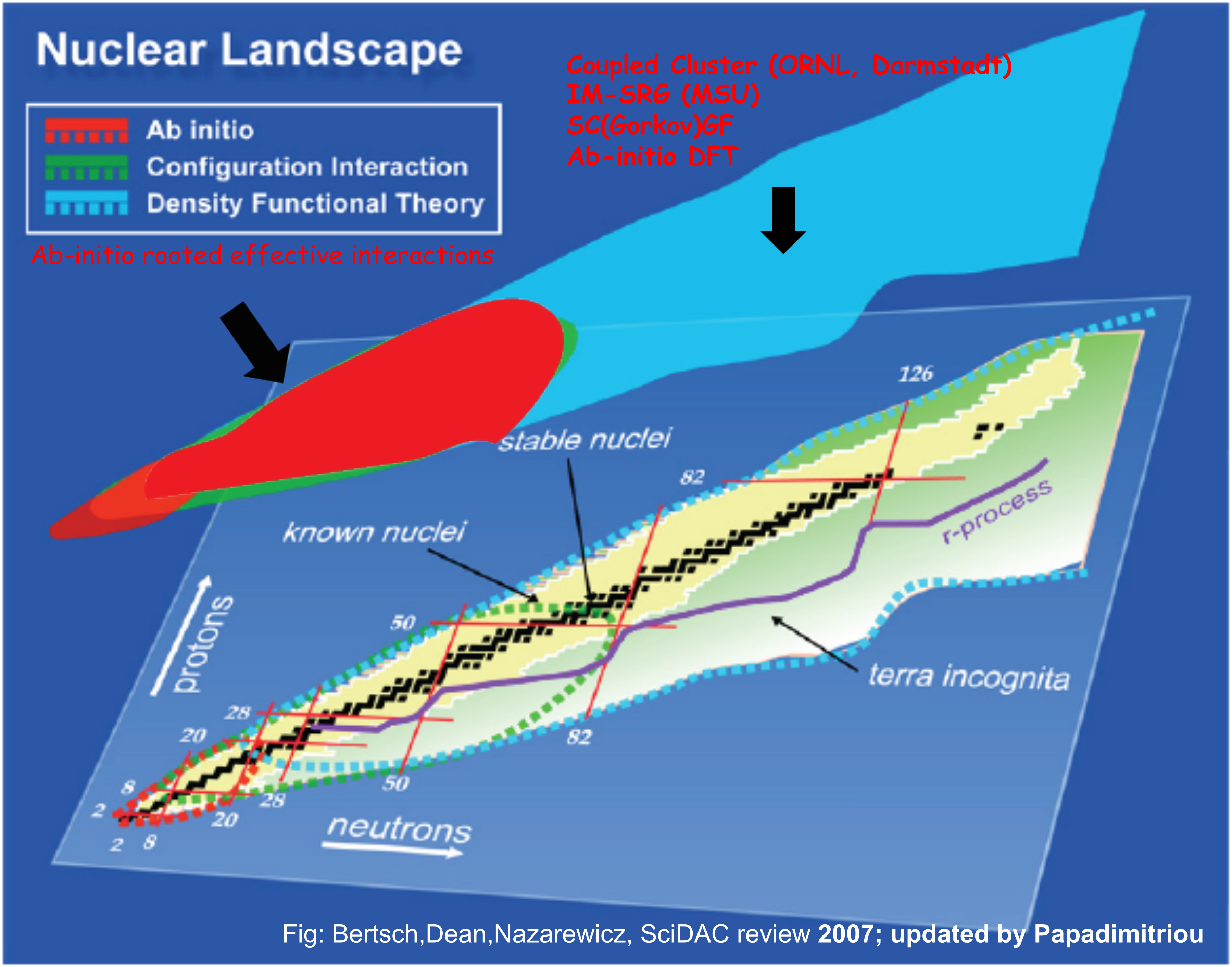
- Confusion in ^{9}He and ^{10}He
- Level structure of ^{12,13}Li
- ^{13}Be puzzle
- Evidence for 2n radioactivity (^{26}O)
- 3-body correlations (^{13}Li, ^{16}Be, ^{26}O)
- Nitrogen Request [^{23}N*, ^{24}N(g.s.)]

Stuff we really want theorists to calculate

accurately

NSCL


Effective Field Theory (pionless, pionful, deltaful,…)
Ab-initio many-body theory: structure & reactions
Predictive nuclear theory with quantified uncertainties for practical and fundamental physics
Computational Science: Fully exploit disruptive technologies
Applied Mathematics: New/improved algorithms


Nuclear Landscape
Ab initio
Configuration Interaction
Density Functional Theory
Ab-initio rooted effective interactions
Coupled Cluster (ORNL, Darmstadt)
IM-SRG (MSU)
SC(Gorkov)GF
Ab-initio DFT
stable nuclei
known nuclei
r-process
terra incognita
protons
neutrons
126
82
50
28
20
8
2
Fig: Bertsch,Dean,Nazarewicz, SciDAC review 2007; updated by Papadimitriou

No-Core Configuration Interaction calculations

Barrett, Navrátil, Vary, *Ab initio no-core shell model*, PPNP69, 131 (2013)

Given a Hamiltonian operator

$$\hat{\mathbf{H}} = \sum_{i<j} \frac{(\vec{p}_i - \vec{p}_j)^2}{2\,m\,A} + \sum_{i<j} V_{ij} + \sum_{i<j<k} V_{ijk} + \ldots$$

solve the eigenvalue problem for wavefunction of A nucleons

$$\hat{\mathbf{H}}\,\Psi(r_1,\ldots,r_A) = \lambda\,\Psi(r_1,\ldots,r_A)$$

- Expand wavefunction in basis states $|\Psi\rangle = \sum a_i |\Phi_i\rangle$
- Diagonalize Hamiltonian matrix $H_{ij} = \langle\Phi_j|\hat{\mathbf{H}}|\Phi_i\rangle$
- No-Core CI: all A nucleons are treated the same
- Complete basis $\longrightarrow$ exact result
- In practice
  - truncate basis
  - study behavior of observables as function of truncation

Basis expansion $\Psi(r_1,\ldots,r_A) = \sum a_i \Phi_i(r_1,\ldots,r_A)$

- Many-Body basis states $\Phi_i(r_1,\ldots,r_A)$ Slater Determinants
- Single-Particle basis states $\phi_\alpha(r_k)$ with $\alpha = (n,l,s,j,m_j)$
- Radial wavefunctions: Harmonic Oscillator (HO), Woods-Saxon, Coulomb-Sturmian, Complex Scaled HO, Berggren,. . .
- M-scheme: Many-Body basis states eigenstates of $\hat{\mathbf{J}}_\mathbf{z}$

$$\hat{\mathbf{J}}_\mathbf{z}|\Phi_i\rangle = M|\Phi_i\rangle = \sum_{k=1}^{A} m_{ik}|\Phi_i\rangle$$

- N_{max} truncation: Many-Body basis states satisfy

$$\sum_{\alpha \text{ occ.}}^{A} (2n+l)_\alpha \le N_0 + N_{\text{max}}$$

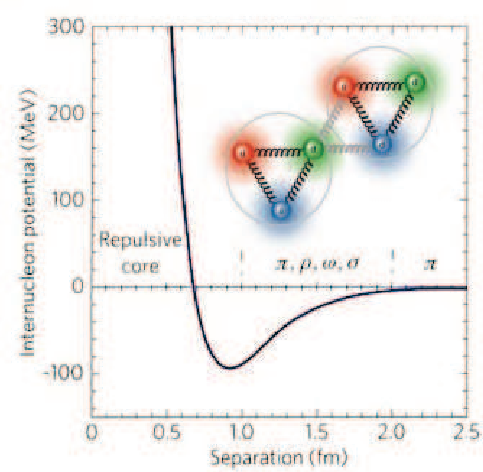
N_{max} runs from zero
to computational limit.
$(N_{\text{max}}, \hbar\Omega)$ fix HO basis

- Alternatives:
  - Full Configuration Interaction (single-particle basis truncation)
  - Importance Truncation — Roth, PRC79, 064324 (2009)
  - No-Core Monte-Carlo Shell Model — Abe *et al*, PRC86, 054301 (2012)
  - SU(3) Truncation — Dytrych *et al*, PRL111, 252501 (2013)

Nuclear interaction

Nuclear potential not well-known,
though in principle calculable from QCD

$$\hat{\mathbf{H}} \quad = \quad \hat{\mathbf{T}}_{\text{rel}} + \sum_{i<j} V_{ij} + \sum_{i<j<k} V_{ijk} + \ldots$$



In practice, alphabet of realistic potentials

- Argonne potentials: AV8′, AV18
  - plus Urbana 3NF (UIX)
  - plus Illinois 3NF (IL7)
- Bonn potentials
- Chiral NN interactions
  - plus chiral 3NF, ideally to the same order
- . . .
- JISP16
- . . .

Major development during the past 5-10 years:
High-precision ab initio calculations now used to
“discover” the correct strong NN+NNN interaction

Controlling the center-of-mass (cm) motion in order to preserve Galilean invariance

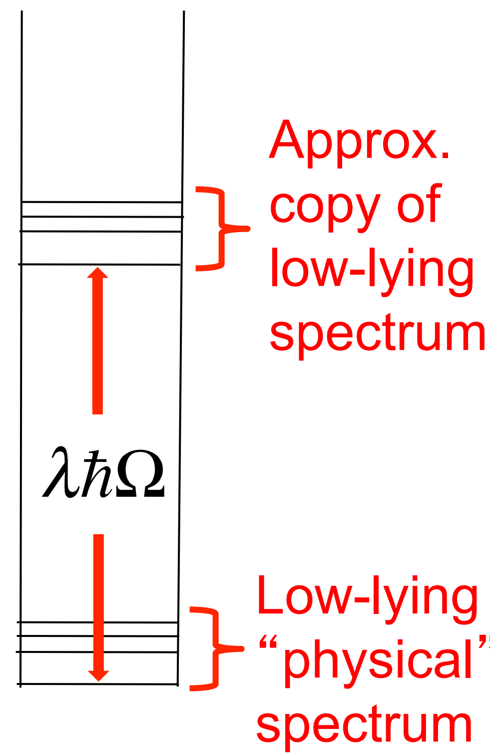
Add a Lagrange multiplier term acting on the cm alone so as not to interfere with the internal motion dynamics

$$H_{eff}\left(N_{\max},\hbar\Omega\right) \equiv P[T_{rel} + V^{a}\left(N_{\max},\hbar\Omega\right)]P$$

$$H = H_{eff}\left(N_{\max},\hbar\Omega\right) + \lambda H_{cm}$$

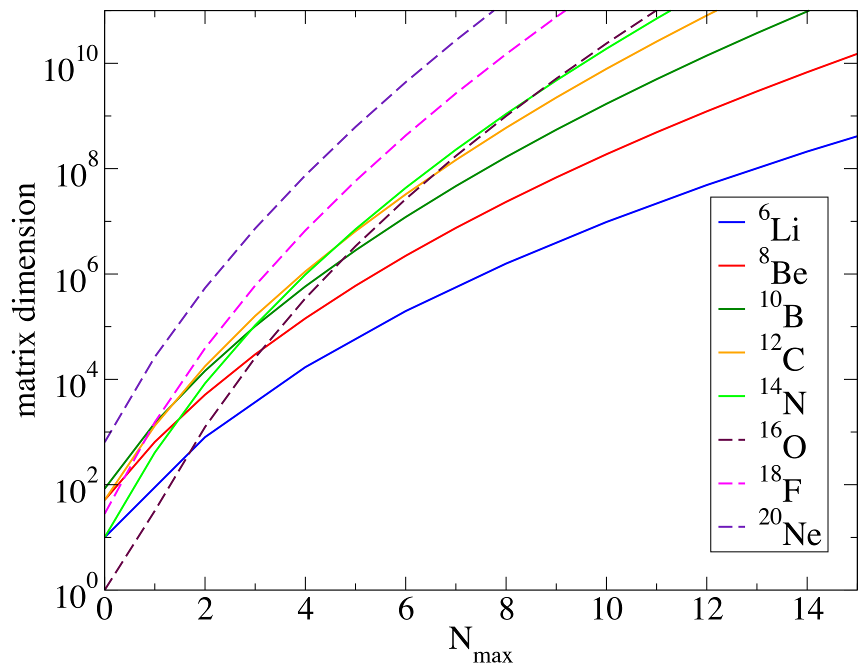
$$H_{cm} = \frac{P^2}{2M_A} + \frac{1}{2}M_A\Omega^2 R^2$$

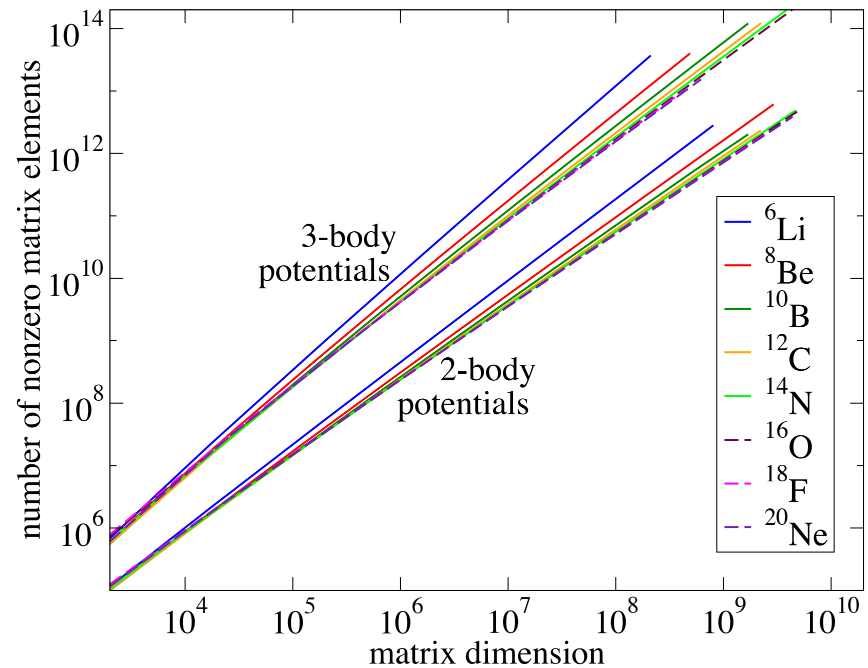
$$\lambda \sim 10 \quad \text{suffices}$$



