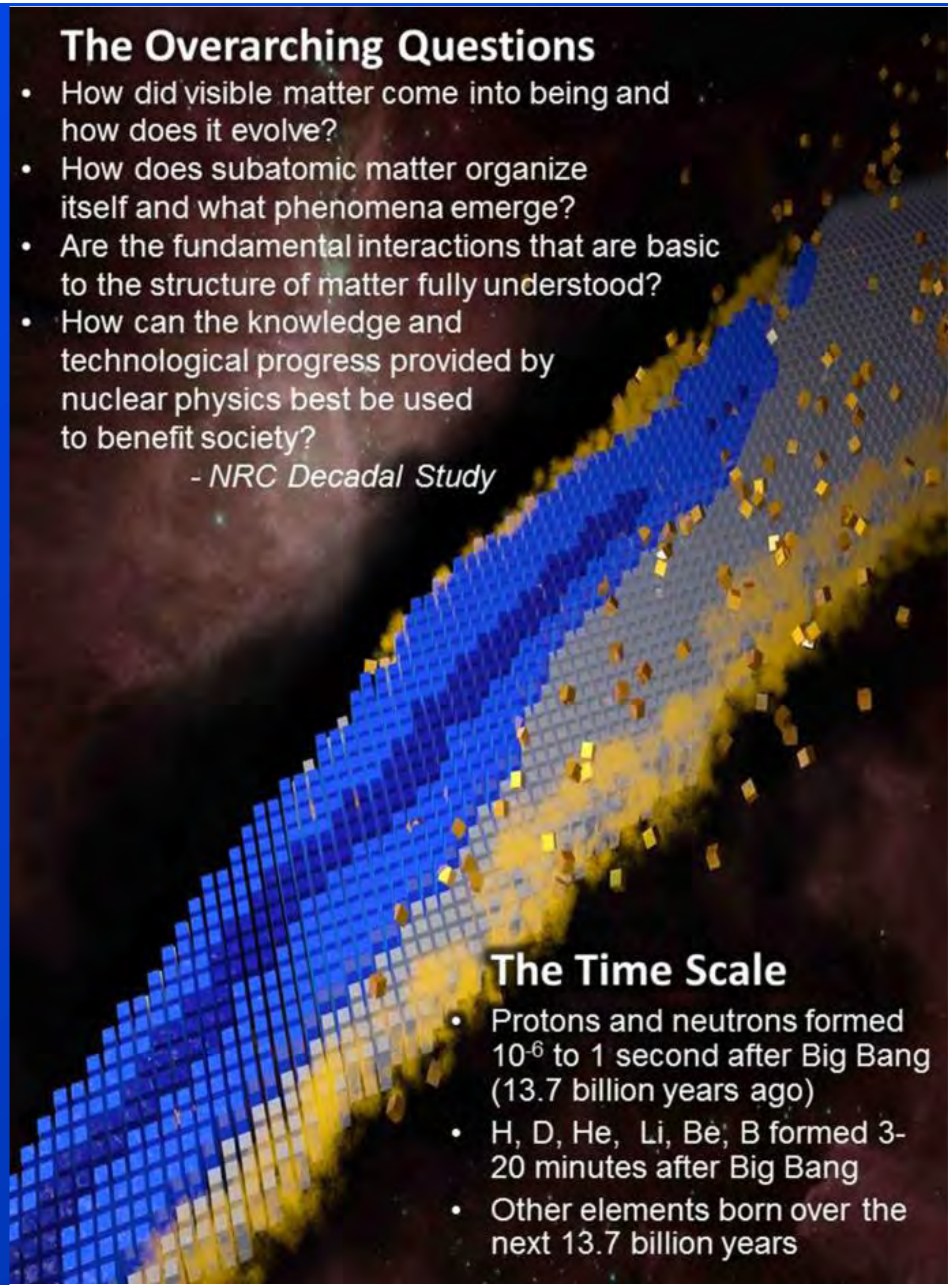
Development and Applications of the ab initio No-Core Shell Model

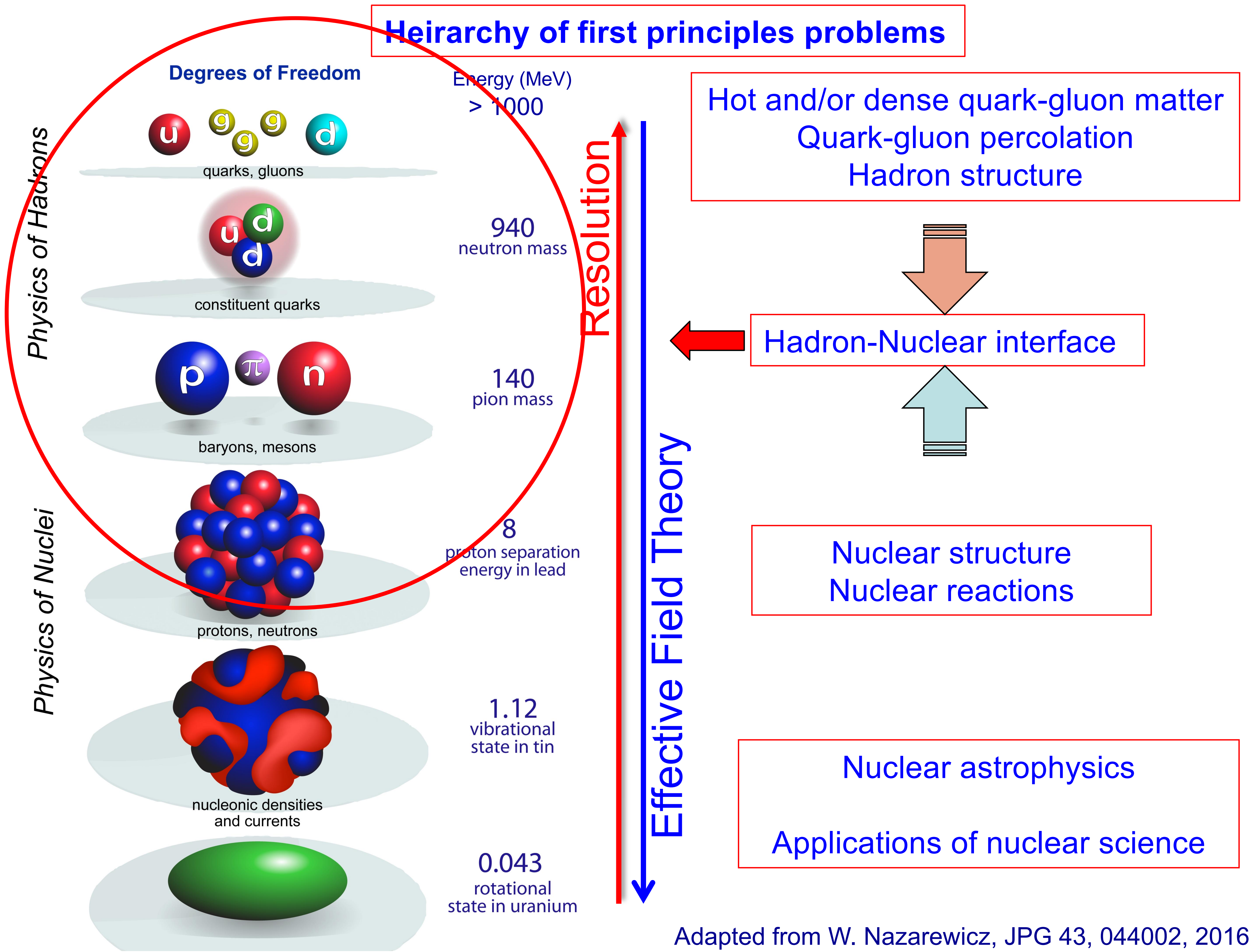
James P. Vary
Iowa State University

Symposium in Honor of the 75^{th} Anniversary of the Shell Model

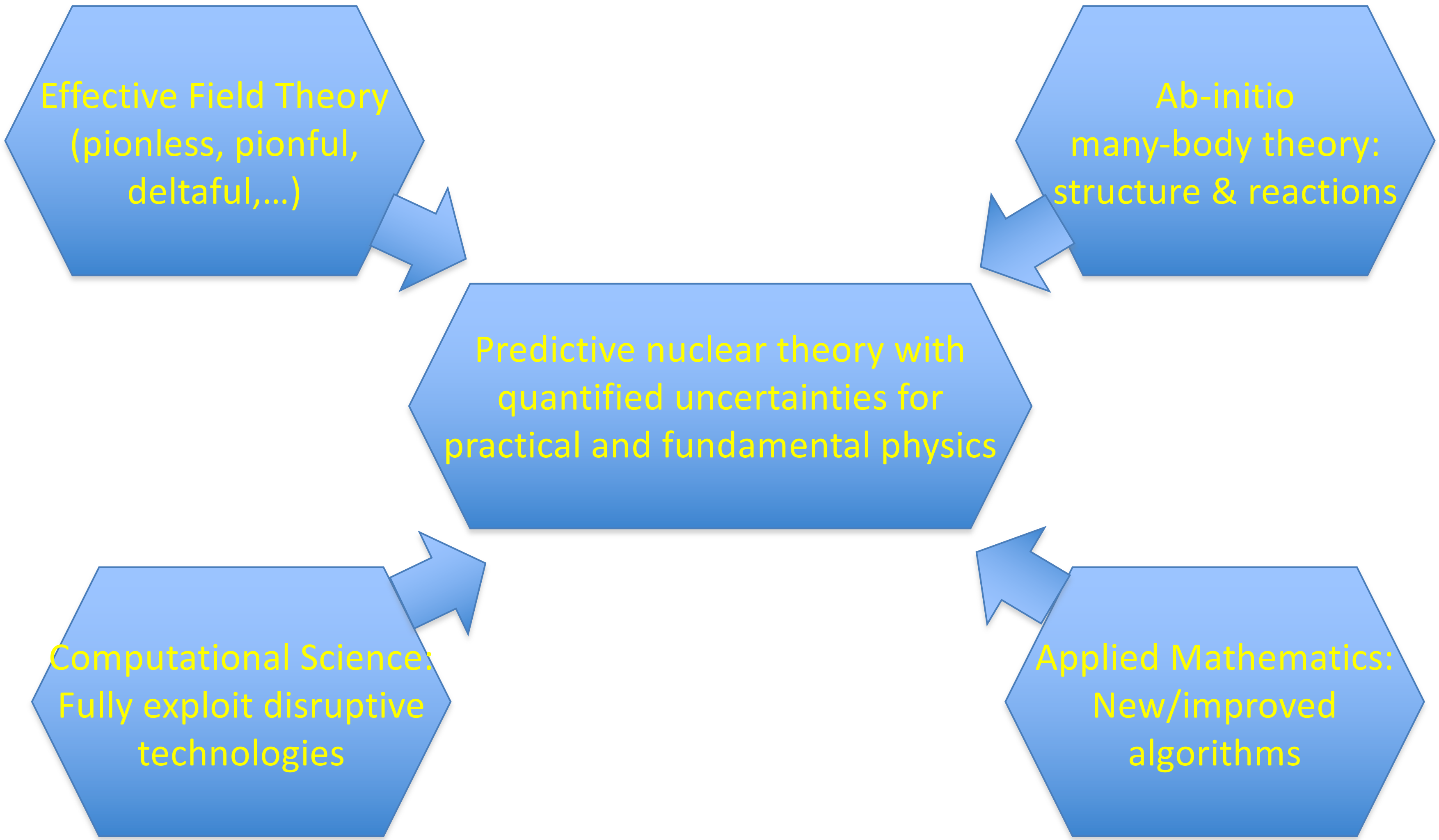
Argonne National Lab

July 19-21, 2024





Heirarchy of first principles problems
Degrees of Freedom
Energy (MeV)
> 1000
quarks, gluons
940
neutron mass
constituent quarks
140
pion mass
baryons, mesons
8
proton separation energy in lead
protons, neutrons
1.12
vibrational state in tin
nucleonic densities and currents
0.043
rotational state in uranium
Physics of Hadrons
Physics of Nuclei
Resolution
Effective Field Theory
Hot and/or dense quark-gluon matter
Quark-gluon percolation
Hadron structure
Hadron-Nuclear interface
Nuclear structure
Nuclear reactions
Nuclear astrophysics
Applications of nuclear science
Adapted from W. Nazarewicz, JPG 43, 044002, 2016



SciDAC/NUCLEI: https://nuclei.mps.ohio-state.edu/

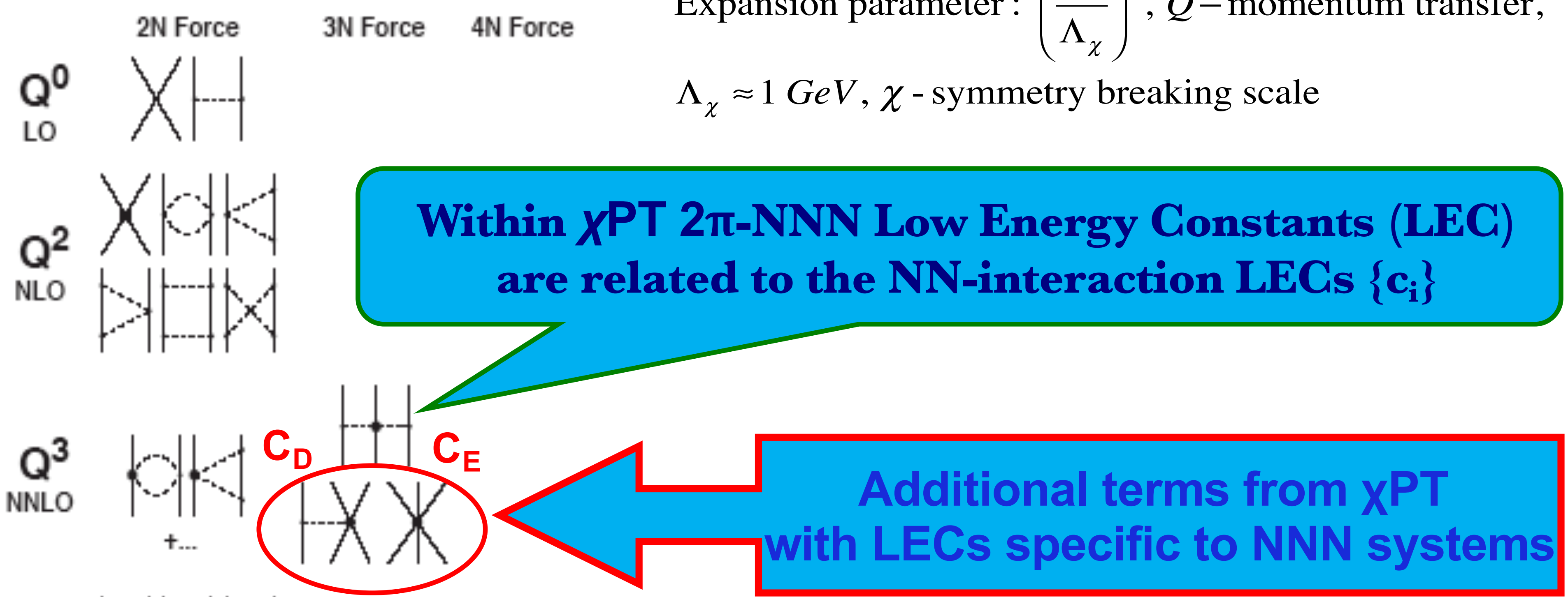
Effective Nucleon Interaction

Chiral Perturbation Theory (χPT)

Weinberg's χPT allows for controlled power series expansion

$$\text{Expansion parameter}: \left(\frac{Q}{\Lambda_\chi}\right)^{\upsilon},\ Q - \text{momentum transfer},$$

$$\Lambda_\chi \approx 1\ GeV,\ \chi \text{ - symmetry breaking scale}$$



Regularization is essential, which is also implicit within the Harmonic Oscillator (HO) wave function basis (see below)

R. Machleidt and D.R. Entem, Phys. Rep. 503, 1 (2011);
E. Epelbaum, H. Krebs, U.-G Meissner, Eur. Phys. J. A51, 53 (2015); Phys. Rev. Lett. 115, 122301 (2015)

Adapted from P. Navratil slide

For our goal: ab initio structure and reactions of rare isotopes

Having introduced realistic NN+NNN interactions, we note that they act over momentum scales that may be too large to be accommodated within a practical (truncated) many-body basis with present-day supercomputers so that some form of softening or renormalization may be required to achieve better convergence.

