No Core CI Calculations for light nuclear systems

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UNEDF SciDAC Collaboration
Universal Nuclear Energy Density Functional

SciDAC project – UNEDF

spokespersons: Rusty Lusk (ANL), Witek Nazarewicz (ORNL/UT)

http://www.unedf.org

National Science Foundation
WHERE DISCOVERIES BEGIN

PetaApps award

PIs: Jerry Draayer (LSU), Umit Catalyurek (OSU)

Masha Sosonkina, James Vary (ISU)

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

INCITE award – Computational Nuclear Structure

PI: James Vary (ISU)

NERSC CPU time

NERSC

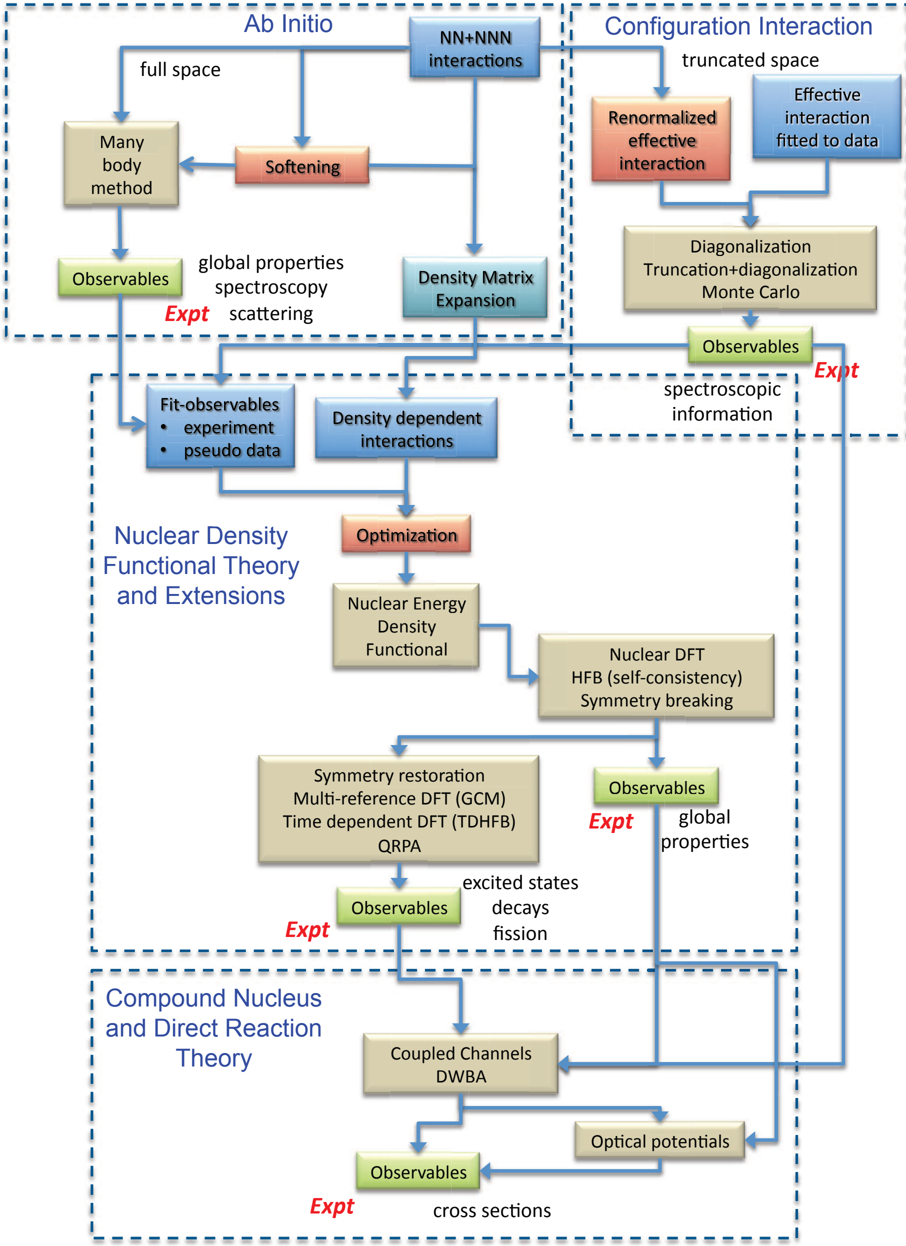
SciDAC/UNEDF – Uniform description of nuclear structure