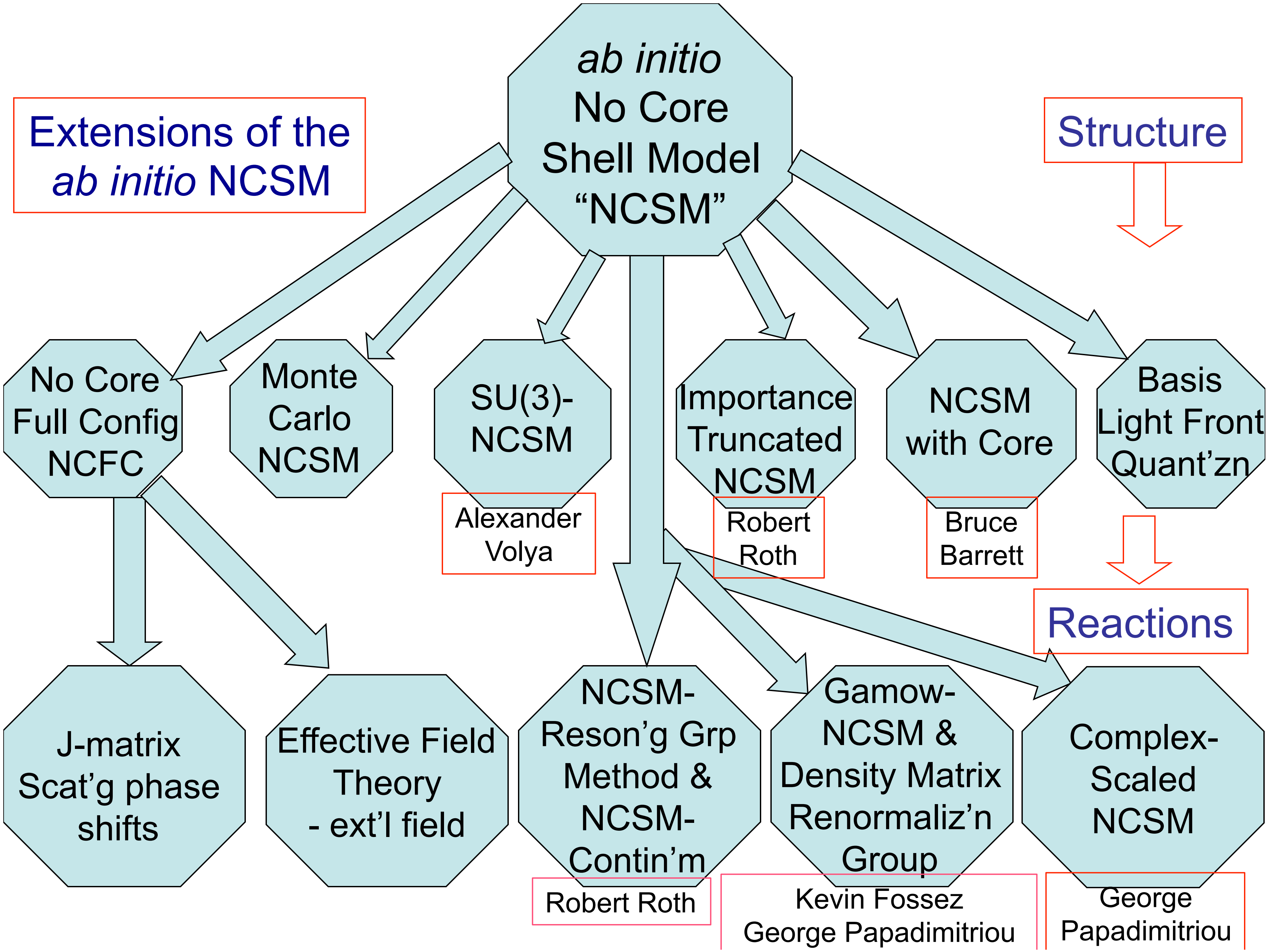
Along with the N_{max} truncation in the HO basis, the Lagrange multiplier term guarantees that all low-lying solutions have eigenfunctions that factorize into a 0s HO wavefunction for the cm times a translationaly invariant wavefunction.

NCSM Main Computational Challenge – Compute/Store Nonzero Matrix Elements





- Increase of basis space dimension with increasing A and N_{max}
  - need calculations up to at least $N_{\text{max}} = 8$
    for meaningful extrapolation and numerical error estimates
- More relevant measure for computational needs
  - number of nonzero matrix elements (NNZ)
  - current limit 10^{13} to 10^{14} (Edison, Mira, Titan)


Extensions of the *ab initio* NCSM
Structure
Reactions
ab initio No Core Shell Model "NCSM"
No Core Full Config NCFC
Monte Carlo NCSM
SU(3)-NCSM
Alexander Volya
Importance Truncated NCSM
Robert Roth
NCSM with Core
Bruce Barrett
Basis Light Front Quant'zn
J-matrix Scat'g phase shifts
Effective Field Theory - ext'l field
NCSM-Reson'g Grp Method & NCSM-Contin'm
Robert Roth
Gamow-NCSM & Density Matrix Renormaliz'n Group
Kevin Fossez
George Papadimitriou
Complex-Scaled NCSM
George Papadimitriou

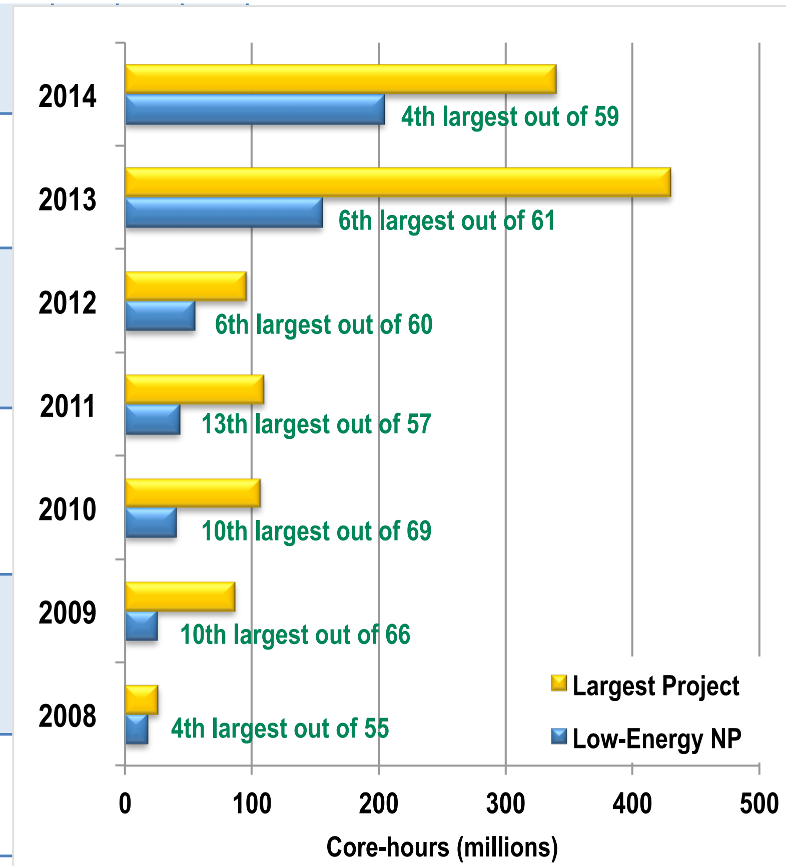
- Hardware advances: Moore’s Law
- Theory/Algorithms/Software advances: Doubles Moore’s Law

Discovery potential and Predictive Power increases geometrically

Low Energy NP Application Areas

Application	Production Run Sizes	Resource	Dense Linear Alg.	Sparse Linear Alg.	Monte Carlo
AGFMC: Argonne Green's Function Monte Carlo	262,144 cores @ 10 hrs	Mira			X
MFDn: Many Fermion Dynamics - nuclear	260K cores @ 4 hrs 500K cores @ 1.33 hrs	Titan Mira		X	
NUCCOR: Nuclear Coupled-Cluster Oak Ridge, m-scheme & spherical	100K cores @ 5 hrs (1 nucleus, multiple parameters)	Titan		X	
DFT Code Suite: Density Functional Theory, mean-field methods	100K cores @ 10 hrs (entire mass table, fission barriers)	Titan	X		
MADNESS: Schroedinger, Lippman-Schwinger and DFT	40,000 cores @ 12 hrs (extreme asymmetric functions)	Titan	X	X	
NCSM_RGM: Resonating Group Method for scattering	98,304 cores @ 8 hrs	Titan	X	X	

- Ab initio Methods (CC, GFMC, NCSM) → pushing the limits to calculate larger nuclei
- Density Functional Theory → reasonable time to solution to calculate the entire mass table



Slide by Hai Ah Nam, ORNL

Computer Science/Applied Math/Physics Collaborations

Main Goal: Solve forefront ab initio nuclear structure/reactions problems
Code: Many-Fermion Dynamics – nuclear (MFDn)

<u>Goals for MFDn (often compete with each other)</u>

- Scalable to ~500,000 cores
- Load balanced
- Optimized for single-node efficiency
- Minimize memory footprint
- Observables calculated accurately
- Minimize cpu-hour cost/case
- Efficient use of GPUs where available
- Minimize time-to-completion

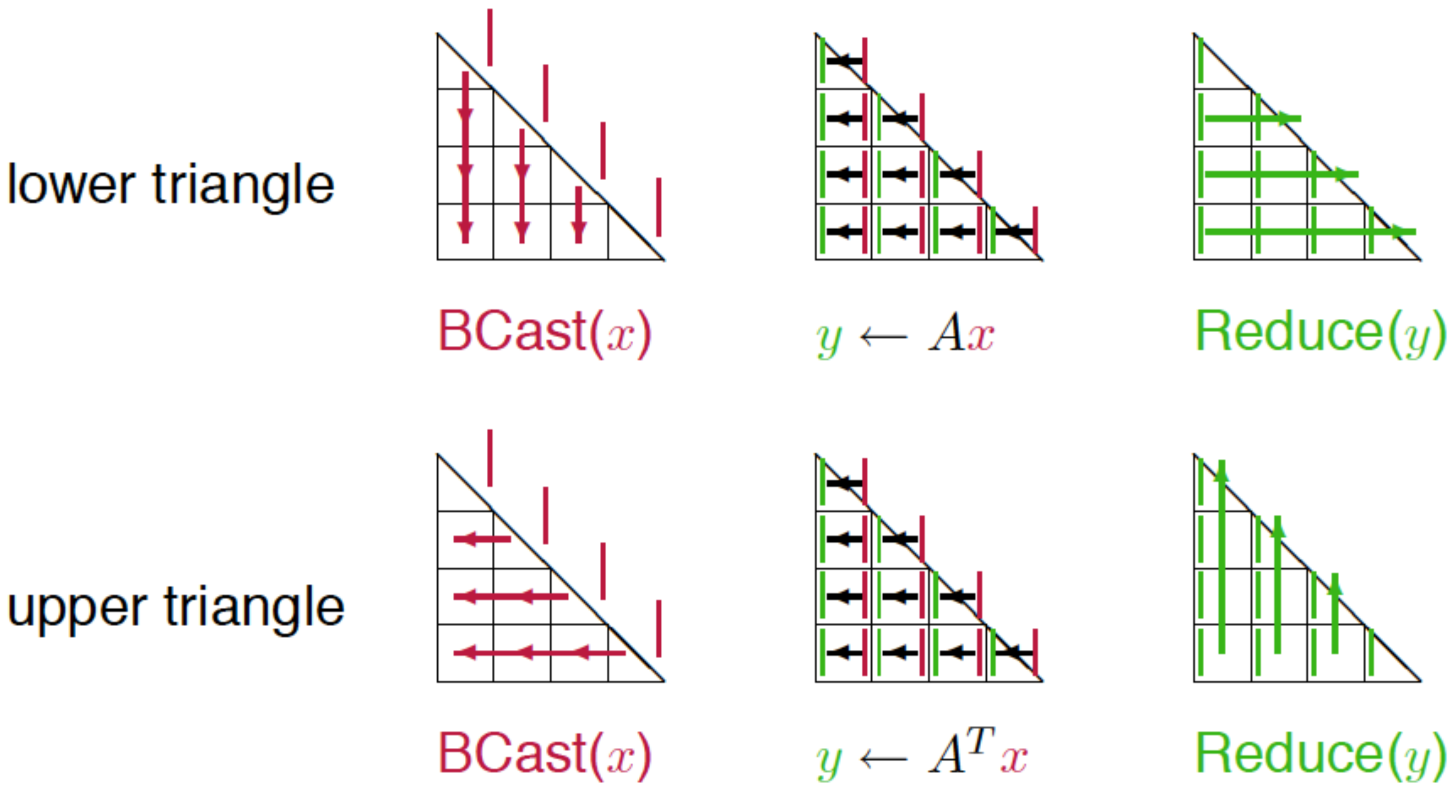
<u>Leading Algorithms Developed/Tested/Implemented/Published</u>

- Multi-level blocking algorithm for basis clustering
- Out-of-core eigensolver using on-node solid-state memory
- Overlap communications and computation within Lanczos
- Topology-aware mapping algorithm
- Extend nuclear physics techniques to relativistic quantum field theory
- Adapt matrix-matrix multiplies to GPUs for 3-nucleon transformations

<u>More than 20 jointly-authored publications to date on algorithms/code developments</u>

MFDn - Communication Topologies for matvec

- Store lower half of symmetric matrix, distributed over $n = d \cdot (d+1)/2$ processors with d "diagonal" proc's
- Communication pattern matrix-vector multiplication



Scalable Eigensolver for Many-Fermion Dynamics - nuclear (MFDn)

ASCR/NP – Applied Math/Computer Science Highlight

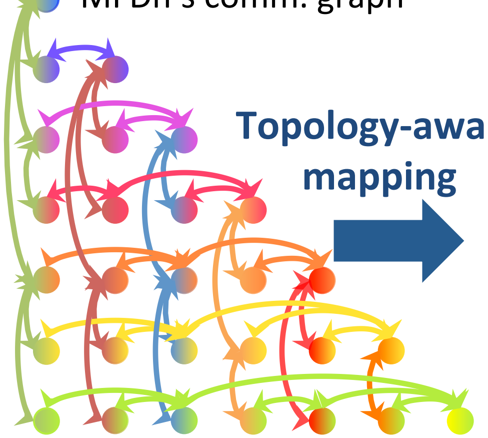
Objective

- Efficient and scalable iterative solvers for extreme-scale eigenvalue problems arising in nuclear physics (MFDn code)

Impact

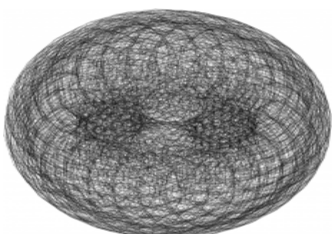
- Drastically reduced communication overheads
- Significant speed-ups over earlier version of MFDn (up to 6x on 18,000 cores)
- Almost perfect strong scaling on up to 260,000 cores on Jaguar

MFDn's comm. graph



Topology-aware mapping

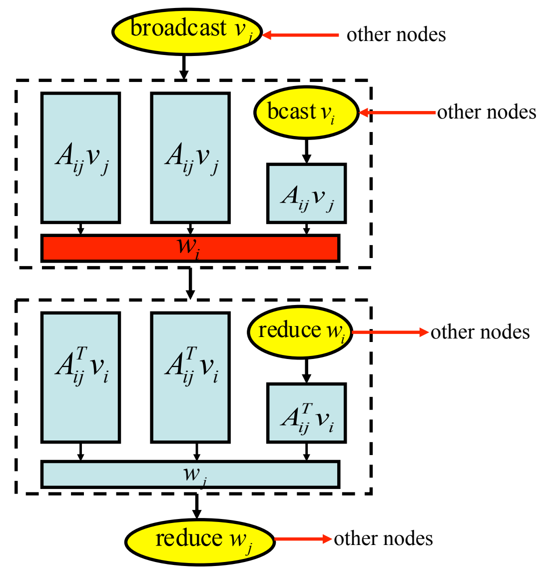
3D torus



Topology-aware mapping of processes to the physical processors becomes more important as the gap between computational power and bandwidth widens. Communication groups are optimized through a column-major ordering of processes on the triangular grid [1].

Communication Hiding

Flow-chart for multi-threaded SpMV computations during the eigensolve phase of MFDn. Expensive communications are overlapped with computations. Explicit communications are carried out over topology-optimized groups [2].