Options include:

A. Okubo-Lee-Suzuki (OLS) – employed here
B. Similarity Renormalization Group (SRG) - employed here
C. V_{lowk} – S. Bogner, T.T.S. Kuo, L. Corragio, and N. Itaco, Phys. Rev. C 65, 051301(R) (2002)
D. Unitary Correlation Operator Method (UCOM)- H. Feldmeier, T. Neff, R. Roth and J. Schnack, Nucl. Phys. A632, 61 (1998)
E. Brueckner G-matrix – P.J. Ellis and E. Osnes, Rev. Mod. Phys. 49, 777 (1977); J.P. Vary, Proceedings of the Predeal International Summer School: Structure and Stability of Nucleon and Nuclear Systems, A.A. Raduta, S. Stoica and I.I. Ursu, Editors. Predeal, Romania (World Scientific Press, Singapore, 1999) p. 70.

No Core Shell Model (NCSM)

A large sparse matrix eigenvalue problem

$$H = T_{rel} + V_{NN} + V_{3N} + \bullet\bullet\bullet$$

$$H|\Psi_i\rangle = E_i|\Psi_i\rangle$$

$$|\Psi_i\rangle = \sum_{n=0}^{\infty} A_n^i |\Phi_n\rangle$$

$$\text{Diagonalize } \{\langle\Phi_m|H|\Phi_n\rangle\}$$

P. Navratil, J. P. Vary and B.R. Barrett, *Phys. Rev. Lett*. **84**, 5728 (2000); *Phys. Rev. C* **62**, 054311 (2000)

- Adopt realistic NN (and NNN) interaction(s) & renormalize as needed - retain induced many-body interactions: Chiral Effective Field Theory (Chiral EFT) interactions
- Adopt the 3-D Harmonic Oscillator (HO) for the single-nucleon basis states, α, β,…
- Evaluate the nuclear Hamiltonian, H, in basis space of HO (Slater) determinants (each determinant manages the bookkeeping of anti-symmetrization)
- Diagonalize this sparse many-body H in its "m-scheme" basis where [$\alpha = (n,l,j,m_j,\tau_z)$]

HO basis space (configurations)

$$|\Phi_n\rangle = [a_\alpha^+ \bullet\bullet\bullet a_\varsigma^+]_n |0\rangle$$

$$n = 1,2,\ldots,10^{10} \text{ or more!}$$

- Evaluate observables and compare with experiment

Comments

- Computationally demanding => needs new algorithms & high-performance computers
- Requires convergence assessments and extrapolation tools to retain predictive power
- Achievable for nuclei up to atomic number of about 20 with largest computers available

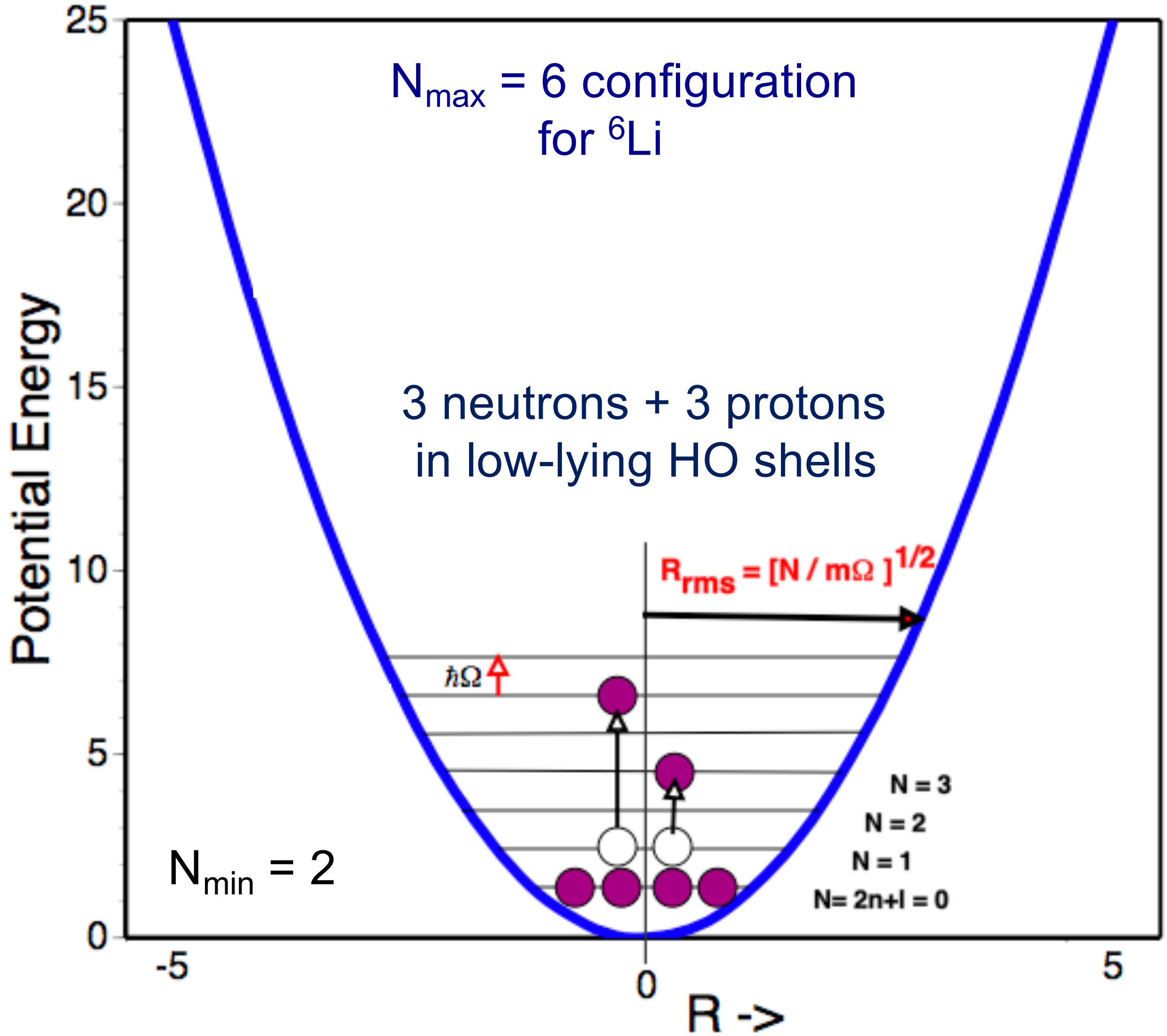
$N_{\min} \equiv$ HO quanta of lowest configuration

$N_{\max} \equiv$ maximum HO quanta above the lowest configuration

Retain configurations with $N_{\min} \leq \sum_{i=1}^{A} (2n_i + l_i) \leq N_{\min} + N_{\max}$

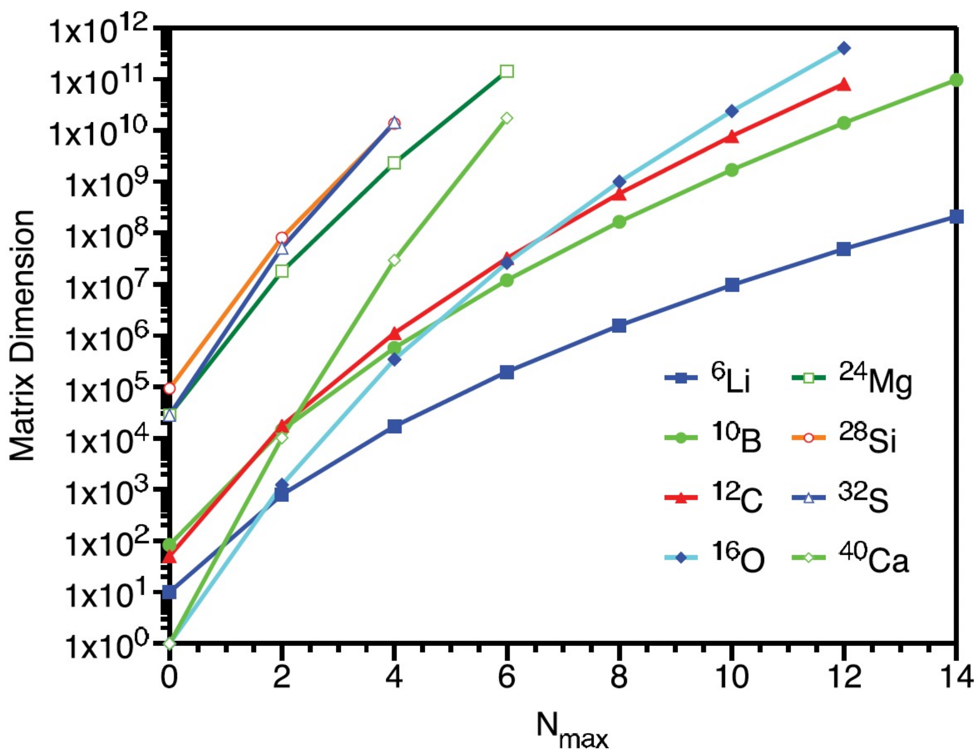
consistent with symmetry constraints (parity, M_J,...)

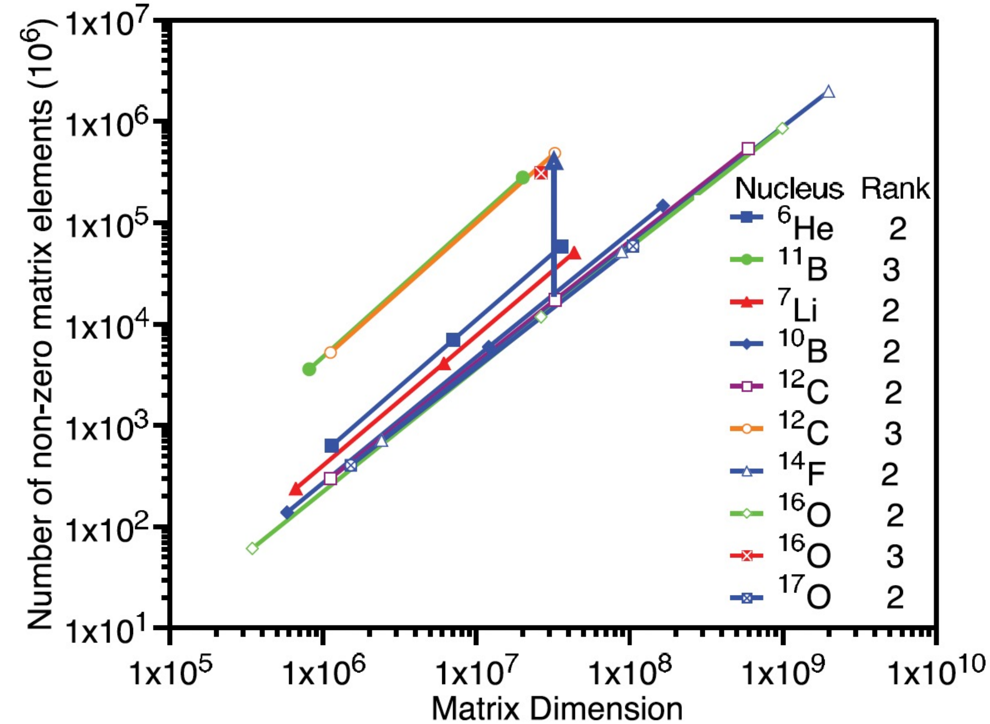
extrapolate: N_{max} -> infinity



Challenge

Exponential increase in Matrix Dimension (D)





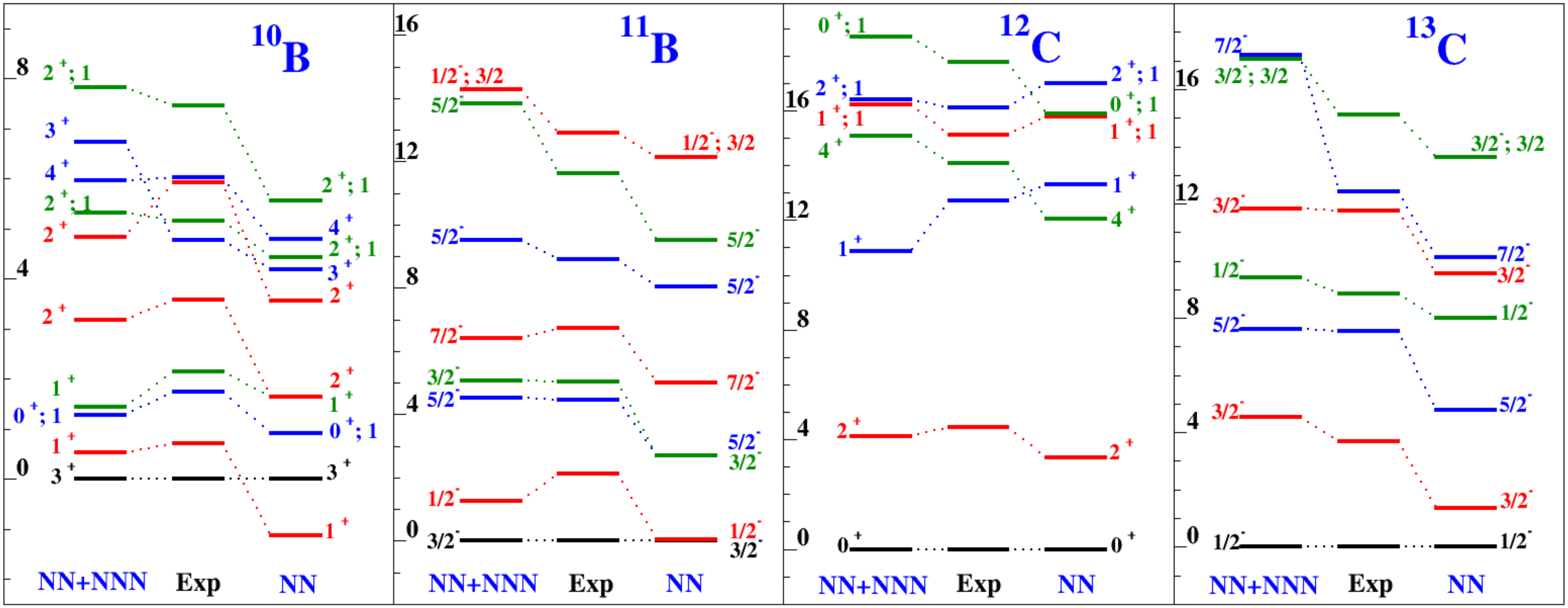
Opportunities

- Memory/cpu time grows only as $D^{3/2}$
- Algorithm development (SciDAC funding)
- Exaflop machines now available (DOE/INCITE competitive awards)
- Improved understanding of Chiral EFT
- Developing methods for extrapolating D->inf (N_{max}->inf)

P. Maris, J.P. Vary and A.M. Shirokov, Phys, Rev. C 79, 014308 (2009); ArXiv:0808.3420

ab initio NCSM with χ_{EFT} Interactions

NNN interactions produce correct ^{10}B ground state spin and overall spectral improvements



$c_D = -1$

P. Navratil, V.G. Gueorguiev, J. P. Vary, W. E. Ormand and A. Nogga, Phys Rev Lett 99, 042501(2007); ArXiV: nucl-th 0701038.