Universal Nuclear Energy Density Functional that spans the entire mass table based on ab initio calculations

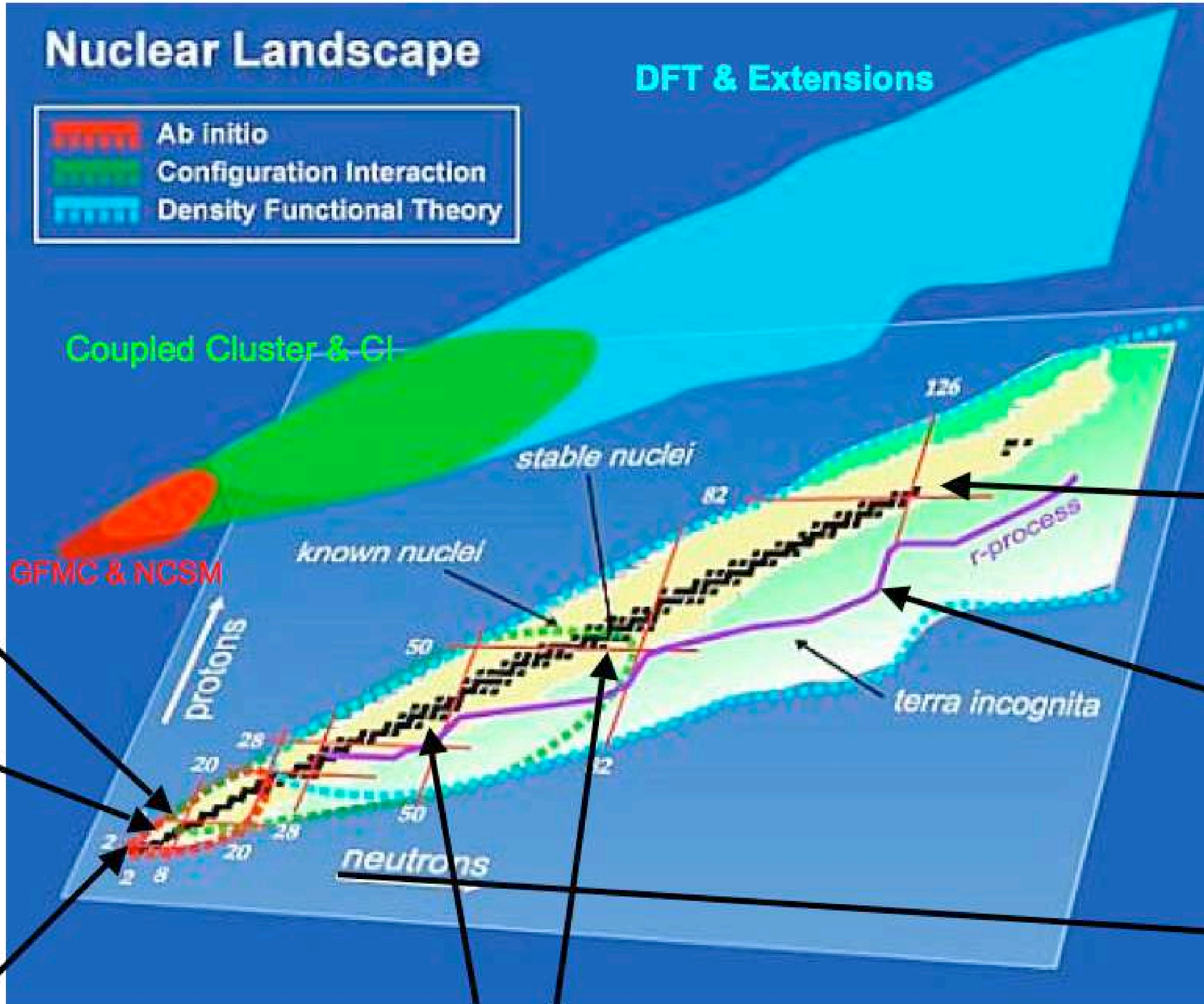
- Greens Function Monte Carlo (Pieper *et al*, ANL)
- No-Core Configuration Interaction calculations
- Coupled Cluster (Papenbrock *et al*, ORNL)

http://www.unedf.org

spokespersons:
R. Lusk (ANL)
W. Nazarewicz (ORNL/UT)