[1] H.M. Aktulga,C. Yang,P. Maris,J.P. Vary,E.G. Ng, “Topology-Aware Mappings for Large-Scale Eigenvalue Problems”, Euro-Par 2012 Conference
[2] H.M. Aktulga,C. Yang,E.G. Ng,P. Maris,J.P. Vary, "Improving the Scalability of a Symmetric Iterative Eigensolver for Multi-core Platforms”, CCP&E 25 (2013)

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FASTMATH

Phenomeological NN interaction: JISP16

JISP16 tuned up to ^{16}O

- Constructed to reproduce np scattering data
- Finite rank seperable potential in H.O. representation
- Nonlocal NN-only potential
- Use Phase-Equivalent Transformations (PET) to tune off-shell interaction to
  - binding energy of ^{3}H and ^{4}He
  - low-lying states of ^{6}Li (JISP6, precursor to JISP16)
  - binding energy of ^{16}O

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Physics Letters B 644 (2007) 33–37

PHYSICS LETTERS B

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Realistic nuclear Hamiltonian: Ab exitu approach

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[c] *Lawrence Livermore National Laboratory, L-414, 7000 East Avenue, Livermore, CA 94551, USA*
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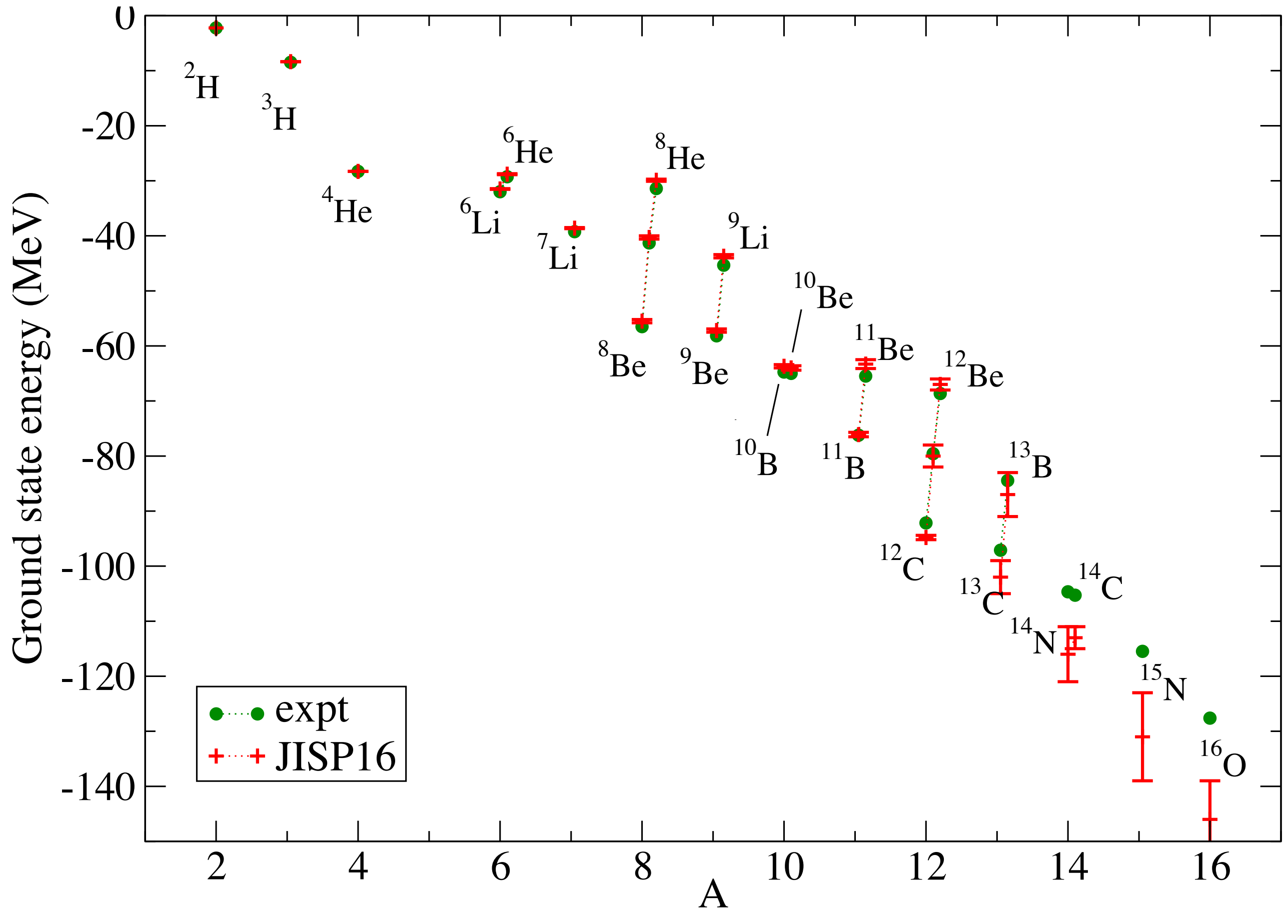
Received 6 March 2006; received in revised form 11 September 2006; accepted 30 October 2006

Ground state energy of p-shell nuclei with JISP16

Compare theory and experiment for 23 nuclei Maris, Vary, IJMPE22, 1330016 (2013)

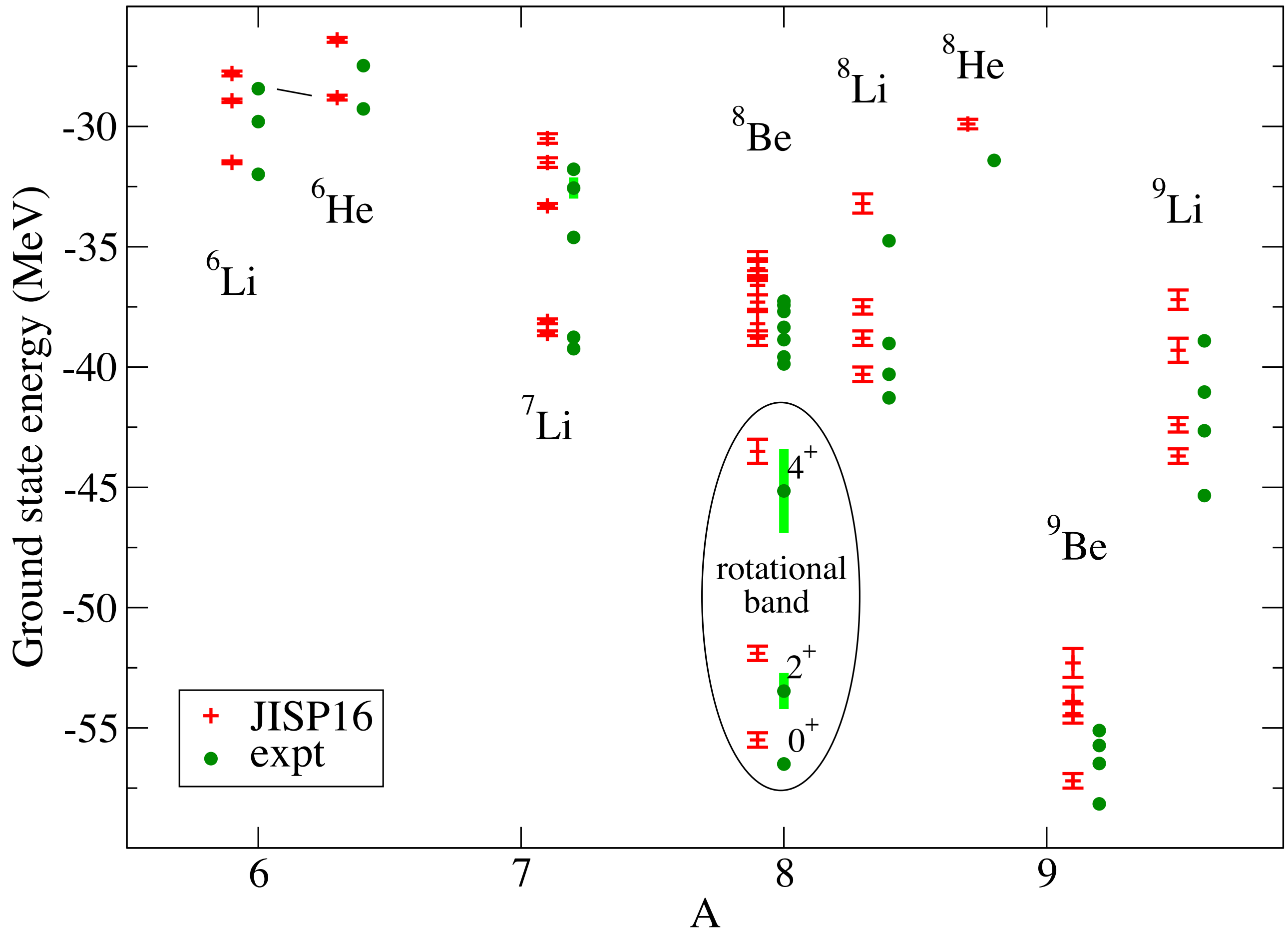


- ^{10}B – most likely JISP16 produces correct 3^{+} ground state, but extrapolation of 1^{+} states not reliable due to mixing of two 1^{+} states
- ^{11}Be – expt. observed parity inversion within error estimates of extrapolation
- ^{12}B and ^{12}N – unclear whether gs is 1^{+} or 2^{+} (expt. at $E_x = 1$ MeV) with JISP16

Energies of narrow A=6 to A=9 states with JISP16

Compare theory and experiment for 33 states

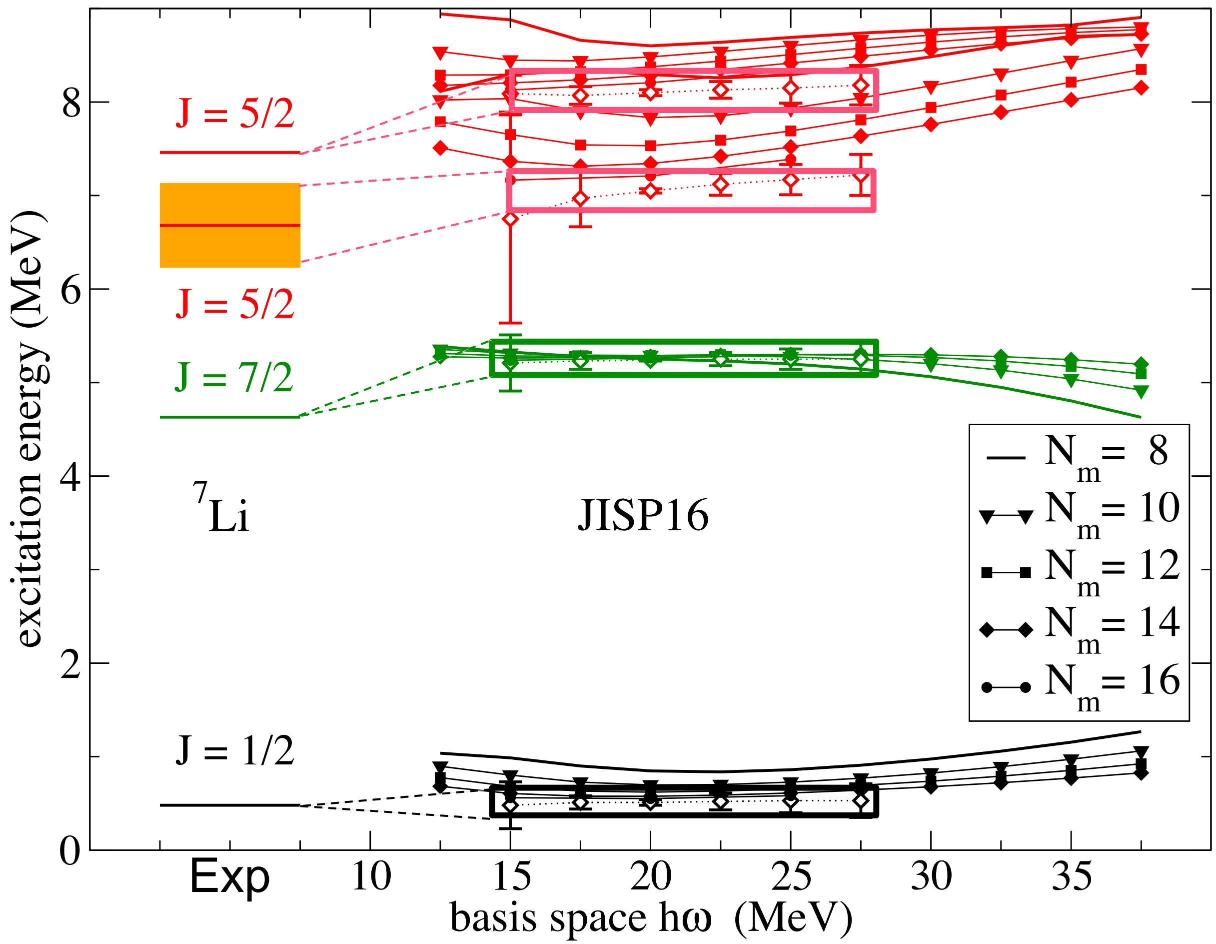
Maris, Vary, IJMPE22, 1330016 (2013)



- Excitation spectrum narrow states in good agreement with data

Excitation spectrum 7Li

Cockrell, Maris, Vary, PRC86 034325 (2012)



- Narrow states well converged, no extrapolation needed
- Broad resonances generally not as well converged; may need to incorporate continuum?

Physics Letters B 719, 179 (2013)

Contents lists available at SciVerse ScienceDirect

Physics Letters B

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Emergence of rotational bands in *ab initio* no-core configuration interaction calculations of light nuclei

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[b] Department of Physics and Astronomy, Iowa State University, Ames, IA 50011-3160, USA