"Proton-Dripping Fluorine-14"

DOE/ASCR/NP – Computational Science Highlight

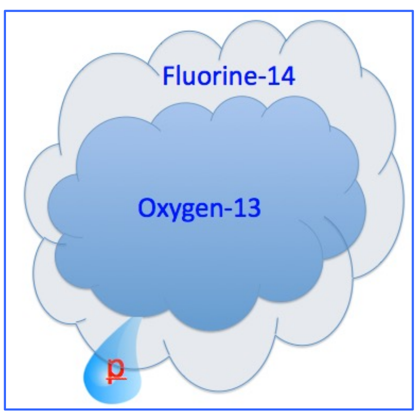
Objectives

- **Apply *ab initio* microscopic nuclear theory's predictive power to major test case**

Impact

- **Deliver robust predictions important for improved energy sources**
- **Provide important guidance for DOE-supported experiments**
- **Compare with new experiment to improve theory of strong interactions**

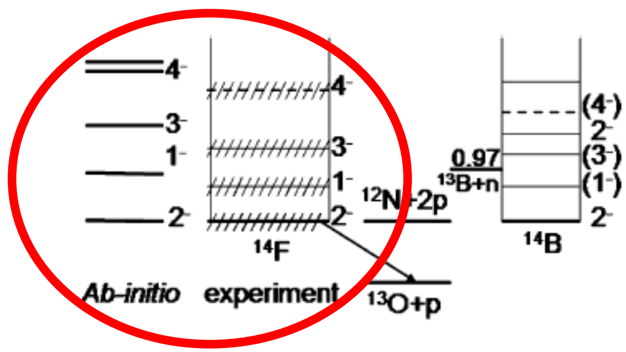
P. Maris, A.M. Shirokov, and J.P. Vary, Phys. Rev. C 81, 021301(R), **Feb. 2010**, uses JISP16 to predict ^{14}F lives a short time in specified states (the "Ab-initio" ladder in the red oval) and decays to Oxygen-13 by emitting a proton.



$^{13}O + p \rightarrow {}^{14}F^{*} \rightarrow {}^{13}O + p$

Experiment validates our published predictions!

V.Z. Goldberg et al., "First observation of 14F", Phys. Lett. B 692, 307 (**August 2010**).



Progress

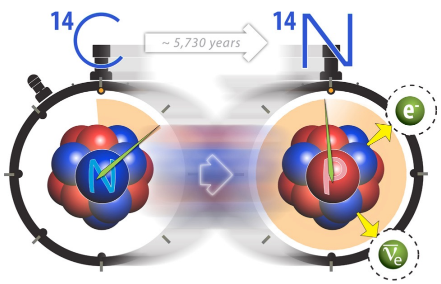
- Dimension of matrix solved for 14 lowest states ~ $2x10^9$
- Solution takes ~ 2.5 hours on 30,000 cores (Cray XT4 Jaguar at ORNL)
- P. Maris, M. Sosonkina, J. P. Vary, E. G. Ng and C. Yang, "Scaling of ab-initio nuclear physics calculations on multicore computer architectures", 2010 Intern. Conf. on Computer Science, Procedia Computer Science 1, 97, May 2010.

PRL 106, 202502 (2011) PHYSICAL REVIEW LETTERS week ending 20 MAY 2011

Origin of the Anomalous Long Lifetime of ^{14}C

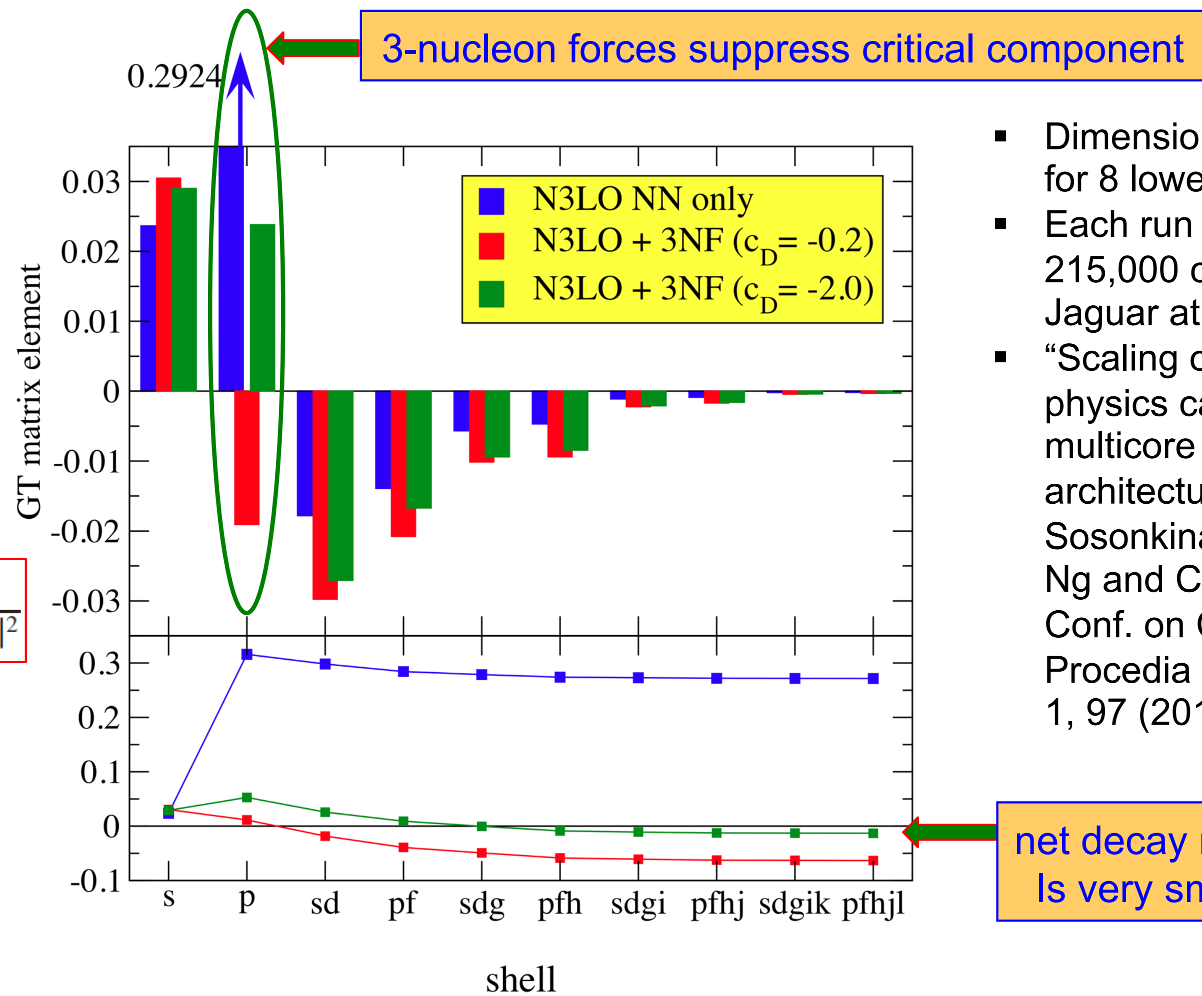
P. Maris,[1] J.P. Vary,[1] P. Navrátil,[2,3] W.E. Ormand,[3,4] H. Nam,[5] and D.J. Dean[5]

- Solves the puzzle of the long but useful lifetime of ^{14}C
- Establishes a major role for strong 3-nucleon forces in nuclei
- Strengthens foundation for guiding experiments



$$T_{1/2} = \frac{1}{f(Z, E_0)} \frac{2\pi^3\hbar^7 \ln 2}{m_e^5 c^4 G_V^2} \frac{1}{g_A^2 |M_{GT}|^2}$$

$$M_{GT} = \sum_k \langle \Psi_f || \sigma(k)\tau_+(k) || \Psi_i \rangle$$



- Dimension of matrix solved for 8 lowest states ~ 1×10^9
- Each run takes ~ 6 hours on 215,000 cores on Cray XT5 Jaguar at ORNL
- "Scaling of *ab initio* nuclear physics calculations on multicore computer architectures," P. Maris, M. Sosonkina, J. P. Vary, E. G. Ng and C. Yang, 2010 Intern. Conf. on Computer Science, Procedia Computer Science 1, 97 (2010)

net decay rate
Is very small

PHYSICAL REVIEW C **103**, 054001 (2021)

Editors' Suggestion

Light nuclei with semilocal momentum-space regularized chiral interactions up to third order

P. Maris,[1,*] E. Epelbaum,[2] R. J. Furnstahl,[3] J. Golak,[4] K. Hebeler,[5,6] T. Hüther,[5] H. Kamada,[7] H. Krebs,[2] Ulf-G. Meißner,[8,9,10]
J. A. Melendez,[3] A. Nogga,[9] P. Reinert,[2] R. Roth,[5] R. Skibiński,[4] V. Soloviov,[4] K. Topolnicki,[4]
J. P. Vary,[1] Yu. Volkotrub,[4] H. Witała,[4] and T. Wolfgruber[5]

The LENPIC team:
www.lenpic.org

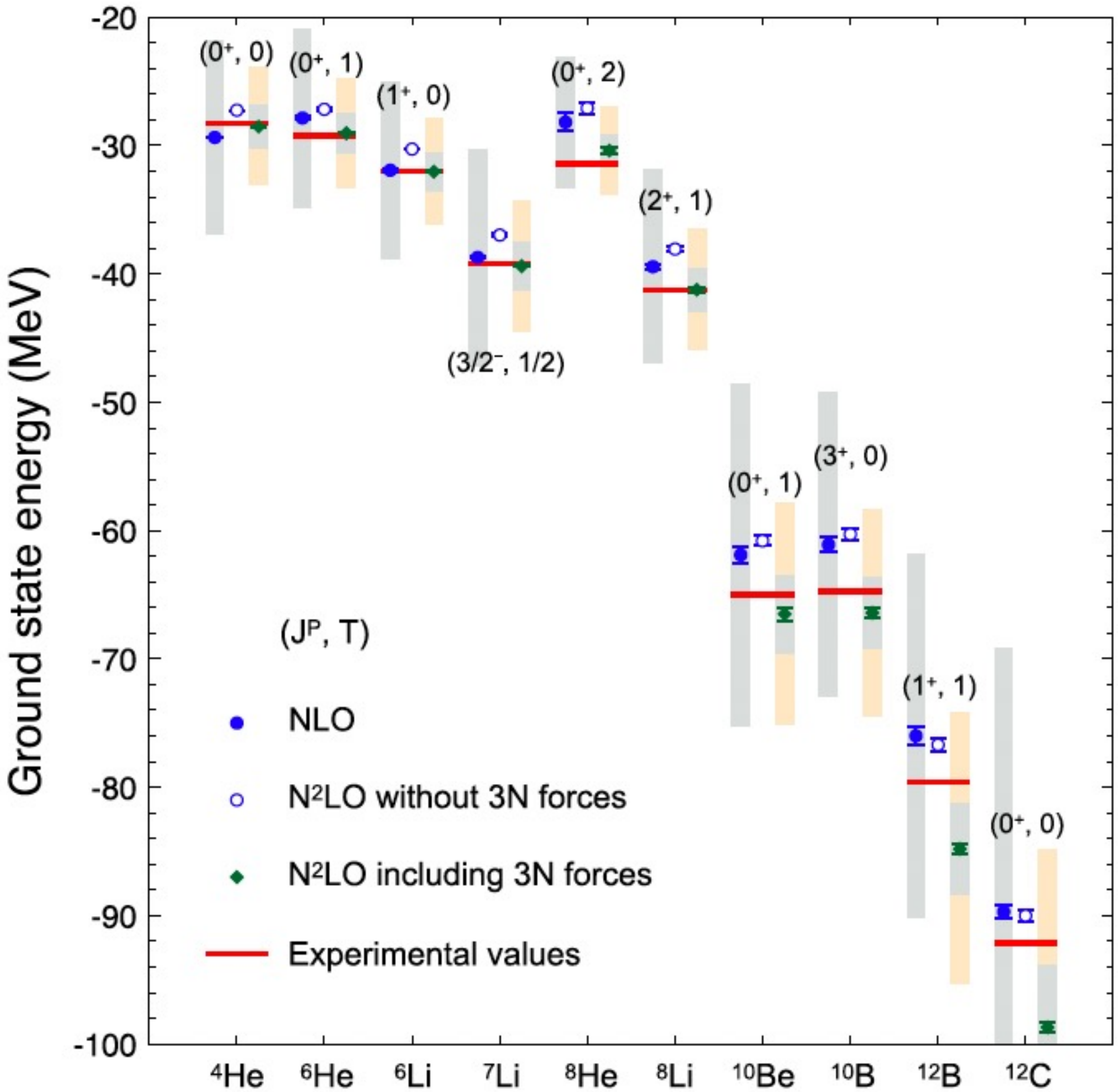
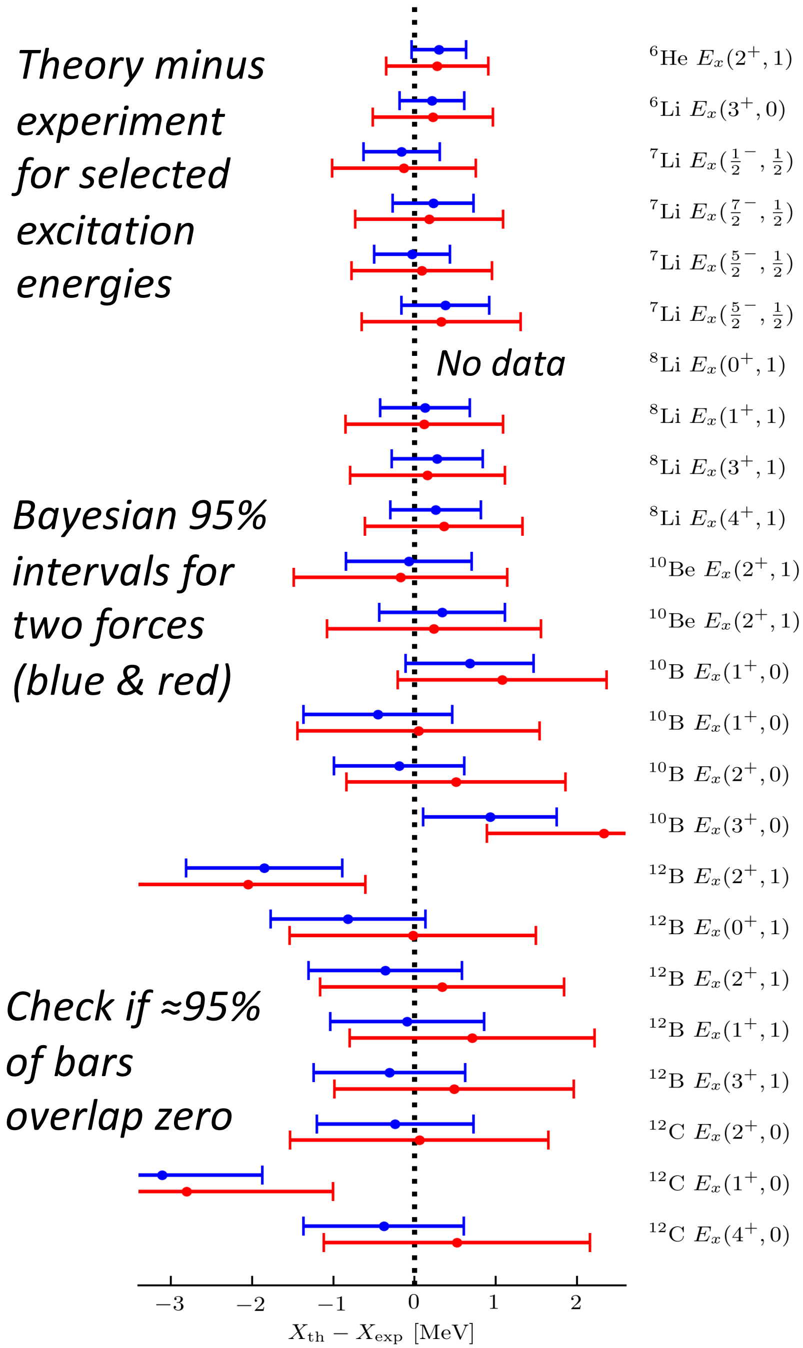


FIG. 8. Calculated ground-state energies in MeV using chiral NLO, and N^{2}LO interactions at $\Lambda = 450$ MeV (blue and green symbols) in comparison with experimental values (red levels). For each nucleus the NLO, and N^{2}LO results are the left and right symbols and bars, respectively. The open blue symbols correspond to incomplete calculations at N^{2}LO using NN-only interactions. Blue and green error bars indicate the NCCI extrapolation uncertainty. All results shown are for $\alpha = 0.08$ fm^4. The light (coral) and dark (gray) shaded bars indicate the 95% and 68% DoB truncation errors, respectively, estimated using the Bayesian model $\bar{C}^{650}_{0.5-10}$ (at NLO we only show the 68% DoB truncation errors because the 95% errors would be off one or even both ends of the scale).