Both natural and unnatural parity bands identified

Employed JISP16 interaction; N_{max} = 10 - 7

K=1/2 bands include Coriolis decoupling parameter:

$$E(J) = E_0 + A\left[J(J+1) + a(-)^{J+1/2}\left(J+\frac{1}{2}\right)\right],$$

$$Q(J) = \frac{3K^2 - J(J+1)}{(J+1)(2J+3)} Q_0,$$

$$B(E2; J_i \to J_f) = \frac{5}{16\pi}(J_i K 20 | J_f K)^2 (eQ_0)^2$$

Black line: Yrast band in collective model fit

Red line: excited band in collective model fit

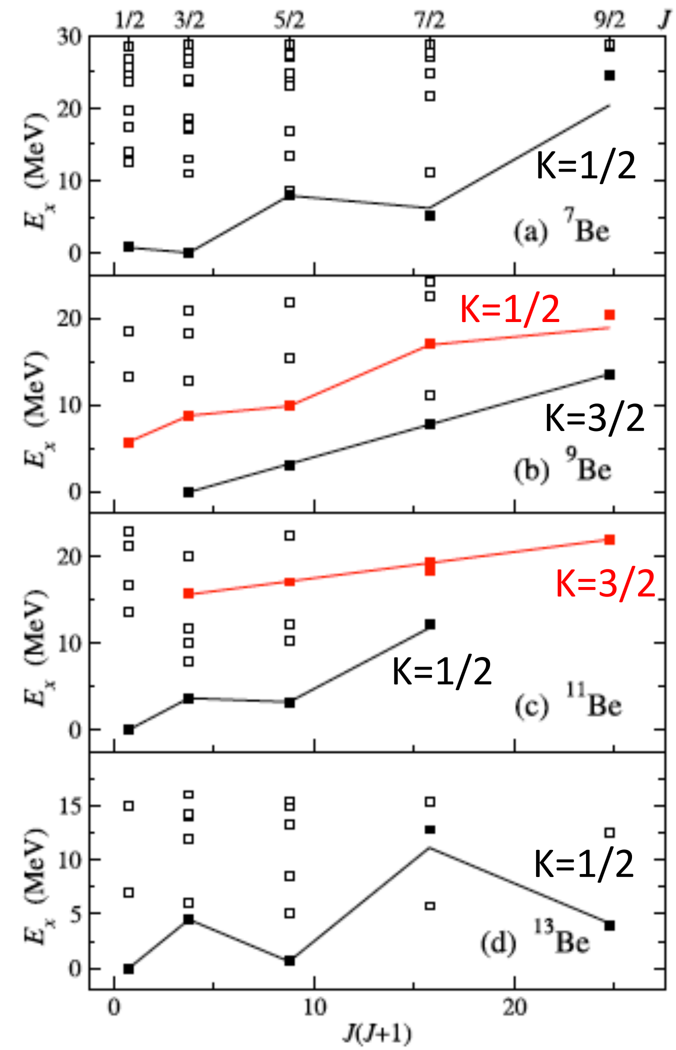
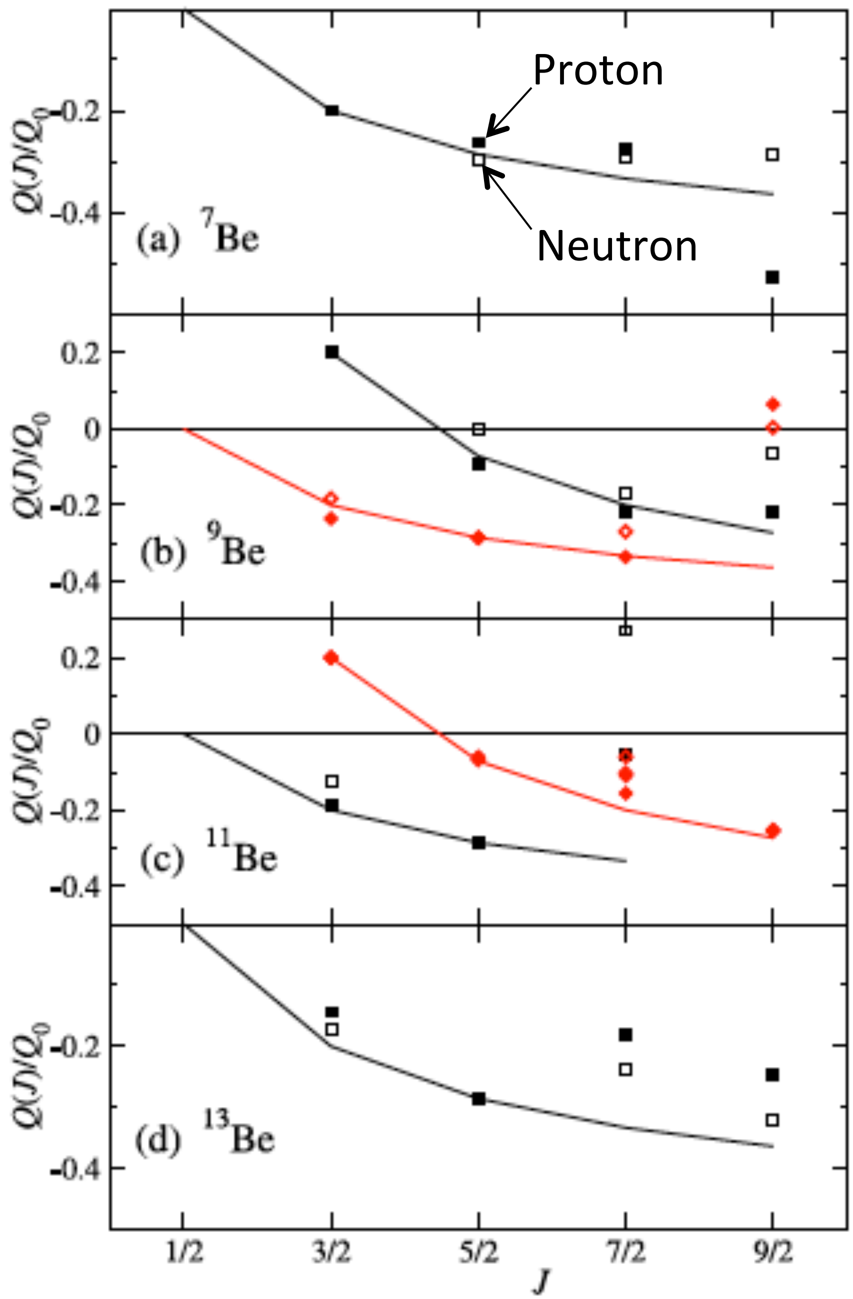


Fig. 1. Excitation energies obtained for states in the *natural* parity spaces of the odd-mass Be isotopes: (a) ^{7}Be, (b) ^{9}Be, (c) ^{11}Be, and (d) ^{13}Be. Energies are plotted with respect to $J(J+1)$ to facilitate identification of rotational energy patterns, while the J values themselves are indicated at top. Filled symbols indicate candidate rotational bandmembers (black for yrast states and red for excited states, in the web version of this Letter). The lines indicate the corresponding best fits for rotational energies. Where quadrupole transition strengths indicate significant two-state mixing (see text), more than one state of a given J is indicated as a bandmember.



Collective model:

$$Q(J) = \frac{3K^2 - J(J+1)}{(J+1)(2J+3)} Q_0,$$

Black line: Yrast band in collective model fit

Red line: excited band in collective model fit

Fig. 3. Quadrupole moments calculated for candidate bandmembers in the *natural* parity spaces of the odd-mass Be isotopes: (a) ^{7}Be, (b) ^{9}Be, (c) ^{11}Be, and (d) ^{13}Be. The states are as identified in Fig. 1 and are shown as black squares for yrast states or red diamonds for excited states (color in the web version of this Letter). Filled symbols indicate proton quadrupole moments, and open symbols indicate neutron quadrupole moments. The curves indicate the theoretical values for a $K = 1/2$ or $K = 3/2$ rotational band, as appropriate, given by (4). Quadrupole moments are normalized to Q_0, which is defined by either the $J = 3/2$ or $J = 5/2$ bandmember (see text).

Note:
Although Q, B(E2) are slowly converging, the ratios within a rotational band appear remarkably stable

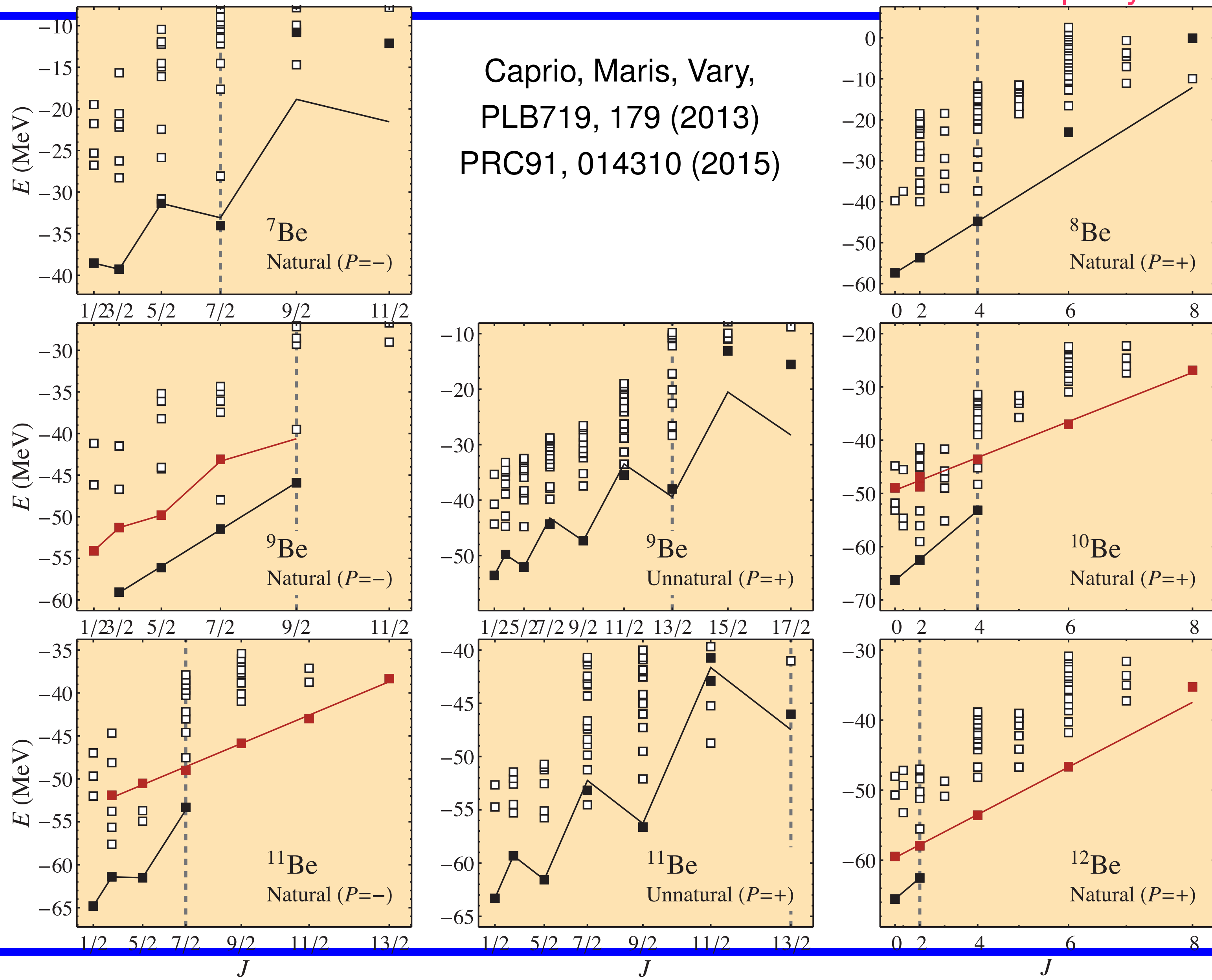
Next challenge: Investigate same phenomena with Chiral EFT interactions

M.A. Caprio, P. Maris and J.P. Vary, Physics Letters B 719, 179 (2013)

Candidate rotational bands: ^{7}Be–^{12}Be

Now include the even nuclei and consider both natural and unnatural parity bands

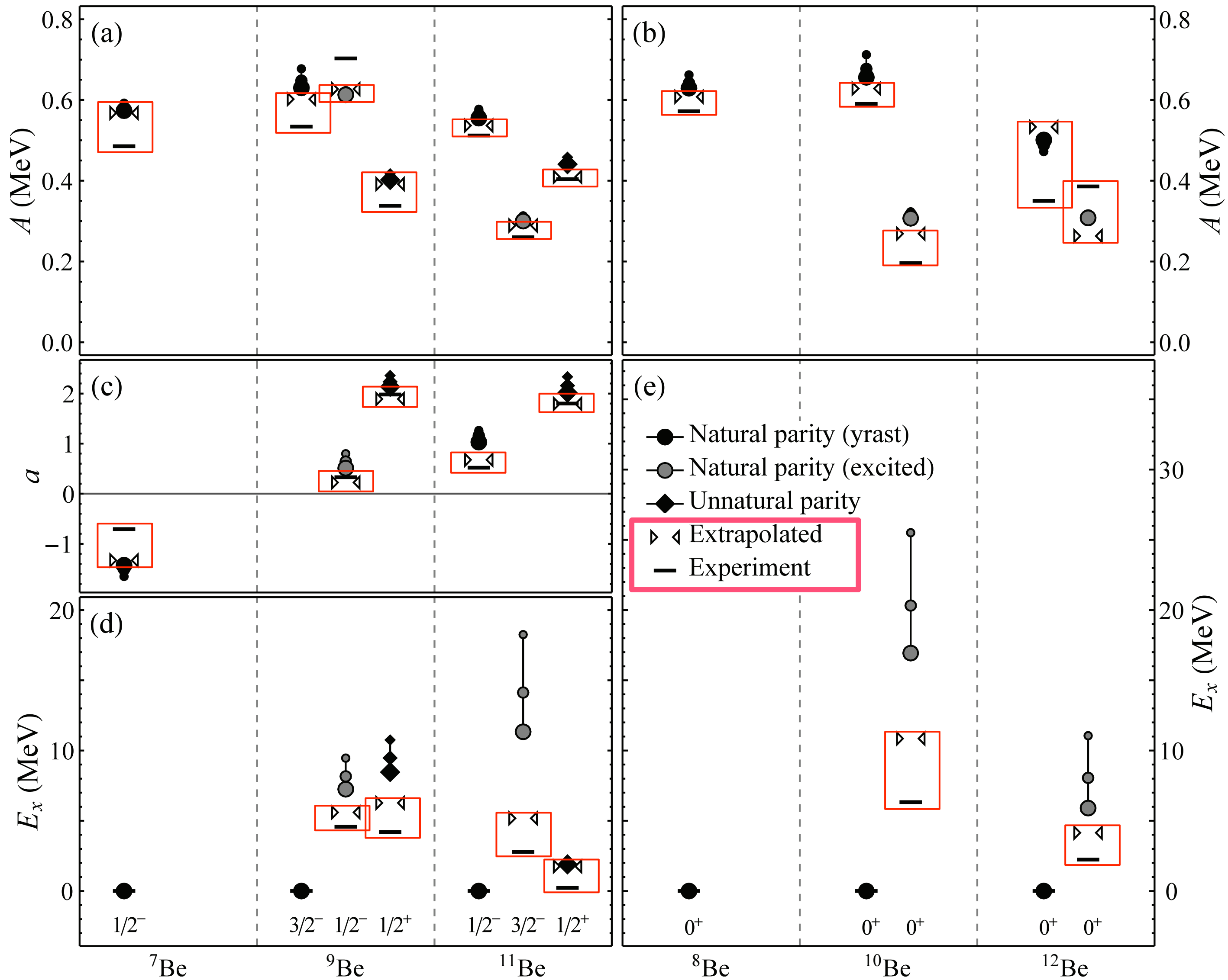
Caprio, Maris, Vary,
PLB719, 179 (2013)
PRC91, 014310 (2015)



Maris, Caprio and Vary, Phys. Rev. C91, 014310 (2015)

Comparison of rotational motion characteristics with experiment

red boxes highlight 23 collective motion observables in 6 Be isotopes

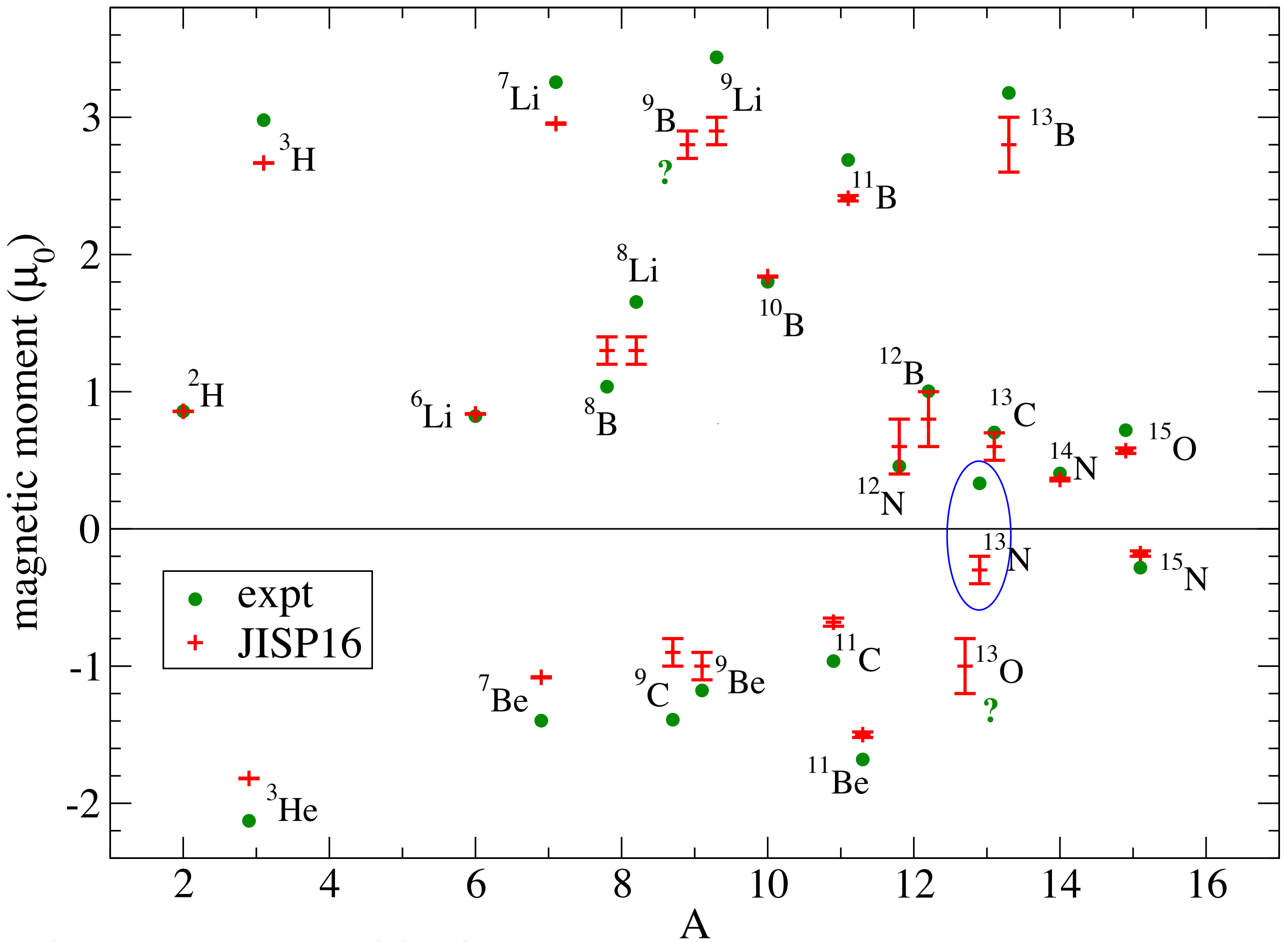


Caprio, Maris, Vary, Smith, arXiv: 1502.01083

Ground state magnetic moments with JISP16

Compare theory and experiment for 22 magnetic moments Maris, Vary, IJMPE22, 1330016 (2013)

$$\mu \quad = \quad \frac{1}{J+1}\Big(\langle \mathbf{J}\cdot\mathbf{L}_p\rangle + 5.586\langle \mathbf{J}\cdot\mathbf{S}_p\rangle - 3.826\langle \mathbf{J}\cdot\mathbf{S}_n\rangle\Big)\,\mu_0$$

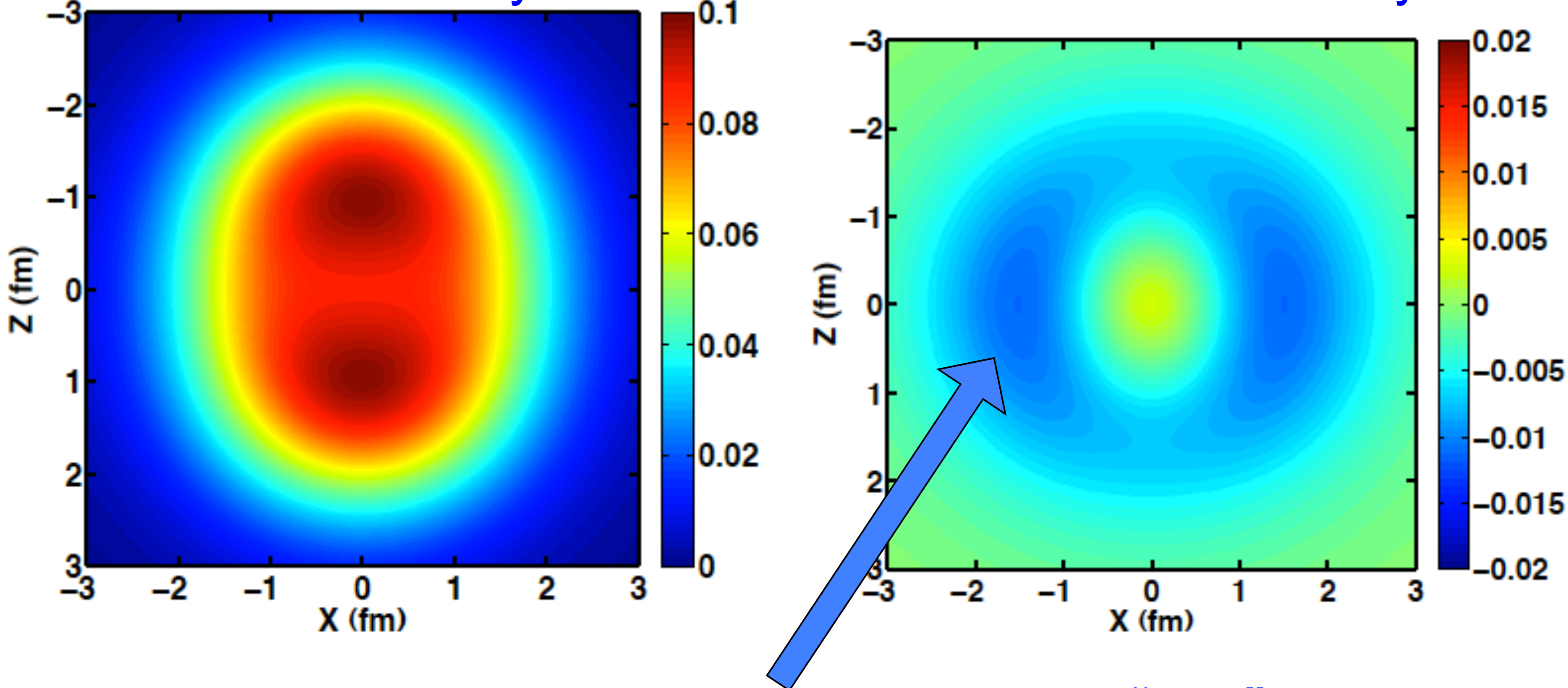


- Good agreement with data, given that we do not have any meson-exchange currents

9Be Translationally invariant gs density
Full 3D densities: rotate around the vertical axis

Total density

Proton-Neutron density



Shows that one neutron provides a “ring” cloud around two alpha clusters binding them together

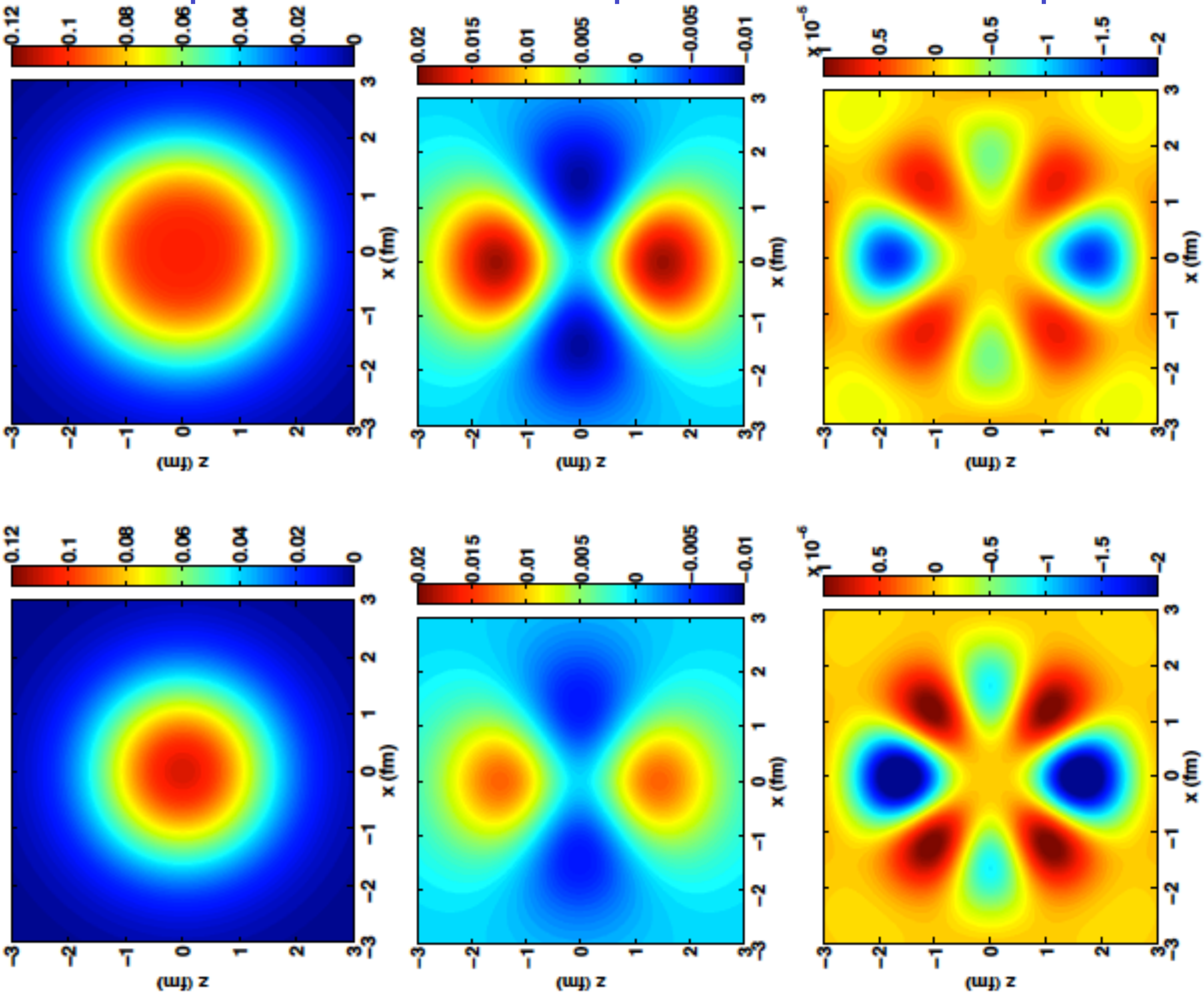
C. Cockrell, J.P. Vary, P. Maris, Phys. Rev. C 86, 034325 (2012); arXiv:1201.0724;
C. Cockrell, PhD, Iowa State University

^{8}Li gs
J=2

Monopole | Quadrupole | Hexadecapole

Neutrons

Protons



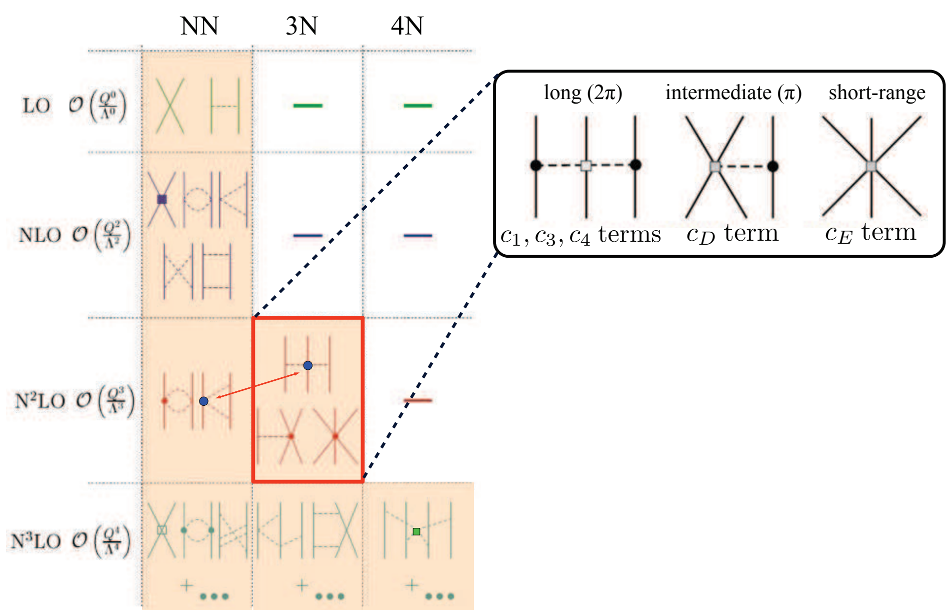
Nuclear interaction from chiral perturbation theory

- Strong interaction in principle calculable from QCD
- Use chiral perturbation theory to obtain effective A-body interaction from QCD Entem and Machleidt, PRC68, 041001 (2003)
  - controlled power series expansion in Q/Λ_χ with $\Lambda_\chi \sim 1$ GeV
  - natural hierarchy for many-body forces

$$V_{NN} \gg V_{NNN} \gg V_{NNNN}$$

  - in principle no free parameters
    - in practice a few undetermined parameters
  - renormalization necessary

Leading-order 3N forces in chiral EFT



Effective Hamiltonian in the NCSM
Okubo-Lee-Suzuki renormalization scheme

$$
\begin{array}{c|cc}
 & P & Q \\
\hline
P & H_{\text{eff}} & 0 \\
Q & 0 & QXHX^{-1}Q
\end{array}
$$

N_{max}

$$H: \quad E_1, E_2, E_3, \ldots E_{d_P}, \ldots E_\infty$$

$$H_{\text{eff}}: \quad E_1, E_2, E_3, \ldots E_{d_P}$$

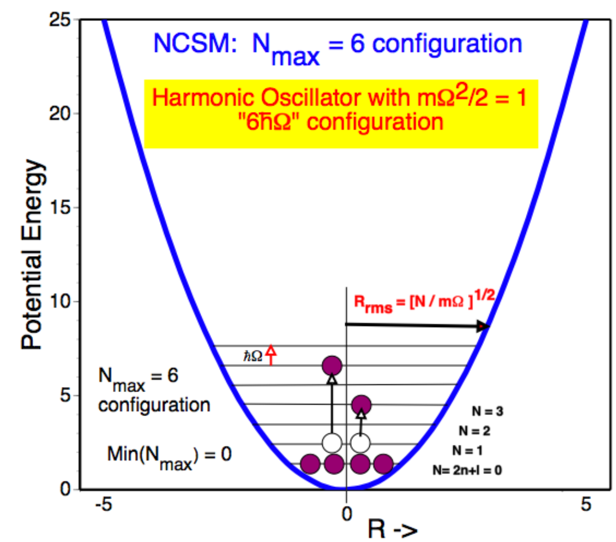
model space dimension

$$QXHX^{-1}P = 0$$

$$H_{\text{eff}} = PXHX^{-1}P$$

unitary $X = \exp[-\arctan h(\omega^+ - \omega)]$

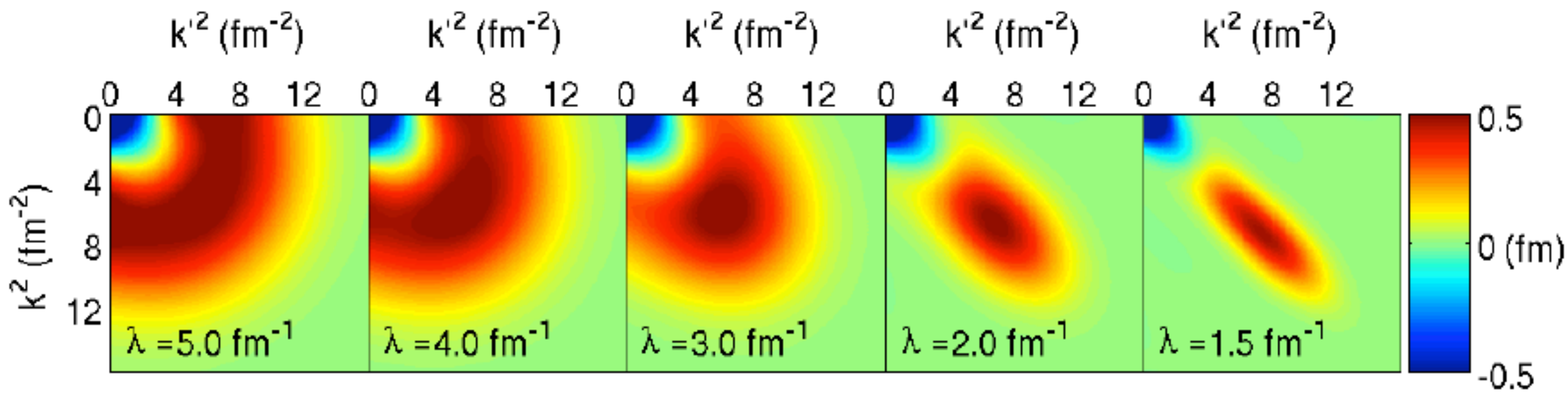
- n-body cluster approximation, $2 \le n \le A$
- $H^{(n)}_{\text{eff}}$ n-body operator
- Two ways of convergence:
  - For $P \rightarrow 1$ $\quad H^{(n)}_{\text{eff}} \rightarrow H$
  - For $n \rightarrow A$ and fixed P: $H^{(n)}_{\text{eff}} \rightarrow H_{\text{eff}}$