Excitation energies from effective field theory with quantified uncertainties

U.S. DEPARTMENT OF ENERGY | Office of Science

NUCLEI — Nuclear Computational Low-Energy Initiative



Objectives

- Predict properties of ground and excited states of light nuclei with robust theoretical error estimates.
- Test consistent LENPIC chiral effective field theory (EFT) interactions with 2- and 3-nucleon forces.
- Extend and test a Bayesian statistical model that learns from the order-by-order EFT convergence pattern to account for correlated excitations.

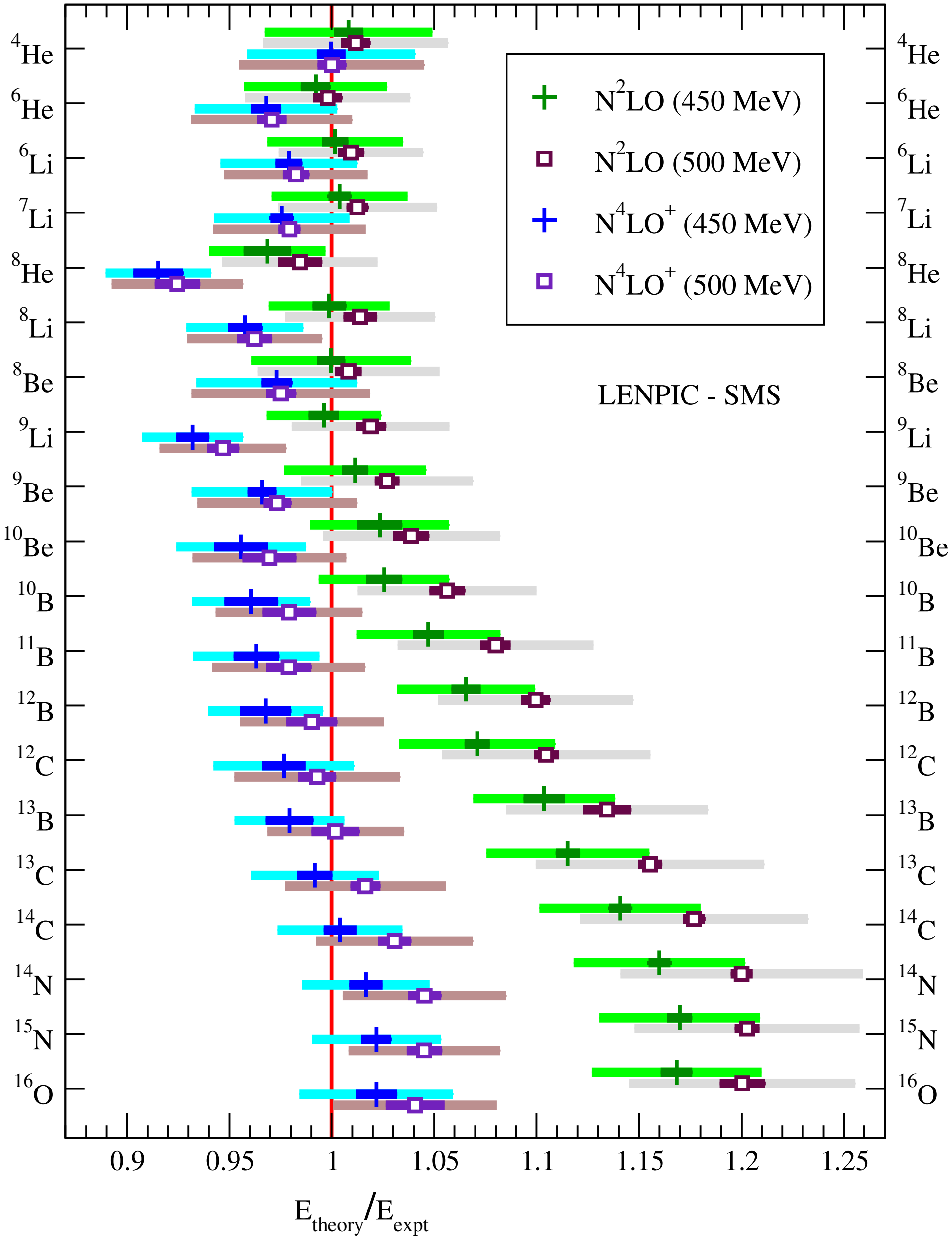
Impact

- First test of novel chiral nucleon-nucleon potentials with consistent three-nucleon forces.
- Demonstrates understanding of theoretical uncertainties due to chiral EFT expansion.
- Accounting for correlations produces agreement with experimental excitation energies (see figure).
- Exceptions in ^{12}C and ^{12}B indicate different theoretical correlations in the nuclear structure.

Accomplishments

P. Maris et al, Phys. Rev. C **103**, 054001 (2021); Editors' Suggestion; arXiv: 2012.12396 [nucl-th]

Binding Energies with LENPIC-SMS chiral EFT



P. Maris, H. Le, A. Nogga, R. Roth, J.P. Vary
Front. Phys. 11, 1098262 (2023)

- NN potential up to N^4LO^+
- 3NFs at N^2LO
- SRG evolved to $\alpha = 0.08$ fm^4
- LECs fitted to
  - NN scattering data
  - ^{3}H binding energy
  - Nd scattering
- Parameter-free predictions
- Error bars
  - numerical uncertainty
  - chiral EFT uncertainty from Bayesian analysis

Adapted from P. Maris, LENPIC Annual Meeting, Bonn, March 11-13, 2024

Daejeon16 NN interaction

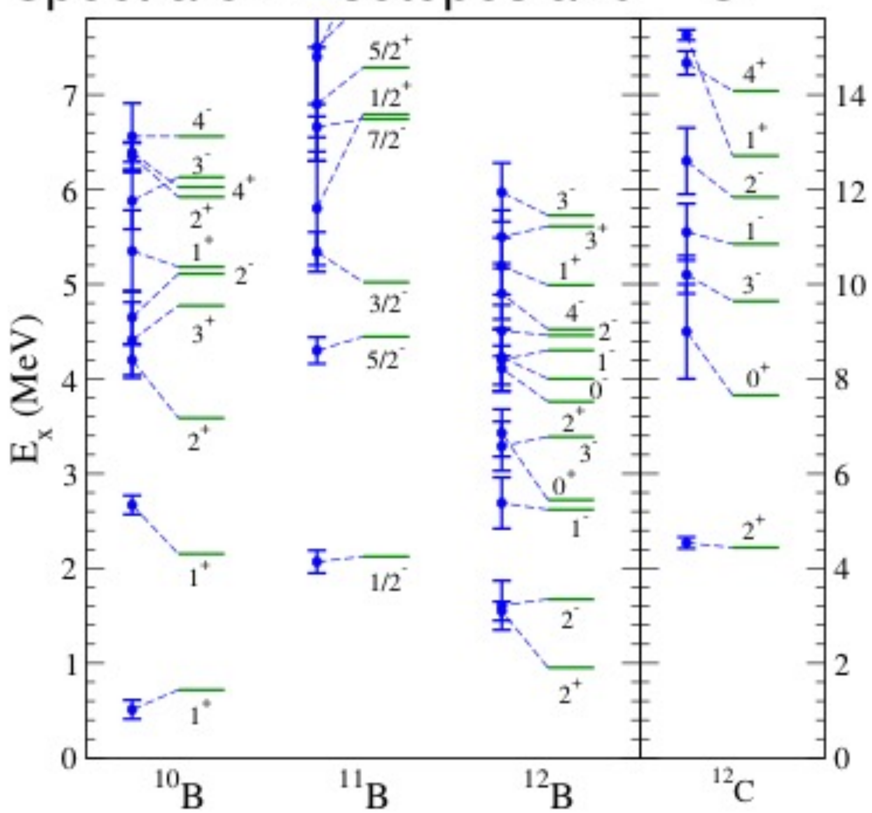
Based on SRG evolution of Entem-Machleidt "500" chiral N3LO to $\lambda = 1.5\ \text{fm}^{-1}$ followed by Phase-Equivalent Transformations (PETs) to fit selected properties of light nuclei.

A.M. Shirokov, I.J. Shin, Y. Kim, M. Sosonkina, P. Maris and J.P. Vary,
"N3LO NN interaction adjusted to light nuclei in ab exitu approach,"
Phys. Letts. B 761, 87 (2016); arXiv: 1605.00413

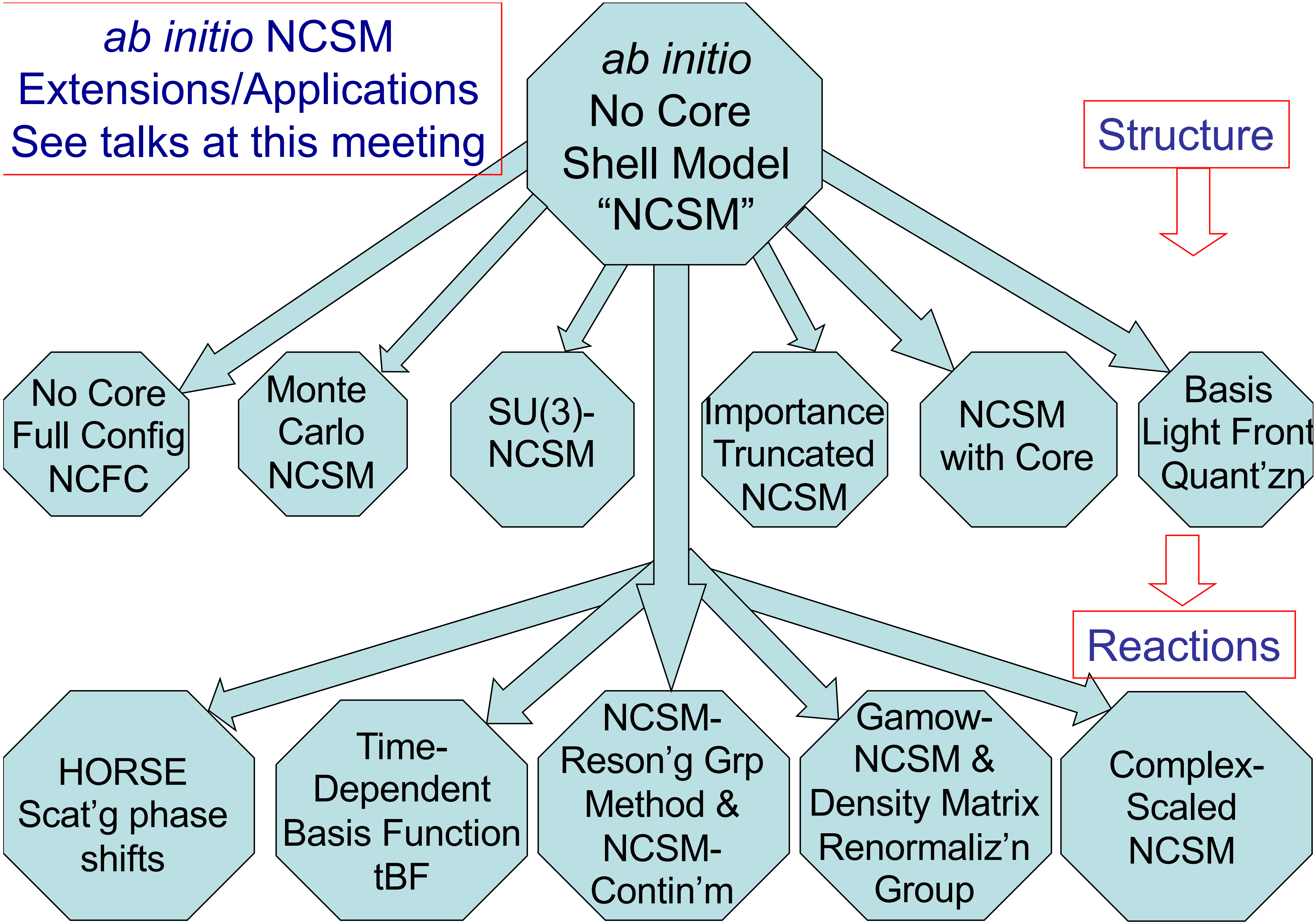
Application to excited states of p-shell nuclei

(Maris, Shin, Vary, in preparation)

Spectra of B isotopes and ^{12}C



- difference of extrapolated E_b
- extrapolation uncertainties: max of E_b uncertainties
- good agreement with positive and negative parity spectra
- need large bases for 'intruder' and 'non-normal parity' states
- spectrum ^{10}B
  - correct gs 3^+ and excited 1^+
  - third 1^+ 'intruder' state
- excited 0^+ state in ^{12}C
  - Hoyle state?
  - see MCNCSM results below



ab initio NCSM
Extensions/Applications
See talks at this meeting
ab initio
No Core
Shell Model
"NCSM"
Structure
Reactions
No Core
Full Config
NCFC
Monte
Carlo
NCSM
SU(3)-
NCSM
Importance
Truncated
NCSM
NCSM
with Core
Basis
Light Front
Quant'zn
HORSE
Scat'g phase
shifts
Time-
Dependent
Basis Function
tBF
NCSM-
Reson'g Grp
Method &
NCSM-
Contin'm
Gamow-
NCSM &
Density Matrix
Renormaliz'n
Group
Complex-
Scaled
NCSM

General idea of the HORSE formalism

"Harmonic Oscillator Representation of Scattering Equations"

$$T \; + \; V$$

NCSM with:

$\lambda(N,\hbar\Omega)$ & $\Lambda(N,\hbar\Omega)$

Infinite set of algebraic equations in HO basis of relative motion:

$$\sum_{n'=0}^{N}\left(T^{l}_{nn'} + V^{l}_{nn'} - \delta_{nn'}E\right) a_{n'l}(E) = 0. \qquad n \leq N-1$$

Matching condition at $n = N$

$$\sum_{n'=0}^{N}\left(T^{l}_{Nn'} + V^{l}_{Nn'} - \delta_{Nn'}E\right) a_{n'l}(E) + T^{l}_{N,N+1}a_{N+1,l}(E) = 0. \quad n \leq N-1$$

Then for $n \geq N+1$

$$\sum_{n'=0}^{\infty}\left(T^{l}_{nn'} - \delta_{nn'}E\right) a_{n'l}(E) = 0,$$ which produces:

$$T^{l}_{n,n-1}a_{n-1,l}(E) + \left(T^{l}_{nn} - E\right)a_{nl}(E) + T^{l}_{n,n+1}a_{n+1,l}(E) = 0.$$

"think outside the box"=> T

Arises as a natural extension of NCSM where both potential and kinetic energies are truncated

This is an exactly solvable algebraic problem!