Adapted from Petr Navratil

Similarity Renormalization Group – NN interaction

- SRG evolution — Bogner, Furnstahl, Perry, PRC 75 (2007) 061001



  - drives interaction towards band-diagonal structure
  - SRG shifts strength between 2-body and many-body forces
- Initial chiral EFT Hamiltonian
  power-counting hierarchy A-body forces

$$V_{NN} \gg V_{NNN} \gg V_{NNNN}$$

Both OLS and SRG derivations of H_{eff} are used extensively in applications

Compare ^{7}Li observables evaluated using OLS versus SRG

Table 4

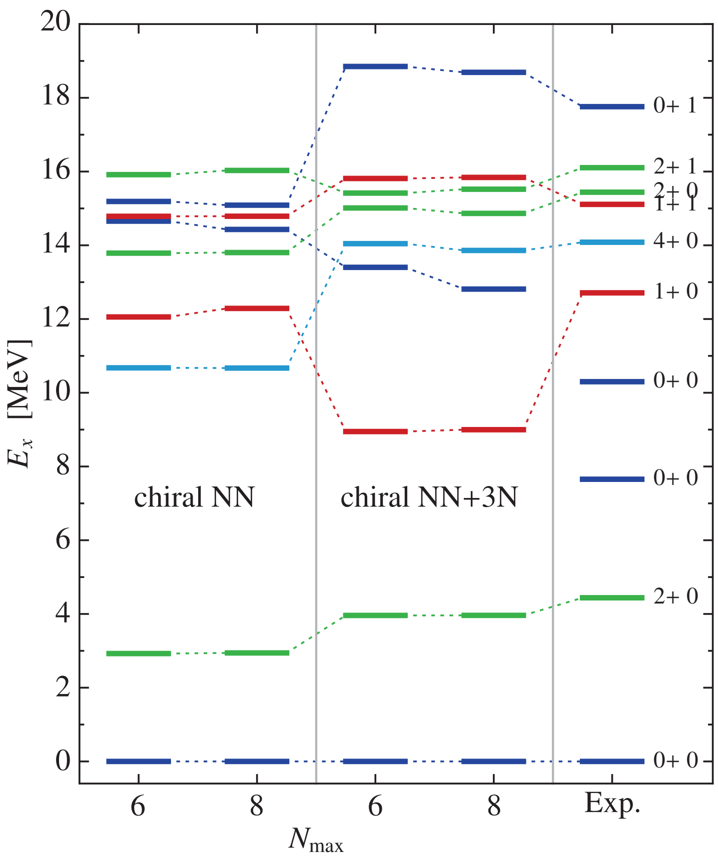
Comparison of ^{7}Li observables between experiment [155–157] and theory. The OLS results with Chiral $NN + NNN$ are calculated at $\hbar\Omega = 13$ MeV in the NCSM up through $N_{\max} = 8$ [153]. The SRG results ($\alpha = 0.08$) with Chiral $NN + NNN$ for $N_{\max} = 8$; 10 calculated at $\hbar\Omega = 16$MeV in the IT-NCSM are reported in Ref. [158]. Results up through $N_{\max} = 14$ with JISP16 [107–109] obtained in the NCFC approach are reported in Ref. [159]. AV18/IL2 results are obtained in the GFMC approach as reported in Refs. [1–4]. The energies are in MeV; the g.s. RMS point-proton radius ($\langle r^2_{pp}\rangle^{1/2}$) is in fm; the quadrupole moments (Q) are in e fm^2; the magnetic moments (μ) are in μ_N; the reduced B(E2) transition probabilities are in e^{2}fm^4; and the reduced B(M1) transition probabilities are in μ_N^2. All listed transitions are to the ground state. The energies with JISP16 are obtained from extrapolations to the infinite basis space, and the magnetic dipole observables are nearly converged, with error estimates as discussed in Ref. [159] (two errors are quoted based on separate methods of estimating the error for excitation energies); the RMS point-proton radius and electric quadrupole observables are evaluated at $\hbar\Omega = 12.5$ MeV with JISP16. The AV18/IL2 results include meson-exchange corrections for the dipole observables (e.g. these corrections change the g.s. magnetic moment from $\approx 2.9\ \mu_N$ to $\approx 3.2\ \mu_N$); CD-Bonn ("CD-B") and INOY results are NCSM results from Refs. [136,163] calculated at $N_{\max} = 12$ and $\hbar\Omega = 11$, 12 and 16 MeV respectively, with the INOY gs energy extrapolated to the infinite basis space.

^{7}Li	Expt.	Chiral $NN + NNN$ Okubo–Lee–Suzuki	Chiral $NN + NNN$ SRG(0.08) $N_{\max} = 8$; 10	AV18/IL2	JISP16	INOY	CD-B
$E_b(\frac{3}{2}^-_1\frac{1}{2})$	39.244	38.60(44)	38.14(1) ; 38.90(2)	38.9(1)	38.57(4)	39.6(4)	35.56
$\langle r^2_{pp}\rangle^{1/2}$	2.30(5)	2.11		2.25(1)	2.2	2.05	2.22
$E_x(\frac{1}{2}^-_1\frac{1}{2})$	0.477	0.382(69;24)	0.332(3) ; 0.312(2)	0.2(1)	0.52(6)	0.51	0.29
$E_x(\frac{7}{2}^-_1\frac{1}{2})$	4.630(1)	5.20(22;12)	4.983(2) ; 4.980(9)	4.9(1)	5.25(5)	5.35	5.49
$E_x(\frac{5}{2}^-_1\frac{1}{2})$	6.680(50)	7.50(16;23)	7.135(9) ; 6.992(10)	6.6(1)	7.1(2)	7.66	7.00
$E_x(\frac{5}{2}^-_2\frac{1}{2})$	7.460(10)	8.31(01;17)	8.063(5) ; 7.981(15)	7.2(1)	8.1(1)	8.65	8.25
$E_x(\frac{3}{2}^-_2\frac{1}{2})$	8.75	10.43(44;28)	10.080(5) ; 9.800(17)			11.27	9.85
$E_x(\frac{1}{2}^-_2\frac{1}{2})$	9.09	11.18(47;33)				11.93	10.46
$E_x(\frac{7}{2}^-_2\frac{1}{2})$	9.57	11.28(24;29)				11.69	11.03
$E_x(\frac{3}{2}^-_1\frac{3}{2})$	11.24	12.46(18;28)				12.83	11.97
$Q(\frac{3}{2}^-)$	−4.06(8)	−2.75	−2.79(4) ; −3.15(8)	−3.6(1)	−3.2	−2.79	−3.20
$Q(\frac{7}{2}^-)$	–	−4.10	−4.19(2) ; −4.46(3)		−5.0		
$Q(\frac{5}{2}^-_1)$	–	−4.28	−4.36(3) ; −4.75(5)		−6.0		
$Q(\frac{5}{2}^-_2)$	–	1.76	1.88(1) ; 1.89(2)		2.3		
$\mu(\frac{3}{2}^-)$	3.256	2.993	2.95(6) ; 3.22(11)	3.168(13)	2.954(5)	3.02	3.01
$\mu(\frac{1}{2}^-)$	–	−0.79	−0.78(2) ; −0.87(4)		−0.76(1)		
$\mu(\frac{7}{2}^-)$	–	3.30	3.33(2) ; 3.41(7)		3.3(1)		
$\mu(\frac{5}{2}^-_1)$	–	−0.98	−0.99(2) ; −1.01(4)		−0.90(2)		
$\mu(\frac{5}{2}^-_2)$	–	−0.38	−0.37(1) ; −0.38(2)		−0.39(5)		
B(E2; $\frac{1}{2}^-$)	15.7(10)	7.30	7.81(9) ; 8.49(12)	16.2(5)	10.2		
B(E2; $\frac{7}{2}^-$)	3.4	3.4	3.67(4) ; 4.14(5)	9.92(14)	5.1		
B(E2; $\frac{5}{2}^-_1$)	–	0.91	0.98(5) ; 1.46(9)		1.5		
B(E2; $\frac{5}{2}^-_2$)	–	0.05	0.05(1) ; 0.04(1)		<0.1		
B(M1; $\frac{1}{2}^-$)	4.92(25)	4.07	4.15(2) ; 4.01(5)	4.92(7)	3.89(2)	4.10	4.13
B(M1; $\frac{5}{2}^-_1$)	–	0.004	0.004(1); 0.004(1)		0.002(1)		
B(M1; $\frac{5}{2}^-_2$)	–	0.043	0.037(1); 0.032(1)		0.02(1)		

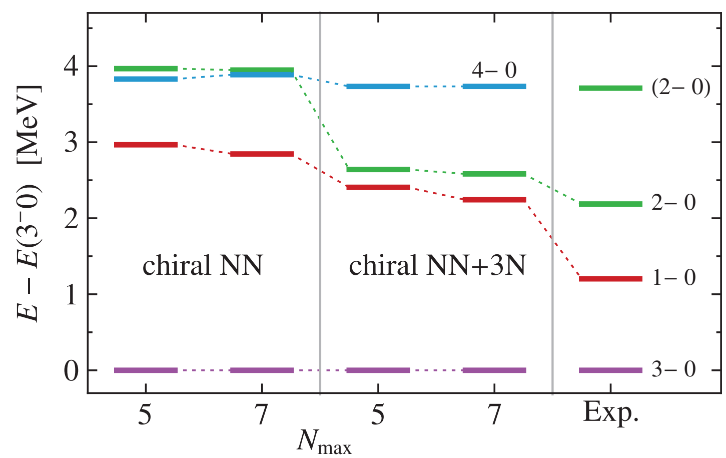
Spectrum of ^{12}C

at SRG parameter $\lambda = 2.0$ fm^{-1} and $\hbar\omega = 20$ MeV

Maris, Vary, Calci, Langhammer, Binder, Roth, Phys. Rev. C90, 014314 (2014)



- chiral NN at N^{3}LO
- chiral 3N at N^{2}LO
- 3N LEC values:
  $c_D = -0.2,\ c_E = -0.205$
- 500 MeV cutoff



- Excitation energies $(1^+, 0)$ and $(0^+, 1)$ sensitive to 3NF
- Negative parity spectrum relative to lowest $(3^-, 0)$ reasonably well converged, and 3NF improves agreement with experiment

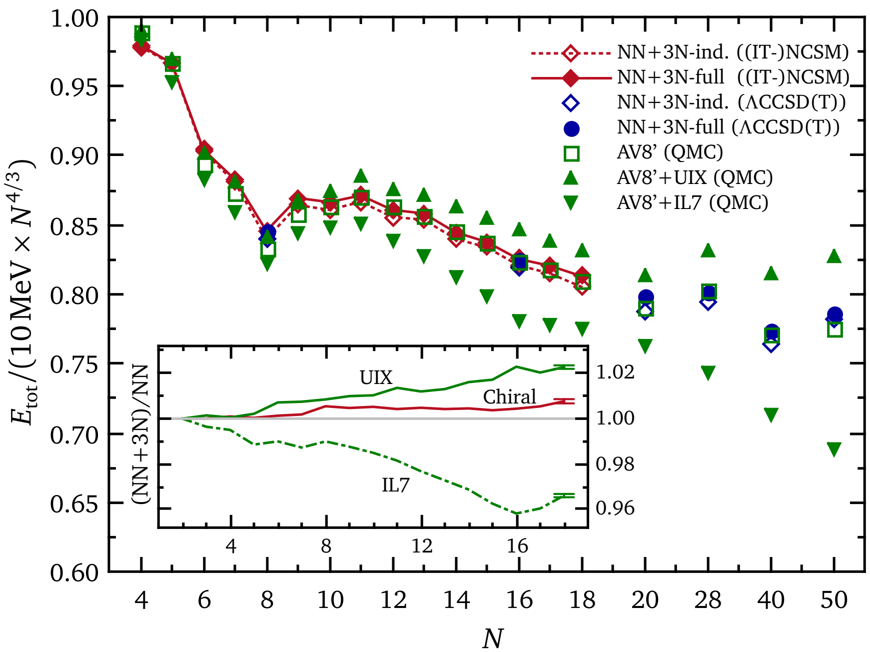
Ab initio Extreme Neutron Matter

Objectives

- Predict properties of neutron-rich systems which relate to exotic nuclei and nuclear astrophysics
- Determine how well high-precision phenomenological strong interactions compare with effective field theory based on QCD
- Produce accurate predictions with quantified uncertainties

Impact

- Improve nuclear energy density functionals used in extensive applications such as fission calculations
- Demonstrate the predictive power of *ab initio* nuclear theory for exotic nuclei with quantified uncertainties
- Guide future experiments at DOE-sponsored rare isotope production facilities



Comparison of ground state energies of systems with N neutrons trapped in a harmonic oscillator with strength 10 MeV. Solid red diamonds and blue dots signify new results with two-nucleon (NN) plus three-nucleon (3N) interactions derived from chiral effective field theory related to QCD. Inset displays the ratio of NN+3N to NN alone for the different interactions. Note that with increasing N, the chiral predictions lie between results from different high-precision phenomenological interactions, i.e. between AV8'+UIX and AV8'+IL7.