Single-State HORSE (SS-HORSE)

$$\sum_{n'=0}^{N} H^{l}_{nn'} \langle n' | \lambda \rangle = E_\lambda \langle n | \lambda \rangle, \qquad n \le N$$

$$(H - E)^{-1}_{nn'} \equiv -G_{nn'} = \sum_{\lambda'=0}^{N} \frac{\langle n | \lambda' \rangle \langle \lambda' | n' \rangle}{E_{\lambda'} - E}$$

← Standard HORSE

$$\tan\delta(E) = -\frac{S_{Nl}(E) - G_{NN} T^{l}_{N,N+1} S_{N+1,l}(E)}{C_{Nl}(E) - G_{NN} T^{l}_{N,N+1} C_{N+1,l}(E)}.$$ Also, S-matrix = $S(G_{NN})$

Suppose $E = E_{\lambda'}$ ← Single-State HORSE

$$\tan\delta(E_\lambda) = \frac{S_{N+1,l}(E_\lambda)}{C_{N+1,l}(E_\lambda)} = (-1)^l q^{2l+1} \Gamma(-l + \tfrac{1}{2}) \frac{L^{l+1/2}_{(N-l)/2}(q^2)}{\Phi(-N/2 - l/2 - 1/2, -l + 1/2; q^2)}$$

where $L^{l+1/2}_{(N-l)/2}$ are associated Laguerre polynomials, Φ are confluent hyper-geometric functions and $q = \sqrt{\dfrac{2E_\lambda}{\hbar\Omega}}$.

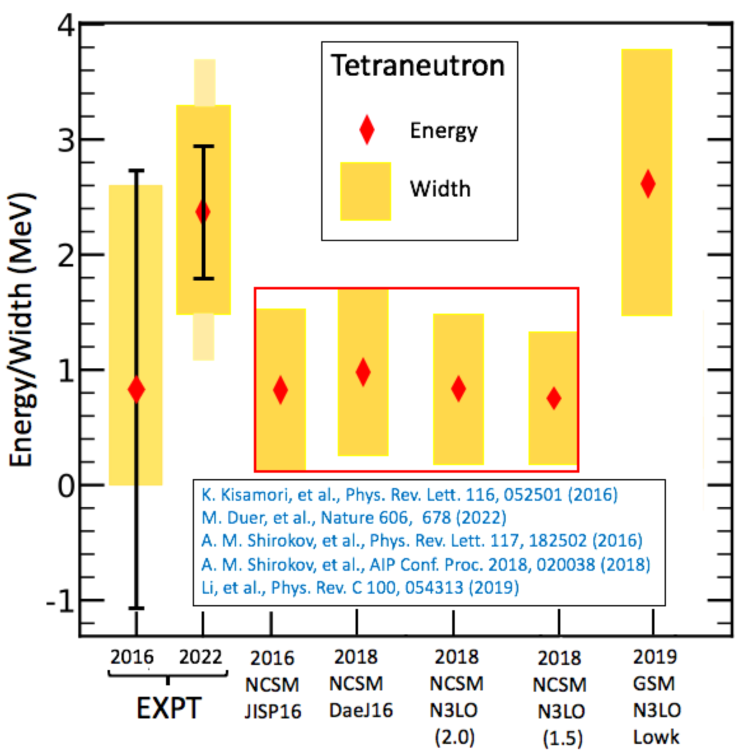
E_λ are (obtained from) eigenvalues of the NCSM (for given $\hbar\Omega$ and N_{max}). Once a scattering channel is defined (sets the continuum energy scale) the phase shift is calculated. Analog of Lüscher's method for a plane-wave basis.

A.M. Shirokov, A.I. Mazur, I.A. Mazur and J.P. Vary, PRC 94, 064320 (2016); arXiv:1608.05885

Tetraneutron discovery confirms prediction

Objectives

- *Ab initio* nuclear theory aims for parameter-free predictions of nuclear properties with controlled uncertainties using supercomputer simulations
- Specific goal is to predict if the tetraneutron (4-neutron system) has a bound state, a low-lying resonance or neither



Experiment and theory for the tetraneutron's resonance energy and width. *Ab initio* No-Core Shell Model (NCSM) and Gamow Shell Model (GSM) predictions use different neutron-neutron interactions and different basis function techniques.

Impact

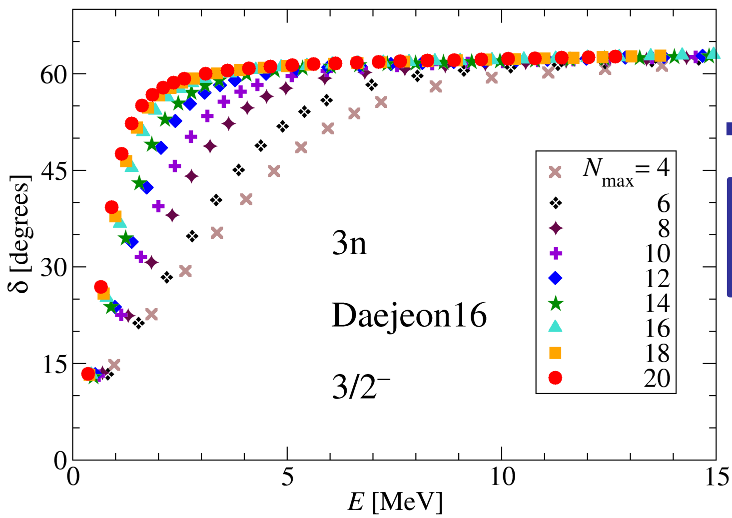
- Discovery in 2022 announced in Nature [1] confirms *ab initio* theory predictions from 2016 [2] of a short-lived tetraneutron resonance at low energy and the absence of a tetraneutron bound state
- Demonstrates the predictive power of *ab initio* nuclear theory since theory and experiment are within their combined uncertainties
- Sets stage for further experimental and theoretical research on new states of matter formed only of neutrons
- Shows need to anticipate a long wait time for experimental confirmation of such an exotic phenomena, ~ 6 years in this case
- Emphasizes the value of DOE supercomputer allocations (NERSC) and support for multi-disciplinary teamwork (SciDAC/NUCLEI)

Accomplishments

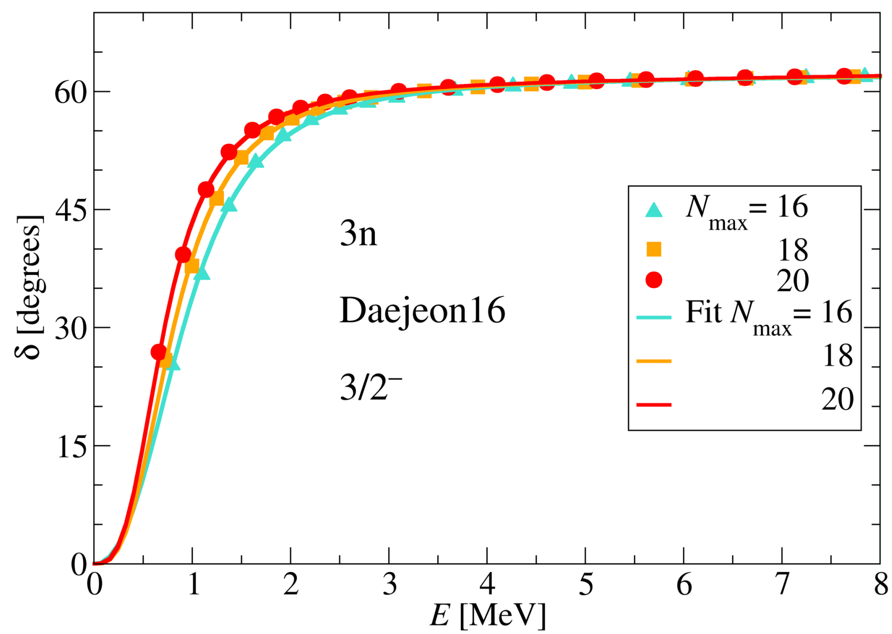
[1] M. Duer, et al., Nature 606, 678 (2022)

[2] A.M. Shirokov, G. Papadimitriou, A.I. Mazur, I.A. Mazur, R. Roth and J.P. Vary, "Prediction for a four-neutron resonance," Phys. Rev. Lett. 117, 182502 (2016)

3n Results with Daejeon16 NN interaction



Selection of points, parameterization



Extraction of S-matrix pole position

N_{max}	$3/2^-$		$1/2^-$	
	E_r [MeV]	Γ [MeV]	E_r [MeV]	Γ [MeV]
16	0.607	1.524	0.606	1.604
18	0.537	1.176	0.531	1.133
20	0.481	0.963	0.481	0.962

I.A. Mazur, M. K. Efimenko, A. I. Mazur, I. J. Shin, V. A. Kulikov,
A. M. Shirokov and J. P. Vary, PRC (to appear); arXiv: 2403.18232

Alpha clusters in Carbon-12 from ab initio theory & statistical learning

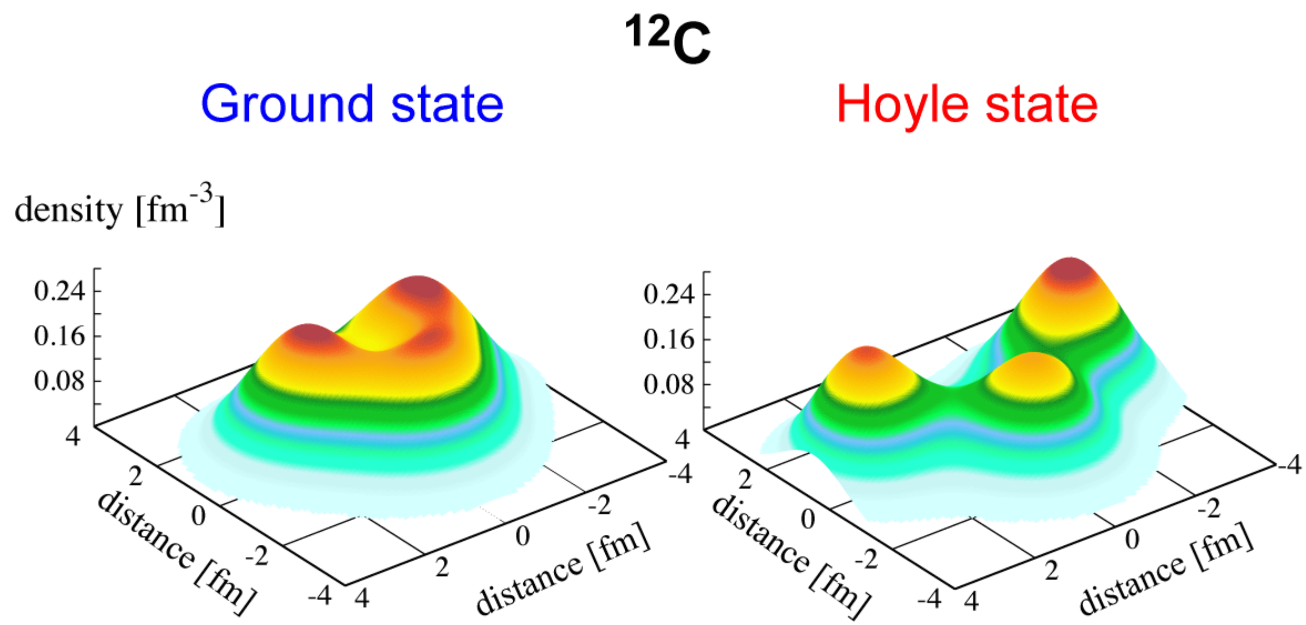
Objectives

- *Ab initio* nuclear theory aims for parameter-free predictions of critical nuclear properties with controlled uncertainties using supercomputer simulations
- Specfic goal is to determine extent of alpha clustering in the Ground state and the Hoyle state of Carbon-12 (^{12}C)

Impact

- Ground state found to have 6% alpha clustering while Hoyle state discovered to be 3-alphas 61% of the time
- With this high percentage of 3-alphas, the Hoyle state is confirmed as a natural gateway state for the cosmic formation of ^{12}C, the key element for organic life
- Statistical learning confirms 3-alpha feature of Hoyle state

Ab initio Monte-Carlo Shell Model results for density contours of 12C Ground state and first excited 0^+ (Hoyle) state using the Daejeon16 two-nucleon potential. Simulations were performed on Fugaku in Japan, the world's largest supercomputer at the time.

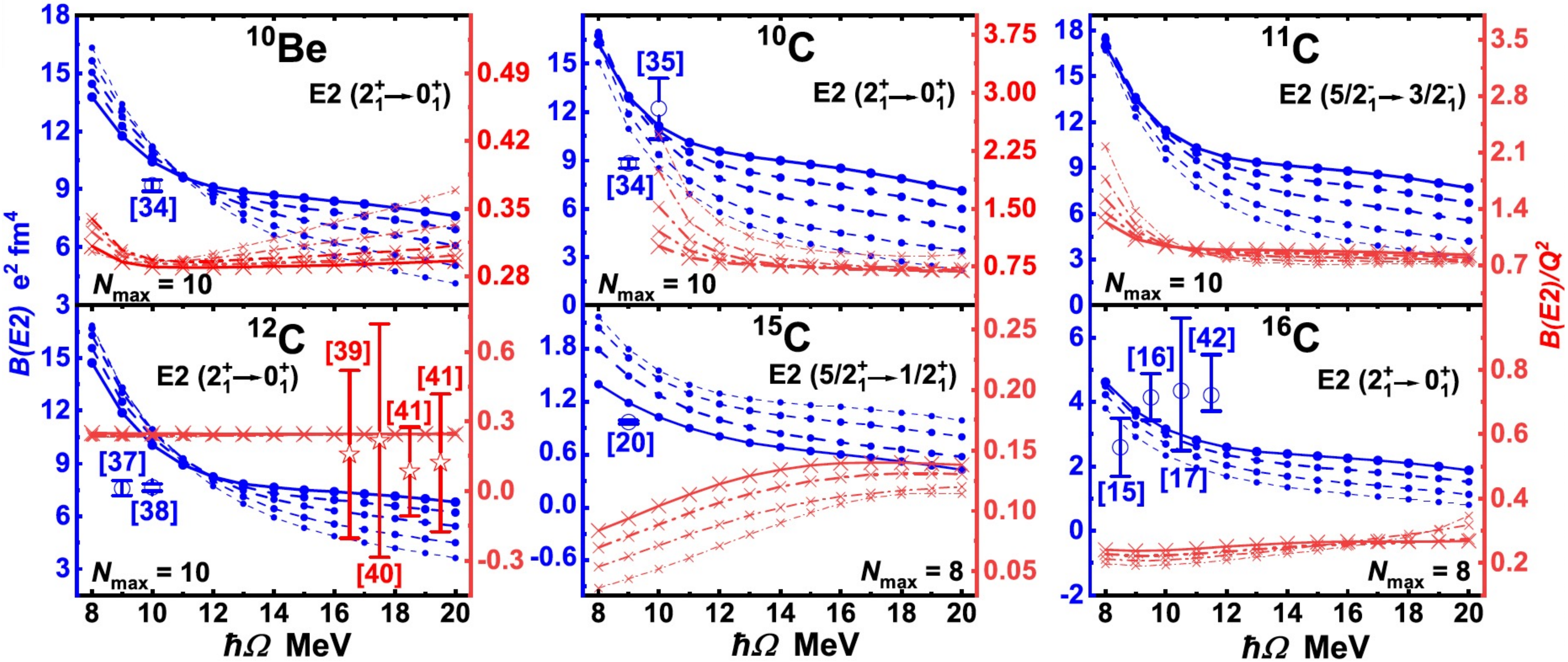


Accomplishments

T. Otsuka, T. Abe, T. Yoshida, Y. Tsunoda, N. Shimizu, N. Itagaki, Y. Utsuno, J. Vary, P. Maris and H. Ueno, "Alpha-Clustering in Atomic Nuclei from First Principles with Statistical Learning and the Hoyle State Character," Nature Communications 13:2234 (2022)

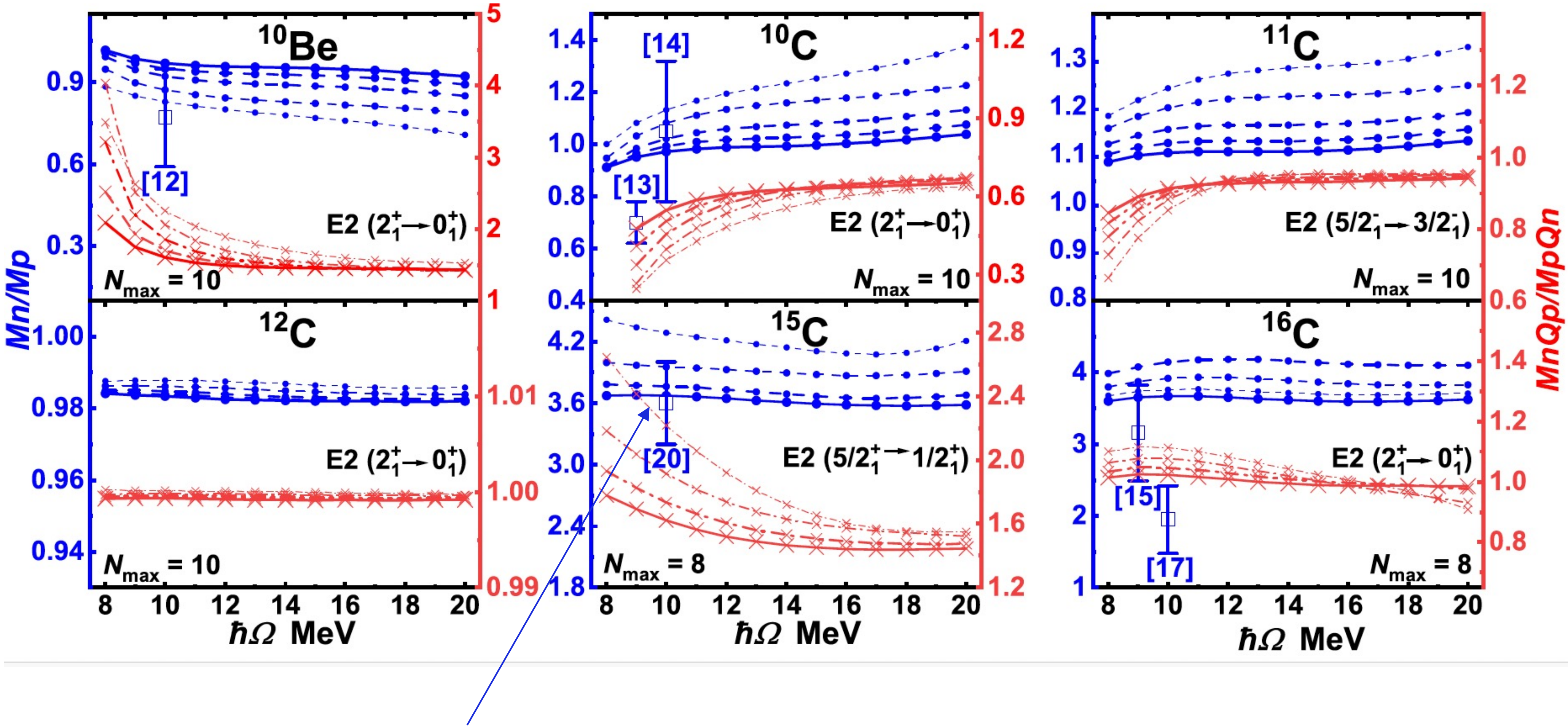
$$\frac{B(E2)}{Q_p^2} = \frac{\langle J_f || \sum_{i\in p} r_i^2 Y_2(\hat{r}_i) || J_i \rangle^2}{\langle J_i || \sum_{i\in p} r_i^2 Y_2(\hat{r}_i) || J_i \rangle^2},$$

Ratios of observables converge better
He Li, et al., arXiv: 2401.05776



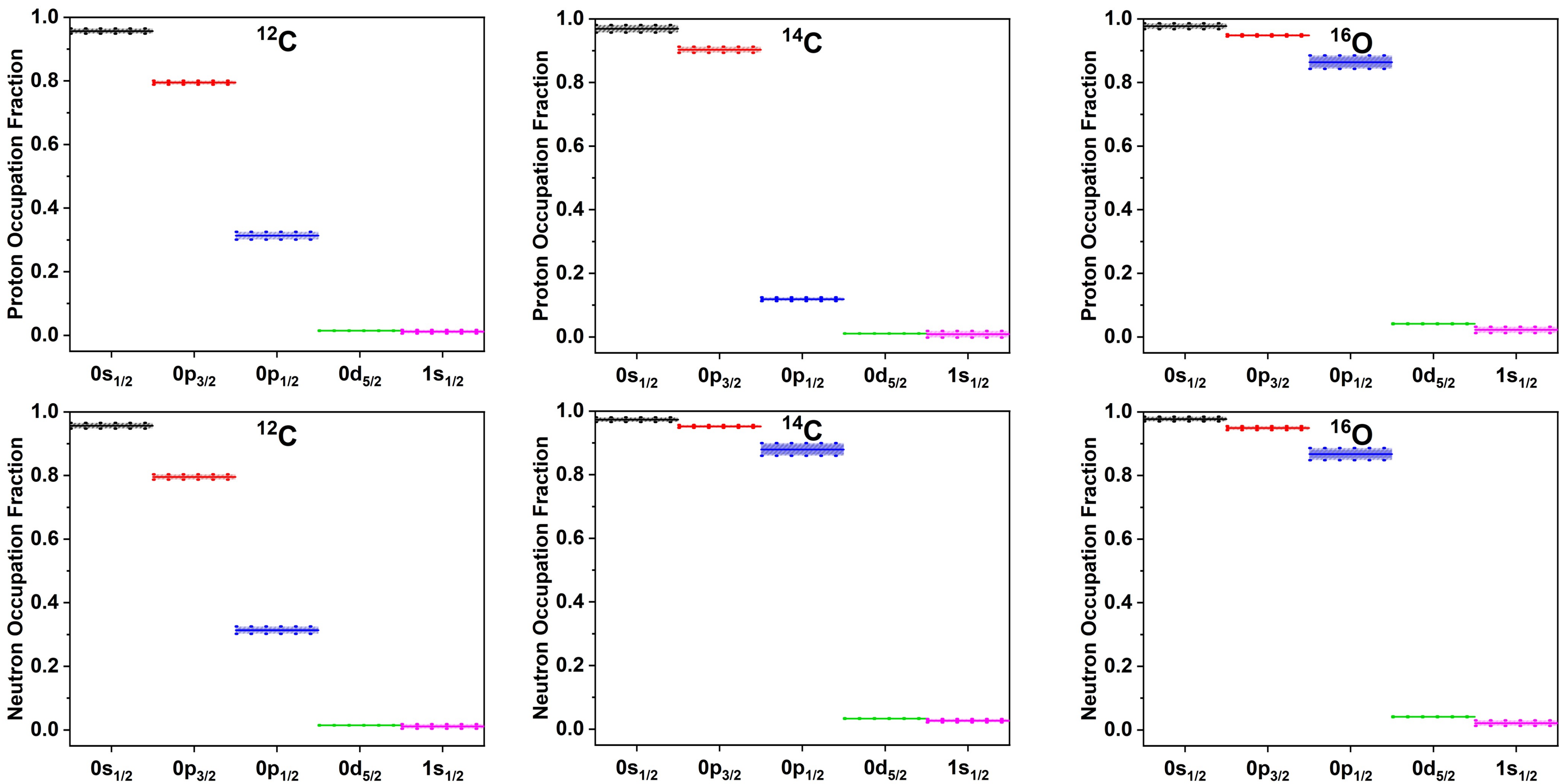
$$\frac{M_n}{M_p} = \frac{\langle J_f || \sum_{i\in n} r_i^2 Y_2(\hat{r}_i) || J_i \rangle}{\langle J_f || \sum_{i\in p} r_i^2 Y_2(\hat{r}_i) || J_i \rangle},$$

Ratios of observables and ratios of ratios converge better
He Li, et al., arXiv: 2401.0577



Jie Chen et al., PRC 106, 064312 (2022)

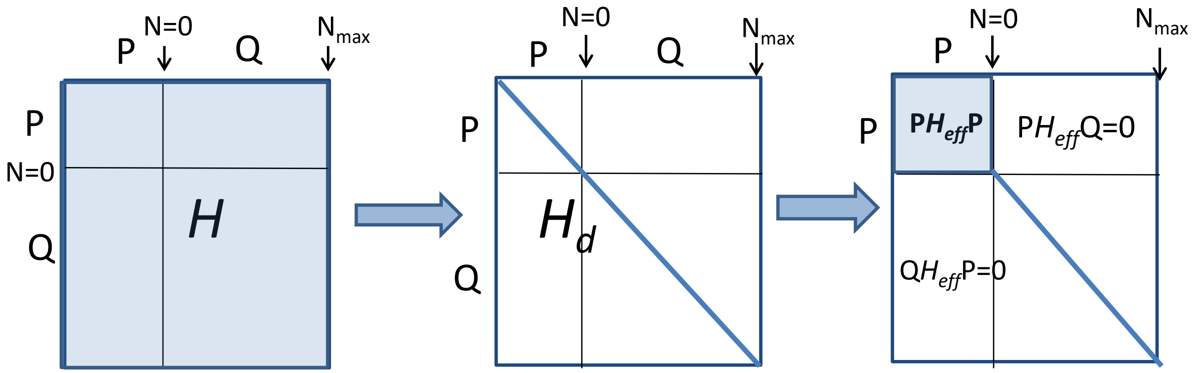
Z = 6 show good subshell closure at N = 8 (i.e. "locally magic")



Ground state occupation fractions of protons (neutrons) in low-lying single particle states in ^{12}C, ^{14}C, and ^{16}O. The NCSM calculations performed in a harmonic oscillator basis using the Daejeon16 *NN* interaction with N_{max} = 10 and $\hbar\Omega$ = 17.5 MeV. We present uncertainties where the lowest (highest) point indicates the minimal (maximal) occupation fraction value in the range from $\hbar\Omega$ = 15 to 20 MeV. *arXiv:2407.09734*

Ab-initio effective interaction from the NCSM

Okubo-Lee-Suzuki (OLS) similarity transformation
of the NCSM solution



$$H_d = UHU^{\dagger} \qquad H_{eff} = \frac{U_P^{\dagger}}{\sqrt{U_P U_P^{\dagger}}} H_d \frac{U_P}{\sqrt{U_P U_P^{\dagger}}}$$

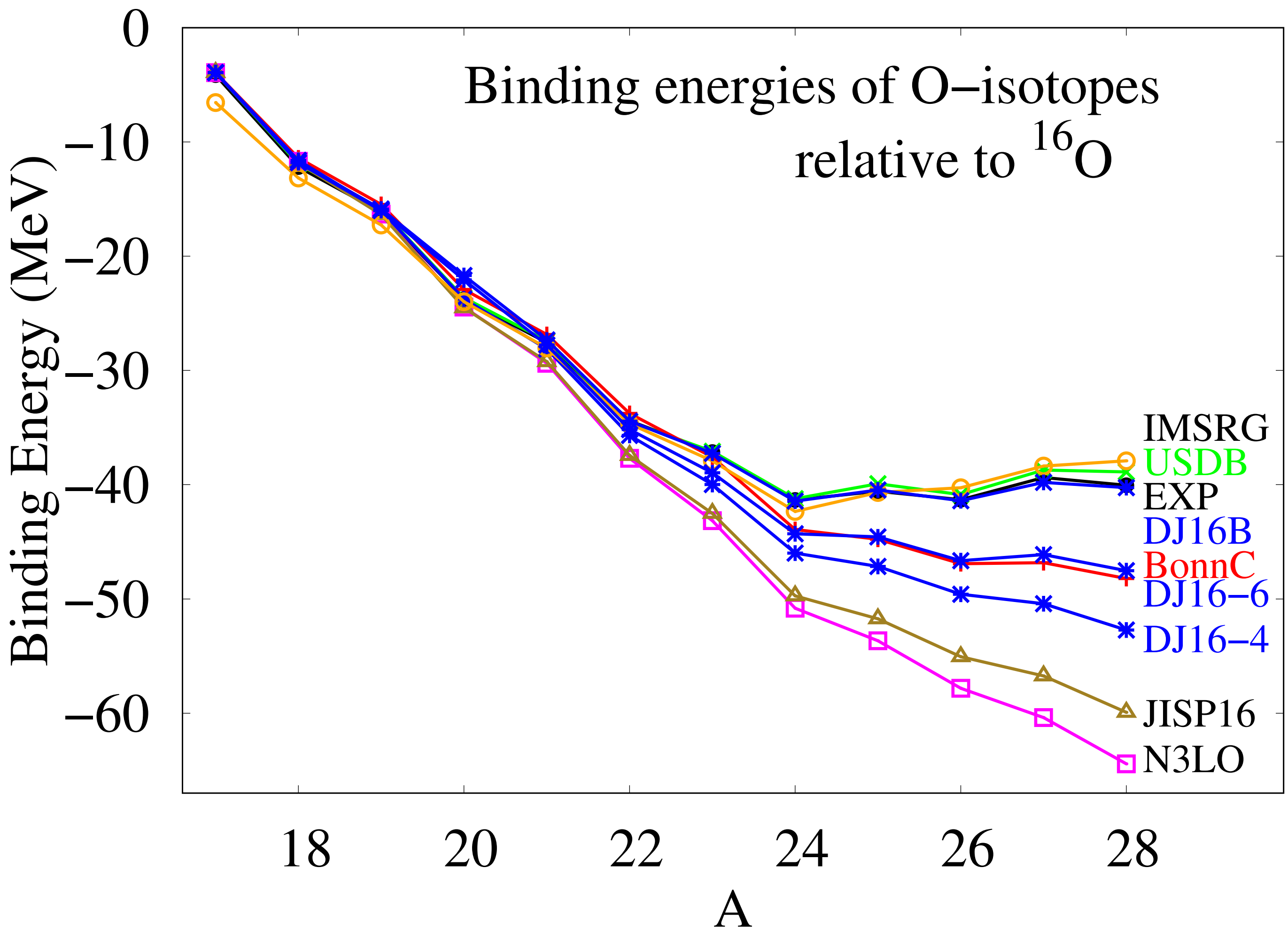
Flow

- NCSM for ^{18}F at $N_{\max}$
- H_{eff} for ^{18}F at $N = 0$ (OLS)
- ^{16}O at $N_{\max}$ (core energy)
- ^{17}O, ^{17}F at $N_{\max}$ (one-body terms)
- ϵ_j, $\langle ij | V_{\text{eff}} | kl \rangle_{JT}$