Accomplishments

1. Demonstrates predictive power of *ab initio* nuclear structure theory.
2. Provides results for next generation nuclear energy density functionals
3. Leads to improved predictions for astrophysical reactions
4. Demonstrates that the role of three-nucleon (3N) interactions in extreme neutron systems is significantly weaker than predicted from high-precision phenomemological interactions

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NUCLEI Nuclear Computational Low-Energy Initiative

References: P. Maris, J.P. Vary, S. Gandolfi, J. Carlson, S.C. Pieper, Phys. Rev. C87, 054318 (2013); H. Potter, S. Fischer, P. Maris, J.P. Vary, S. Binder, A. Calci, J. Langhammer and R.Roth, arXiv:1406.1160;

Contact: jvary@iastate.edu

Reducing the basis dimension

- Symmetry-Adapted No-Core Shell Model

  Dytrych *et al*, PRL111, 252501 (2013)

- No-Core Monte-Carlo Shell Model

  Abe, Maris, Otsuka, Shimizu, Utsuno, Vary, PRC86, 054301 (2012)

  - based on FCI truncation, not on $N_{\max}$ truncation
  - reduce basis to (few) hundred highly optimized states
  - coupled-J basis
  - leads to small but dense matrix

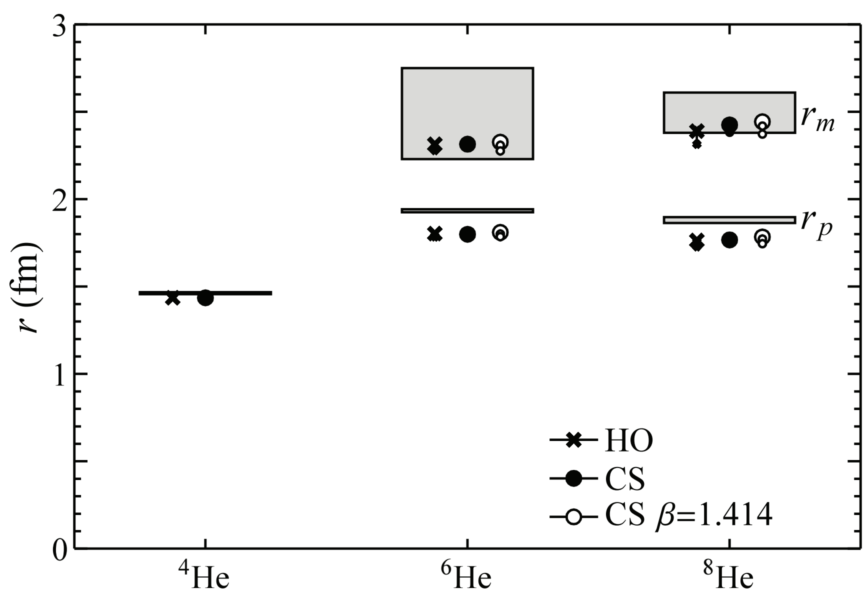
- Importance Truncated NCSM — Roth, PRC79, 064324 (2009)
  - based on $N_{\max}$ truncation
  - reduce basis dimension by (several) order(s) of magnitude
  - many-body states single Slater Determinants in M-scheme

Caveat: Uncertainty Quantification

- Can the numerical errors due to reduced basis dimension be quantified within the computational framework?

Radii of He isotopes with JISP16

Caprio, Maris, Vary, PRC90, 034305 (2014)



- Radii exctracted from crossover point for three highest $N_{\max}$ values
- HO and CS basis in good agreement with each other
- Qualitative agreement with data
- Note: matter radii in agreement with elastic scattering measurement/extraction of experimental radius

Future plans

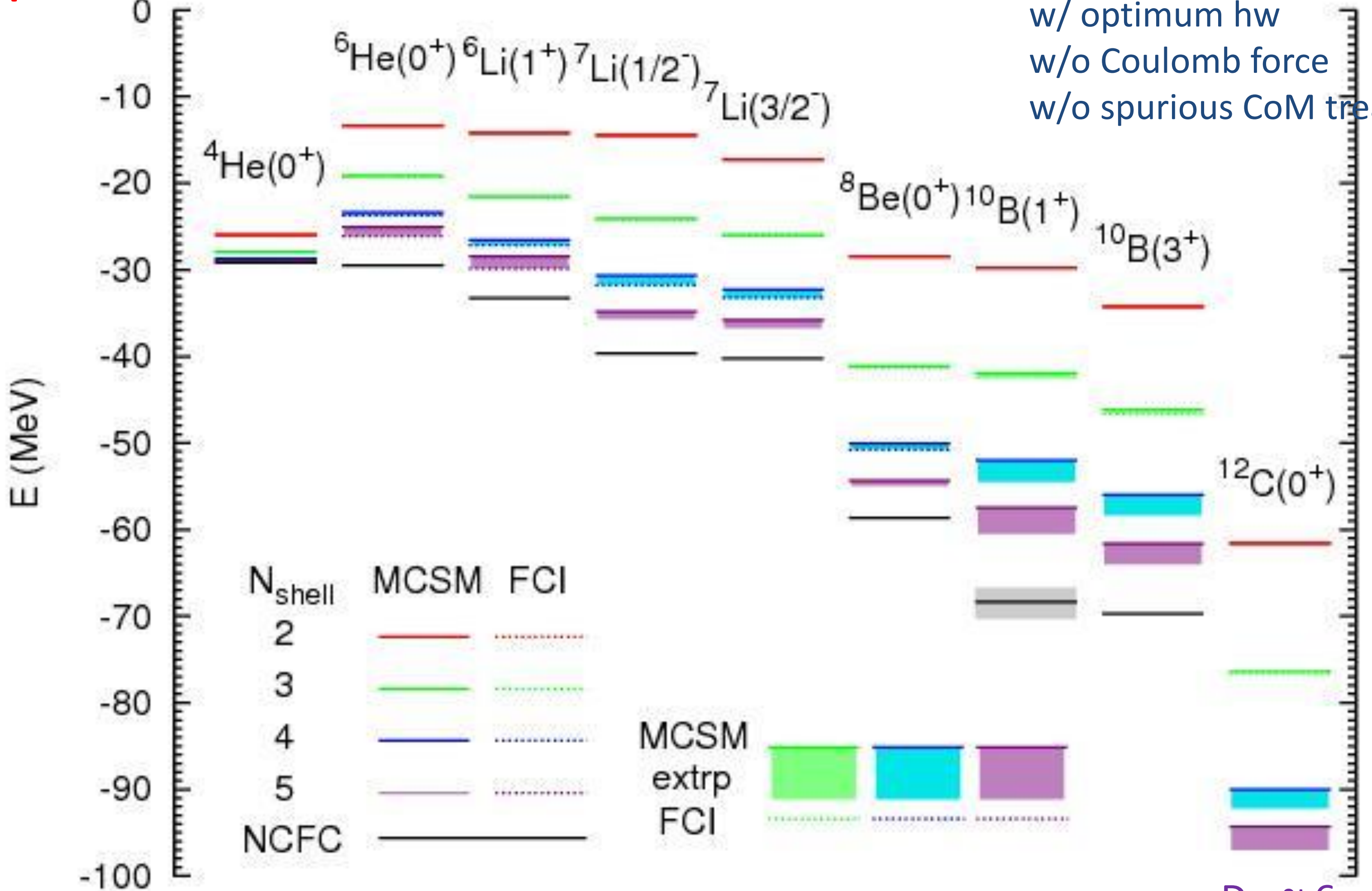
- Explore different basis truncation schemes
- Apply to chiral NN and 3N interactions

Energies of the Light Nuclei

Abe, Maris, Otsuka, Shimizu, Utsuno, Vary, EPJ Web of Conferences 66, 02001 (2014); NTSE-2014

K computer

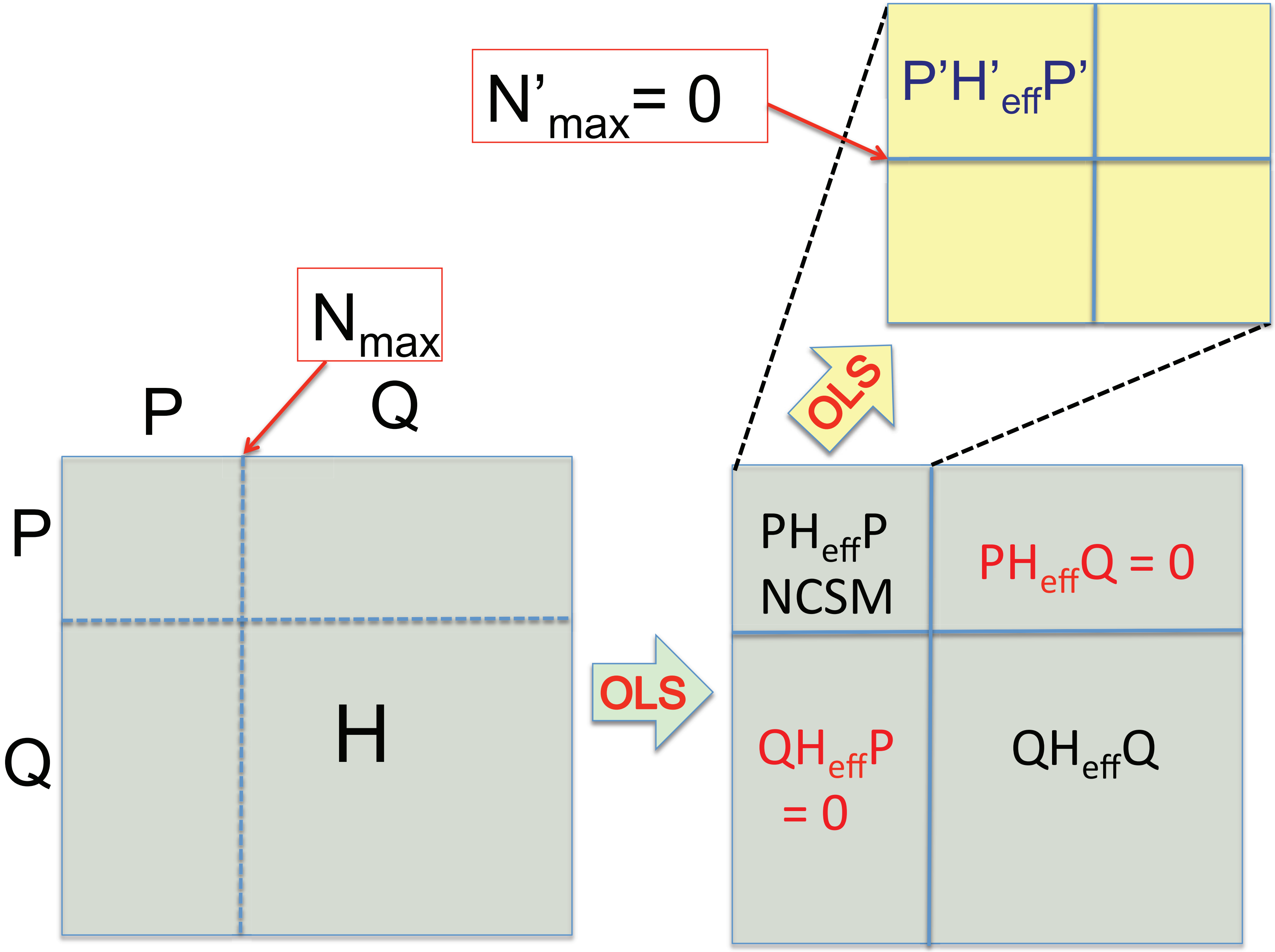
JISP16 NN int.
w/ optimum hw
w/o Coulomb force
w/o spurious CoM treatment



$D_M \sim 6 \times 10^{14}$

Some MCSM results are not reachable in the current FCI

Double OLS reduction of the basis to a "conventional" shell model valence space



Dikmen, Lisetskiy, Barrett, Maris, Shirokov, Vary, PRC accepted; arXiv 1502:00700

Effective interactions in *sd*-shell from *ab-initio* shell model with a core

PRC accepted: arXiv:1502.00700

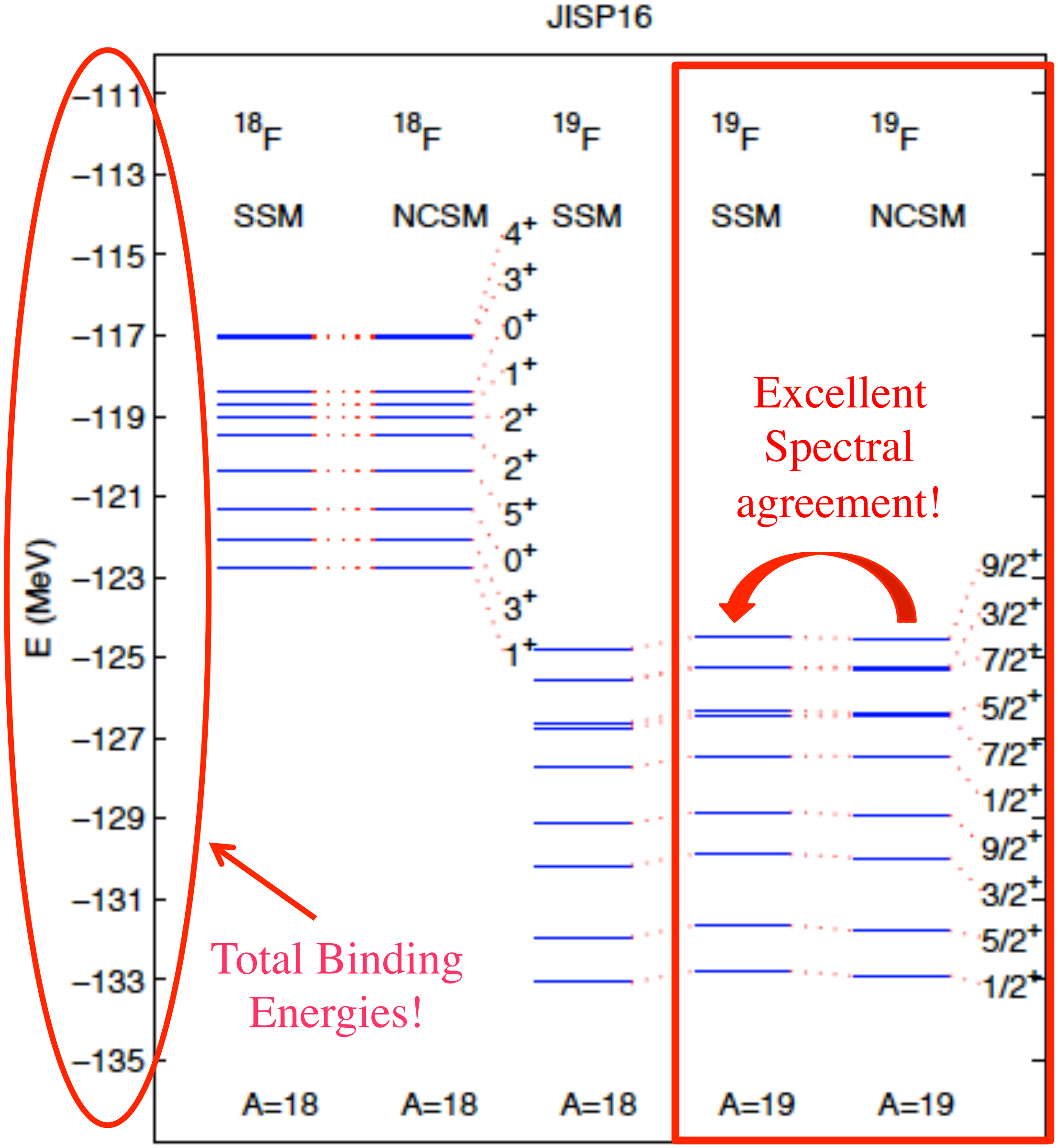
E. Dikmen,[1,2,*] A. F. Lisetskiy,[2,†] B. R. Barrett,[2] P. Maris,[3] A. M. Shirokov,[3,4,5] and J. P. Vary[3]

Aim: Regain valence-core separation but retain full ab initio NCSM

=> "Double OLS" Approach

Now extend to s-d shell the successful p-shell applications

p-shell application:
A. F. Lisetskiy, B. R. Barrett, M. K. G. Kruse, P. Navratil, I. Stetcu, J. P. Vary, Phys. Rev. C. 78, 044302 (2008); arXiv:0808.2187



Qualitative Benchmarks of Derived Single-Particle Energies

E. Dikmen, et al., Double OLS NCSM
hw = 14 MeV

TABLE II: Proton and neutron single-particle energies (in MeV) for JISP16 effective interaction obtained for the mass of $A = 18$ and $A = 19$.

	$A = 18$, $E_{\text{core}} = -115.529$			$A = 19$, $E_{\text{core}} = -115.319$		
j_i	$\frac{1}{2}$	$\frac{5}{2}$	$\frac{3}{2}$	$\frac{1}{2}$	$\frac{5}{2}$	$\frac{3}{2}$
$\epsilon^n_{j_i}$	-3.068	-2.270	6.262	-3.044	-2.248	6.289
$\epsilon^p_{j_i}$	0.603	1.398	9.748	0.627	1.419	9.774

TABLE III: Proton and neutron single-particle energies (in MeV) for chiral N3LO effective interaction obtained for the mass of $A = 18$ and $A = 19$.

	$A = 18$, $E_{\text{core}} = -118.469$			$A = 19$, $E_{\text{core}} = -118.306$		
j_i	$\frac{1}{2}$	$\frac{5}{2}$	$\frac{3}{2}$	$\frac{1}{2}$	$\frac{5}{2}$	$\frac{3}{2}$
$\epsilon^n_{j_i}$	-3.638	-3.042	3.763	-3.625	-3.031	3.770
$\epsilon^p_{j_i}$	0.044	0.690	7.299	0.057	0.700	7.307

H. Hergert, et al., IM-SRG
hw = 20 MeV
Chiral NN + 3N

	17	18	19	JISP16 19	N3LO 19
$\nu 1s_{1/2}$	-3.090	-3.055	-3.034	-3.044	-3.625
$\nu 0d_{3/2}$	2.940	2.973	2.991	6.289	3.770
$\nu 0d_{5/2}$	-4.643	-4.616	-4.606	-2.248	-3.031
$\pi 1s_{1/2}$	0.255	0.292	0.314	0.627	0.057
$\pi 0d_{3/2}$	6.035	6.071	6.093	9.774	7.307
$\pi 0d_{5/2}$	-0.909	-0.880	-0.869	1.419	0.700

Conclude:
S-orbits are comparable to within ~0.5 MeV
Spin-orbit splittings range: 6.5 – 8.5 MeV
Centroids of d-orbits differ by 1.5 – 2.5 MeV

Next Generation Ab Initio Structure Applications – Aim for Precision

Electroweak processes
Beyond the Standard Model tests (e.g. CKM unitarity => v_{ud} determination)
Neutrinoful and neutrinoless double beta-decay

Each puts major demands on theory, algorithms and computational resources
Growing demands => larger collaborating teams, growing computational resources,
Increase in the multi-disciplinary character, . . .

Calculation of three-body forces at N^{3}LO

Low
Energy
Nuclear
Physics
International
Collaboration

J. Golak, R. Skibinski, K. Tolponicki, H. Witala

E. Epelbaum, H. Krebs

A. Nogga

R. Furnstahl

S. Binder, A. Calci, K. Hebeler, J. Langhammer, R. Roth

P. Maris, J. Vary

H. Kamada

Goal

Calculate matrix elements of 3NF in a partial-wave decomposed form which is suitable for different few- and many-body frameworks

---

Challenge

Due to the large number of matrix elements, the calculation is extremely expensive.

Strategy

Develop an efficient code which allows to treat arbitrary local 3N interactions.
(Krebs and Hebeler)

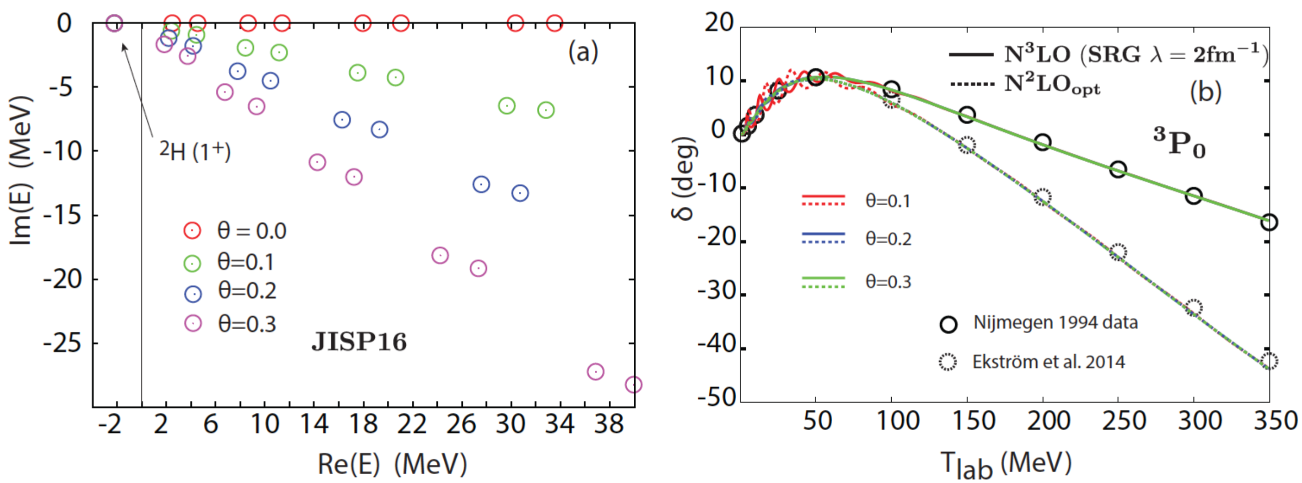
Nuclear Scattering Made Predictive and Convenient

Objectives

- Develop a convenient unified framework to solve nuclear structure and nuclear scattering using realistic nuclear interactions.
- Predict nuclear properties in the vicinity of the drip-lines where resonant states play critical roles.
- Leverage the increase of computing power and the new architectures at DOE-sponsored supercomputing facilities to achieve the efficient diagonalization of large complex symmetric matrices.

Impact

- Advances *ab initio* nuclear physics by implementing a powerful and convenient technique that will provide model independent predictions for structure and scattering properties.
- Use existing bound state many-body solvers and technology, developed for realistic two-nucleon and three-nucleon forces, to solve important scattering problems.
- Assess the quality of modern realistic nuclear forces in systems with high neutron to proton asymmetry and provide solid theoretical justification for new experiments.



(a) Distribution of eigenvalues of a Complex Scaled (CS) realistic JISP16 non-local interaction for the neutron-proton system. The deuteron bound state is invariant with respect to the rotation angle θ (indicated by the arrow) whereas continuum states are distinguished by their approximate 2θ trajectory. **(b)** Evaluation of the elastic scattering $^3P_0$ phase-shifts using CS chiral N^{3}LO and N^{2}LO$_{opt}$ interactions. The convergence of the phase-shifts as a function of the CS rotation parameter θ is rapid. Accurate scattering observables are predicted with calculations performed in a convenient Harmonic Oscillator basis.

Accomplishments

1. First application of Complex Scaling (CS) with realistic nuclear interactions.
2. First demonstration of the validity of ABC theorem for non-local interactions. The ABC theorem is the cornerstone of CS method.
3. Solved for elastic scattering phase-shifts using complex-energy solutions from non-local interactions in a Harmonic Oscillator basis
4. Opened the pathway for *ab initio* description of nuclear scattering with a natural ability to include three-nucleon interactions and without the complication of imposing boundary conditions.

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References: G. Papadimitriou and J.P. Vary, Phys. Rev. C Rapid Communications 91, 021001 (2015). arXiv:1412.0071

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3P1 Resonances (T=1)
Three different NN interactions

Physics Letters B 746 (2015) 121–126

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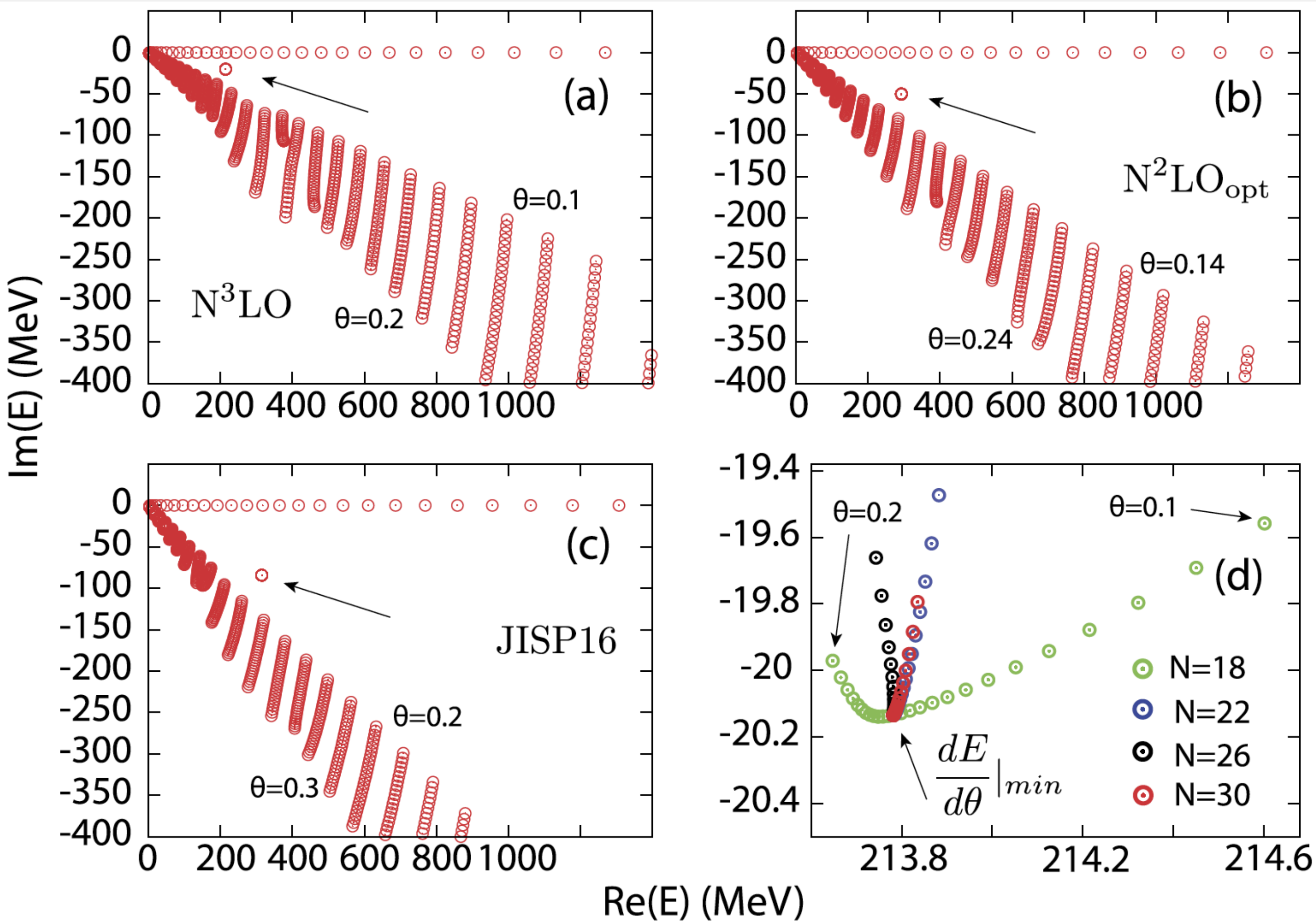
Nucleon–nucleon resonances at intermediate energies using a complex energy formalism

G. Papadimitriou*, J.P. Vary



Conclusions/Outlook

✧ Accomplishments include emergent phenomena & predictive power

✧ Impressive recent progress in deriving NN and NNN interactions with Chiral EFT

✧ Much work needs to be done to improve upon these interactions, the corresponding electroweak observables and the many-body approaches to fully exploit the discovery potential

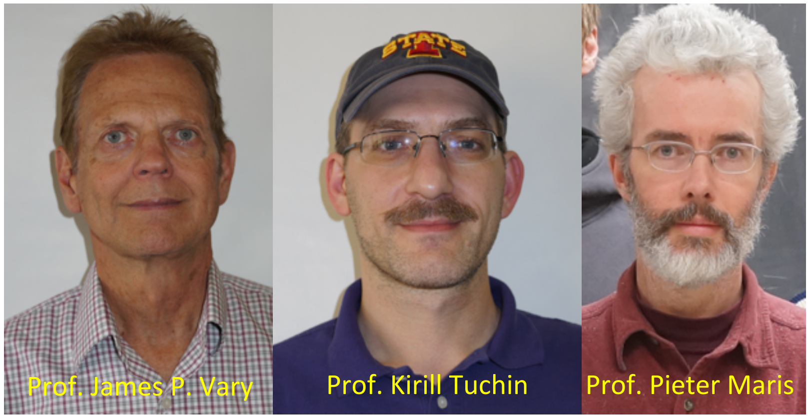
✧ Collaborations of Chiral EFT theorists and ab-initio many-body theorists underway to improve the properties of the Chiral EFT interactions (LENPIC)

✧ Collaborations of nuclear theorists with computer scientists and applied mathematicians must continue to overcome challenges

✧ Increasing computational resources needed (3NFs, 4NFs are major challenges)

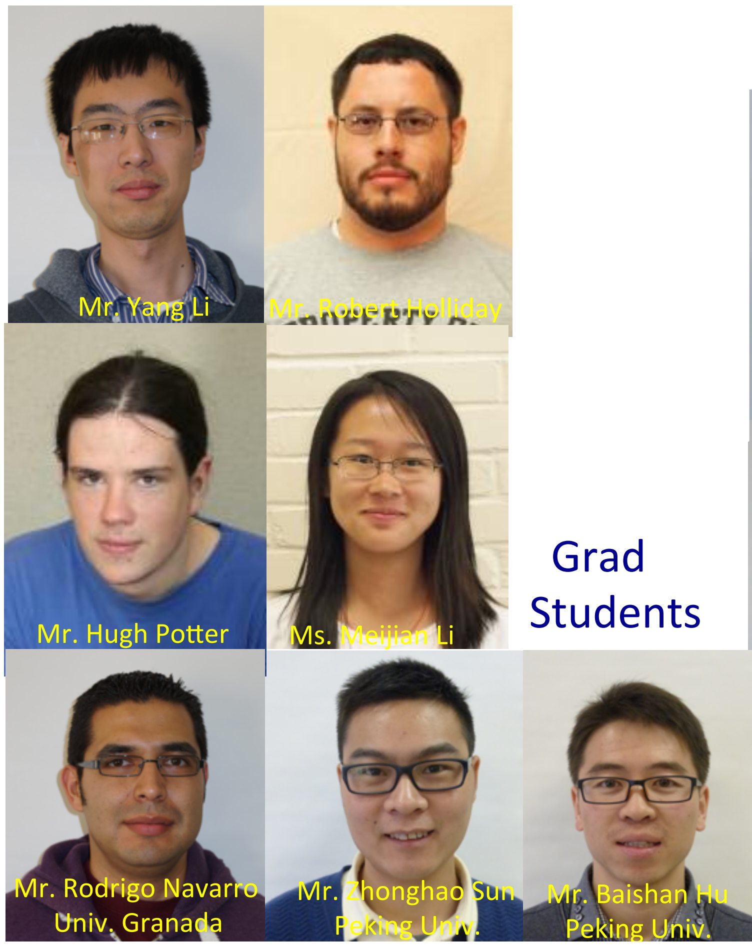
Iowa State University Nuclear Theory Group Fall 2014 & Spring 2015

Faculty



Scientist/Lecturer

Scientist (ret)



Grad Students

Visiting Faculty

Postdocs