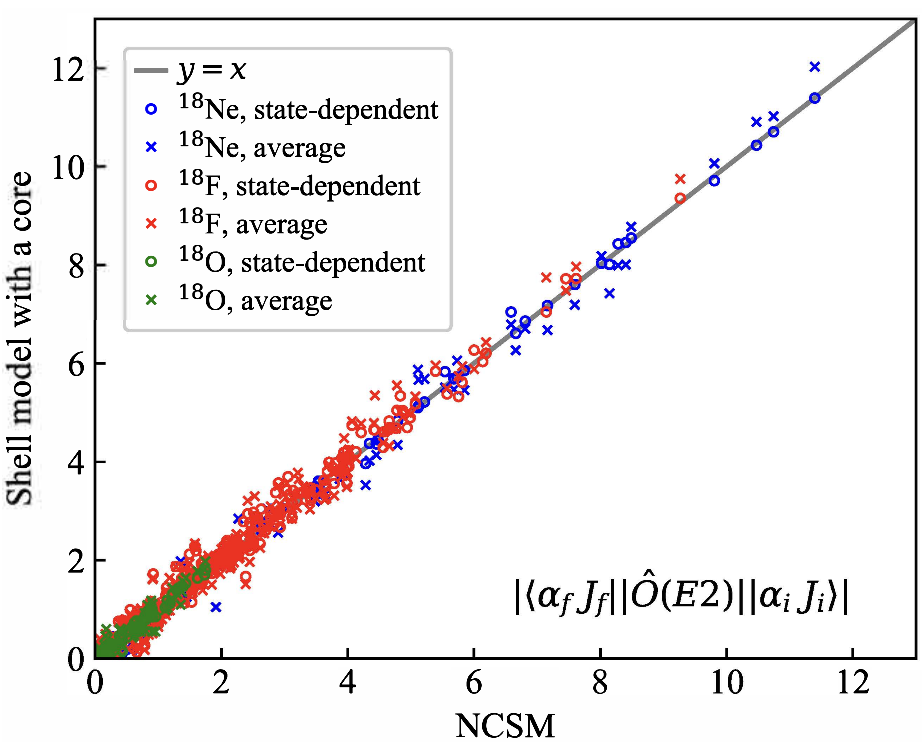
Okubo, Progr. Theor. Phys. 12 (1954); Suzuki, Lee, Prog. Theor. Phys. 68 (1980)
Dikmen, Lisetskiy, Barrett, Maris, Shirokov, Vary, PRC91, 064301 (2015)
Vary, Basili, Du, Lockner, Maris, Pal, Sarker, PRC98, 065502 (2018)
Smirnova, Barrett, Kim, Shin, Shirokov, Dikmen, Maris, Vary, PRC100, 054329 (2019)
Shin, Smirnova, Shirokov, Yang, Barrett, Li, Kim, Maris and Vary, arXiv: 2306.17289

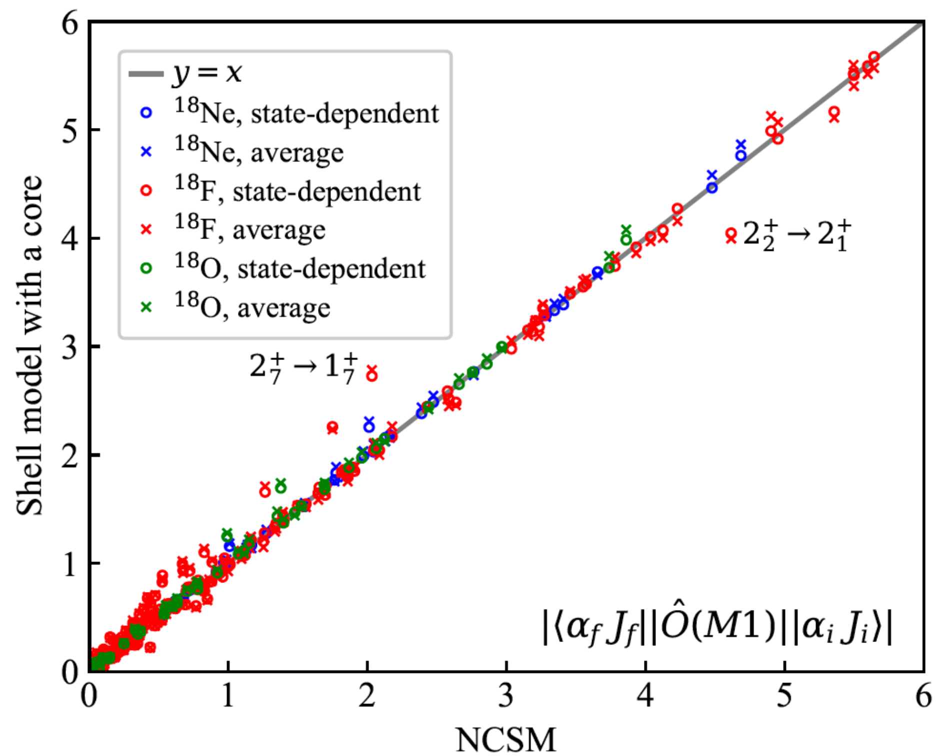
Binding energies of O-isotopes

rms(DJ16-6) ≈ 3671 keV;   rms(DJ16B) ≈ 235 keV; rms(USDB) ≈ 467 keV



Full NCSM E2 and M1 reduced transition matrix elements vs valence space results with effective charges derived from A=17 NCSM calculations.
Daejeon 16 in Nmax = 4 space with hw = 14 MeV





Zhen Li, N.A. Smirnova, A.M. Shirokov, I.J. Shin, B.R. Barrett, P. Maris and J.P. Vary, Arima Memorial Volume, World Scientific Publishing, Singapore; arXiv: 2205.15939

Scattering with the time-dependent basis function (tBF) approach

1. *Ab initio* structure calculation

$$H_0|\beta_i\rangle = E_i|\beta_i\rangle$$

$$H_0 = T_{rel} + V$$

⇓

$$\{|\beta_1\rangle, |\beta_2\rangle, \cdots, |\beta_n\rangle\}$$

2. Time-dependent

$$i\frac{d}{dt}|\psi(t)\rangle = H(t)|\psi(t)\rangle$$

$$H(t) = T_{rel} + V + V_I(t)$$

⇓

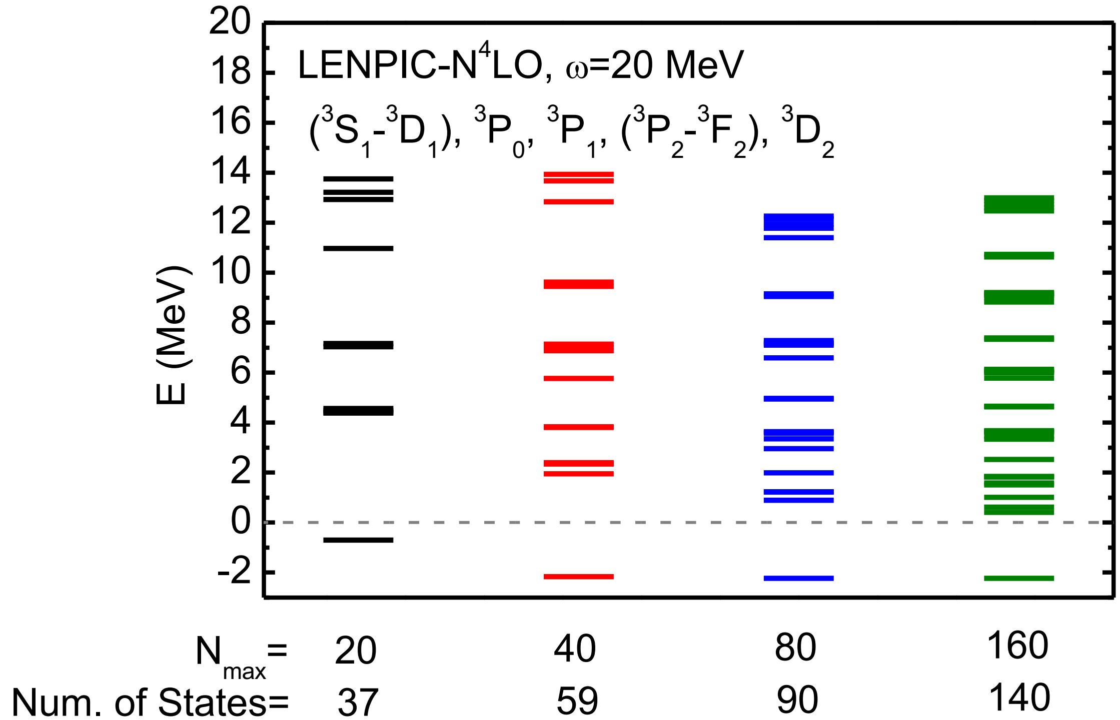
- State vector becomes amplitudes
- Operators become matrices

- Natural extension of the NCSM
- Non perturbative
- *Ab initio*
- Full quantal coherence

$V_I(t)$

- Weijie Du, Peng Yin, Yang Li, Guangyao Chen, Wei Zuo, Xingbo Zhao, and James P. Vary, *Phys. Rev. C* **97**, 064620 (2018);
- Weijie Du, Peng Yin, Guangyao Chen, Xingbo Zhao, and James P. Vary, *in Proceedings of the International Conference "Nuclear Theory in the Supercomputing Era–2016" (NTSE-2016), Khabarovsk, Russia, September 19–23,* 2016.
- Peng Yin, Weijie Du, Wei Zuo, Xingbo Zhao and James P. Vary, J. Phys. G Nucl. Part. Phys. 49, 125102 (2022);& 2208.00267

Deuteron ground state and scattering states



- Deuteron spectrum below E_{cut}=14 MeV, calculated by LENPIC-N4LO
- The deuteron ground state is well converged at large N_{max} and consistent with the experimental value;
- As the basis truncation increases, the discretized continuum states become increasingly dense; low-lying states tend to zero

Peng Yin et al., arXiv: 2208.00267

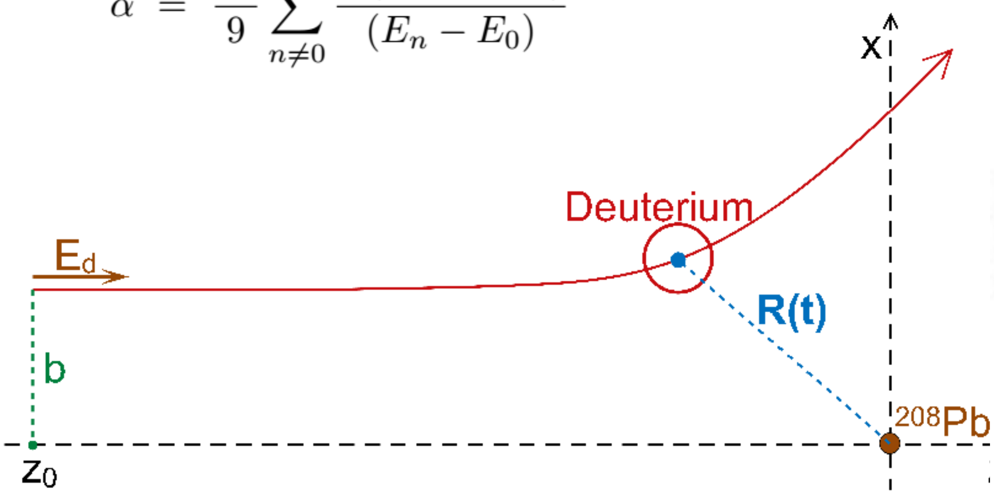
d+^{208}Pb scattering below Coulomb barrier
tBF with no adjustable parameters

Solve EOM for CM motion in external field:

$$V_{pot} = V_c + V_{pol}$$

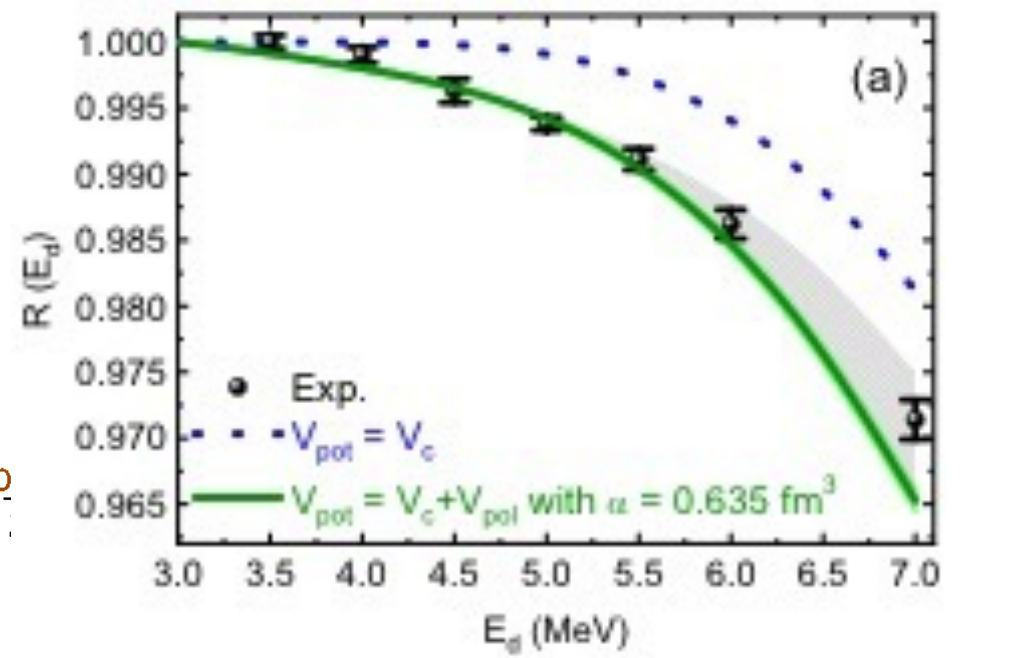
$$V_{pol} = -\frac{1}{2}\alpha Z^2 e^2 \frac{1}{(r^2 + r_0^2)^2}$$

$$\alpha = \frac{8\pi}{9}\sum_{n\neq 0}\frac{B(E1; 0 \to n)}{(E_n - E_0)}$$



$V_I(t) =$ time-dependent electric dipole field acting on np relative coordinates

$$R(E_d) = \frac{\sigma(E_d = 3\text{ MeV}, \theta_1 = 60°)}{\sigma(E_d = 3\text{ MeV}, \theta_2 = 150°)}\frac{\sigma(E_d, \theta_2 = 150°)}{\sigma(E_d, \theta_1 = 60°)}$$



- Scattering states of *np* system: LENPIC N4LO in 3DHO basis with large N_{max}
- Rutherford + polarization potential trajectory of CM
- Scattering basis space: coherent superposition of hundreds of states
- E1 transition included; M1 transitions found to be very weak in comparison

Peng Yin, Weijie Du, Wei Zuo, Xingbo Zhao and James P. Vary, J. Phys. G Nucl. Part. Phys. 49 125102 (2022);
Peng Yin et al., arXiv: 2208.00267

What lies ahead for nuclear theory across energy scales?

- Need for increased theory effort at deriving and validating EFTs
  Expand multi-disciplinary and multi-national collaborative efforts

- Need for enhanced computational power to greatly expand basis spaces
  Artificial Intelligence and/or Quantum Computing can be keys to progress

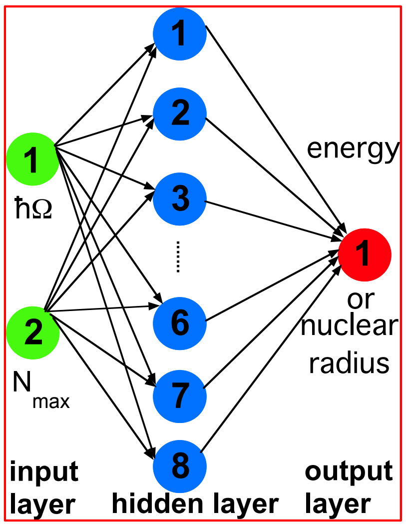
Deep Learning for Nuclear Binding Energy and Radius

Scientific Achievement

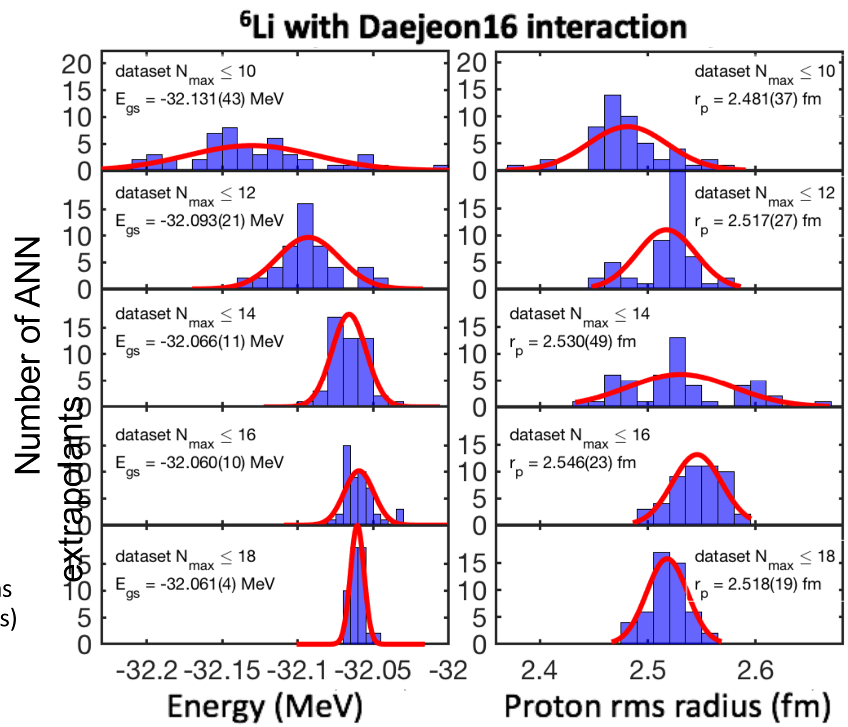
- Developed artificial neural networks (ANNs) for extending the application range of the *ab initio* No-Core Shell Model (NCSM)
- Demonstrated predictive power of ANNs for converged solutions of weakly converging simulations of the nuclear radius
- Provided a new paradigm for matching deep learning with results from high performance computing simulations

Significance and Impact

- Guides experimental programs at DOE's rare isotope facilities
- Extends the predictive power of *ab initio* nuclear theory beyond the reach of current high performance computing simulations
- Establishes foundation for deep learning tools in nuclear theory useful for a wide range of applications



Neural network **(above)** used to successfully extrapolate the ^{6}**Li** ground state energy and rms radius from modest basis spaces (N_{max} datasets) to extreme basis spaces achieving basis parameter independence (histograms of extrapolation ensembles in **right figure**).

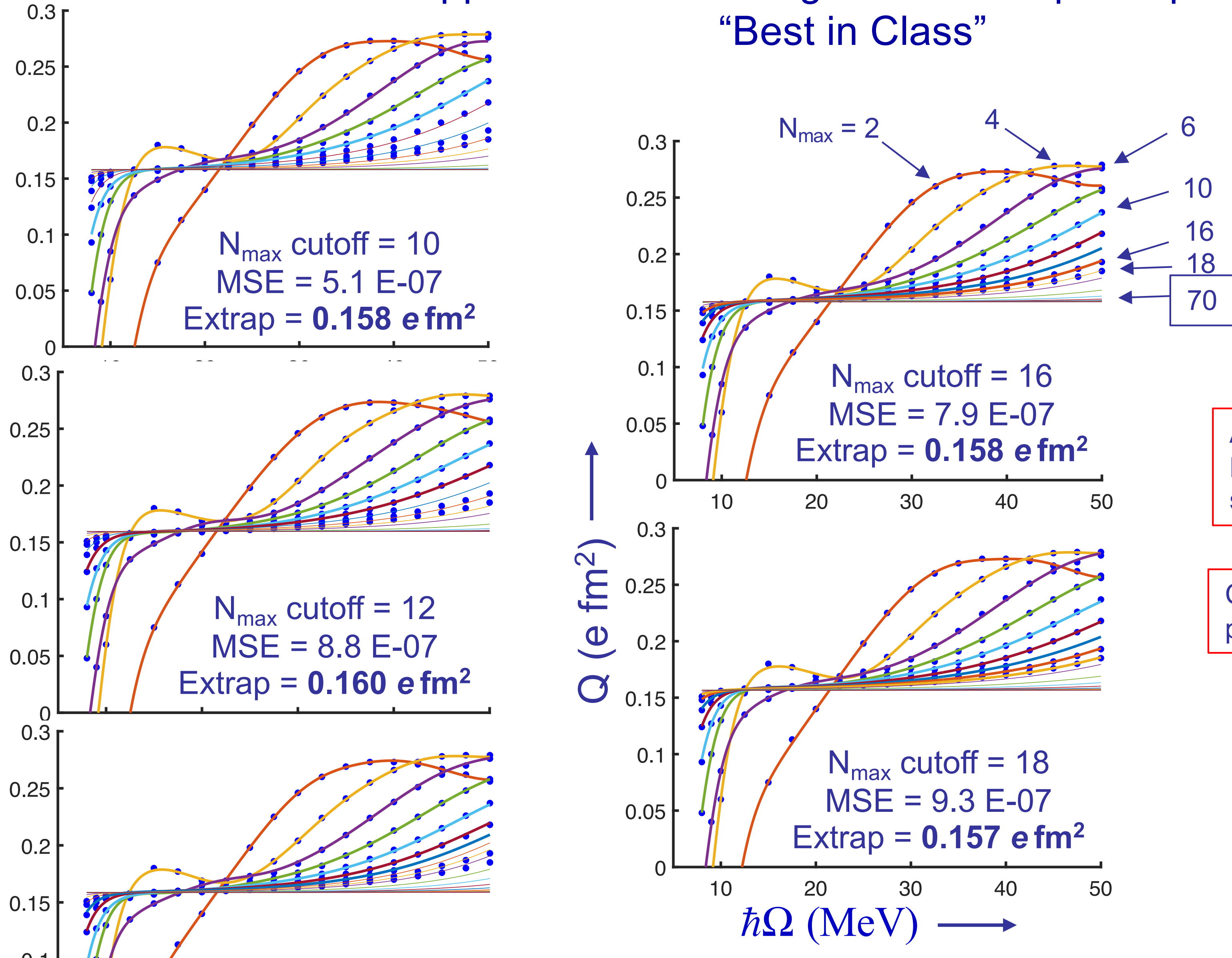


Research Details

- Develop ANNs that extend the reach of high performance computing simulations of nuclei
- Predict properties of nuclei based on *ab initio* structure calculations in achievable basis spaces
- Produce accurate predictions of nuclear properties with quantified uncertainties using fundamental inter-nucleon interactions such as Daejeon16

Ref: G. A. Negoita, et al., Phys. Rev. C **99**, 054308 (2019); https://journals.aps.org/prc/pdf/10.1103/PhysRevC.99.054308

Initial application to the ^{6}Li ground state quadrupole moment
“Best in Class”

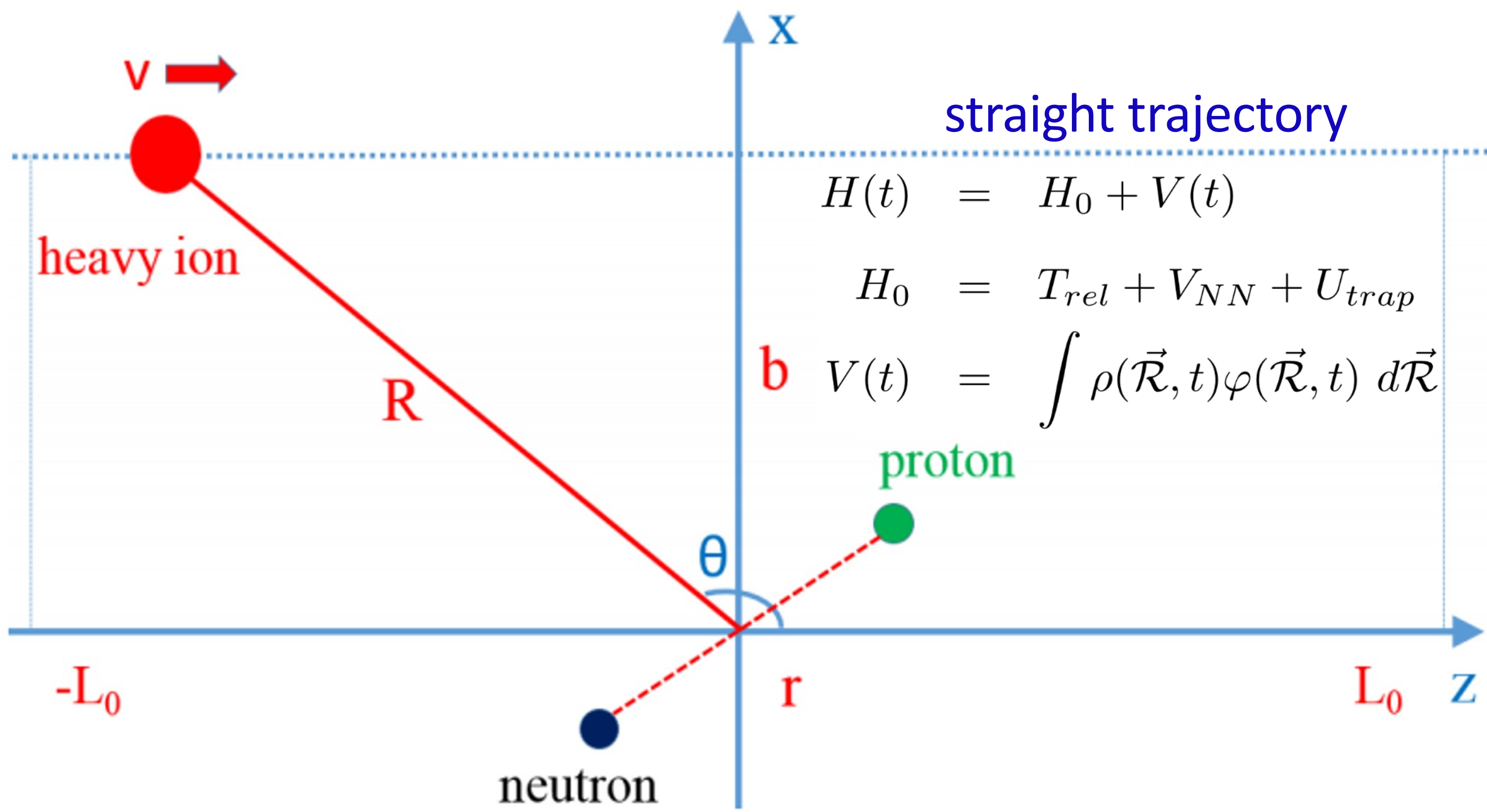


ANN predictions for N_{max} = 20, 25, . . . 65, 70 shown in all graphs

Converged sequence of ANN predictions: Q = 0.157(2) *e* fm^2

M. Lockner, R. McCarty, et al., in preparation

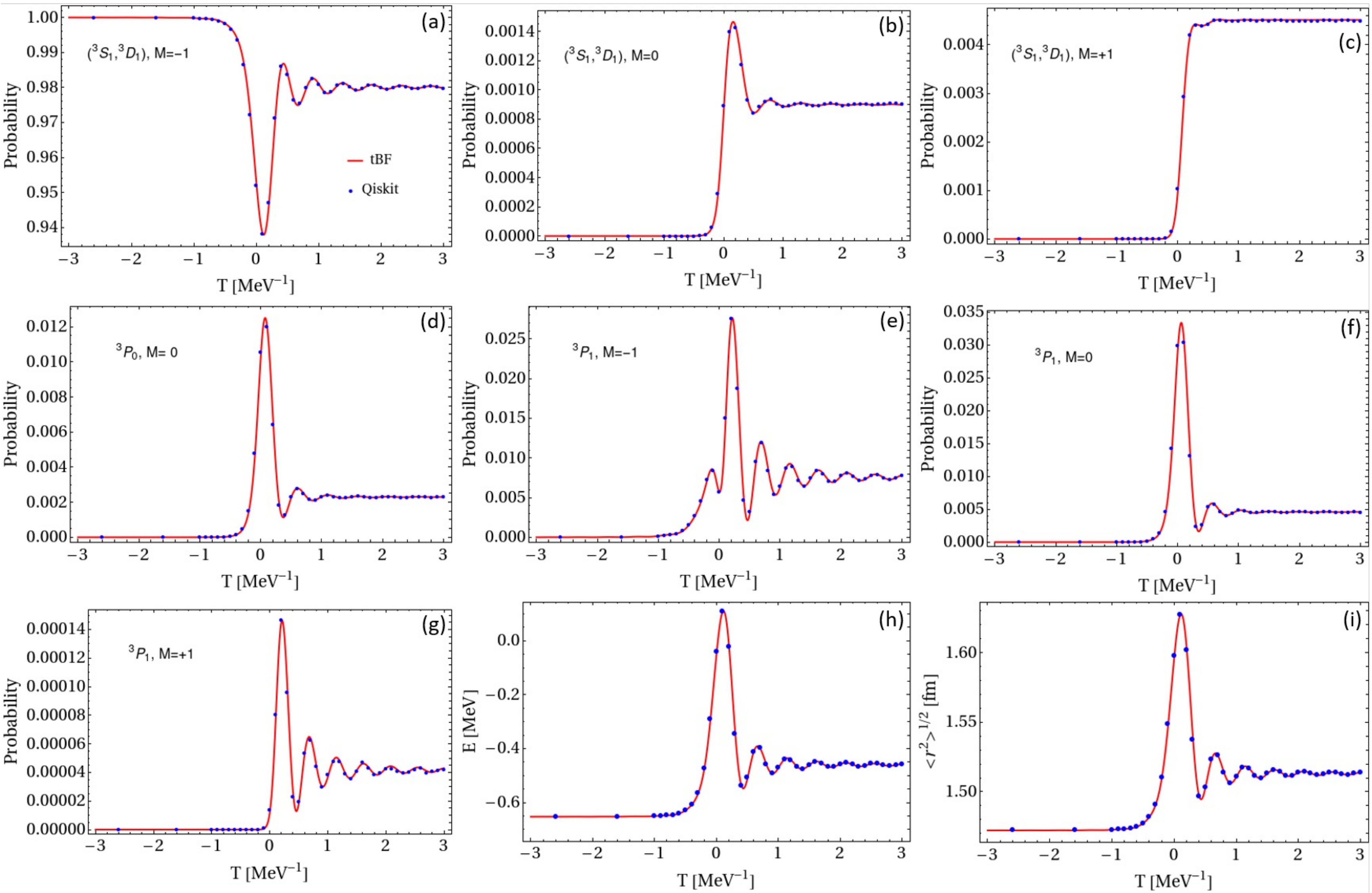
tBF on Quantum Computers
Demonstration case: Coulomb excitation of deuterium by peripheral scattering on a heavy ion



- H_0: Target (deuteron in trap) Hamiltonian
- φ: Coulomb field from heavy ion (U^{92+}) sensed by target
- ρ: Charge density distribution of target
- Limited to 7 deuteron states

Previously solved with tBF: Weijie Du *et al.*, Phys. Rev. C 97, 064620 (2018)

Transition probabilities and observables



Weijie Du, James P. Vary, Xingbo Zhao and Wei Zuo, , Phys. Rev. A 104, 012611 (2021)

Many outstanding nuclear physics
puzzles and discoveries remain

Origin of the successful nuclear shell model
Clustering phenomena
Nuclear reactions and breakup
Astrophysical processes & drip lines
Precision Nuclear Theory as a window on
Physics beyond the Standard Model

A comprehensive program
of theory vs experiment
needed to maximize discovery potential

Thank you for your attention

I welcome your questions