"Digital FRIB" and beyond



Astro

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

Hoyle

Standard Model

QCD/χEFT

0ν-$\beta\beta$ Beyond Standard Model

Nuclear Energy

fission

Astro

r-process

neutron star crust

Configuration Interaction Methods

- Expand wave function in basis states $|\Psi\rangle = \sum a_i |\psi_i\rangle$
- Express Hamiltonian in basis $\langle\psi_j|\hat{\mathbf{H}}|\psi_i\rangle = H_{ij}$
- Diagonalize Hamiltonian matrix H_{ij}
- Complete basis $\longrightarrow$ exact result
  - caveat: complete basis is infinite dimensional

- In practice
  - truncate basis
  - study behavior of observables as function of truncation

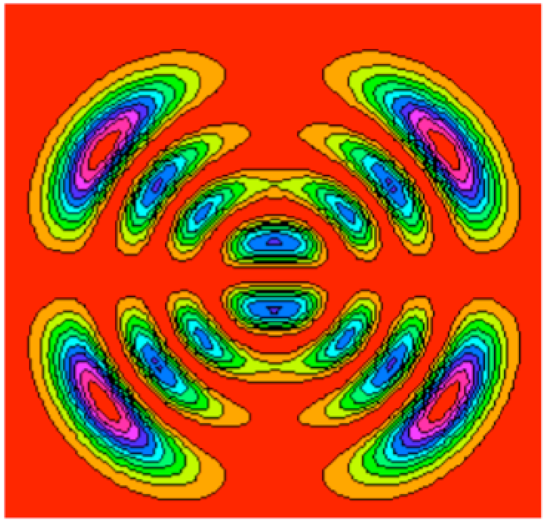
- Computational challenge
  - construct large ($10^{10} \times 10^{10}$) sparse symmetric real matrix H_{ij}
  - use Lanczos algorithm
    to obtain lowest eigenvalues & eigenvectors

Many-Body Basis Space

- Expand wave function in basis states $|\Psi\rangle = \sum a_i |\psi_i\rangle$
- Many-Body basis states $|\psi_i\rangle$
  - Slater Determinants of single-particle states $|\phi\rangle$

$$|\psi\rangle \quad = \quad |\phi_1\rangle \otimes \ldots \otimes |\phi_A\rangle$$

  - single-particle basis states eigenstates of SU(2) operators $\hat{\mathbf{L}}^2$, $\hat{\mathbf{S}}^2$, $\hat{\mathbf{J}}^2 = (\hat{\mathbf{L}} + \hat{\mathbf{S}})^2$, and $\hat{\mathbf{J}}_z$ w. quantum numbers $|\phi\rangle \;=\; |n, l, s, j, m\rangle$
  - radial wavefunctions: Harmonic Oscillator



sample harmonic oscillator basis function

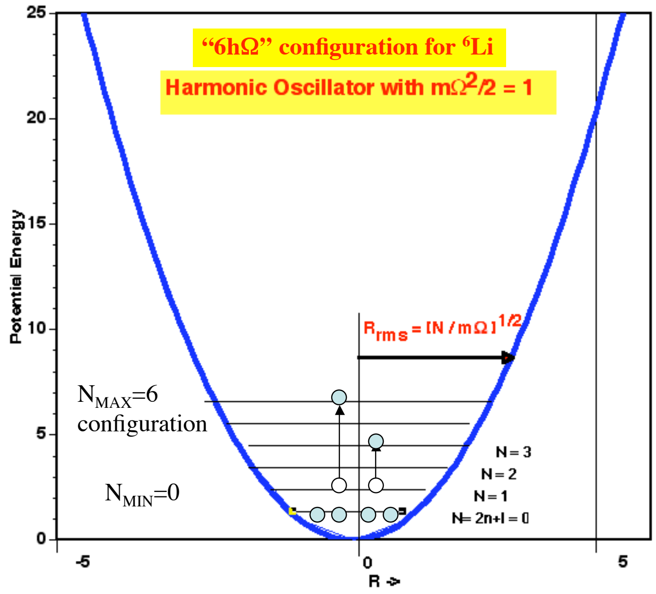
- M-scheme: many-body basis states eigenstates of $\hat{\mathbf{J}}_z$

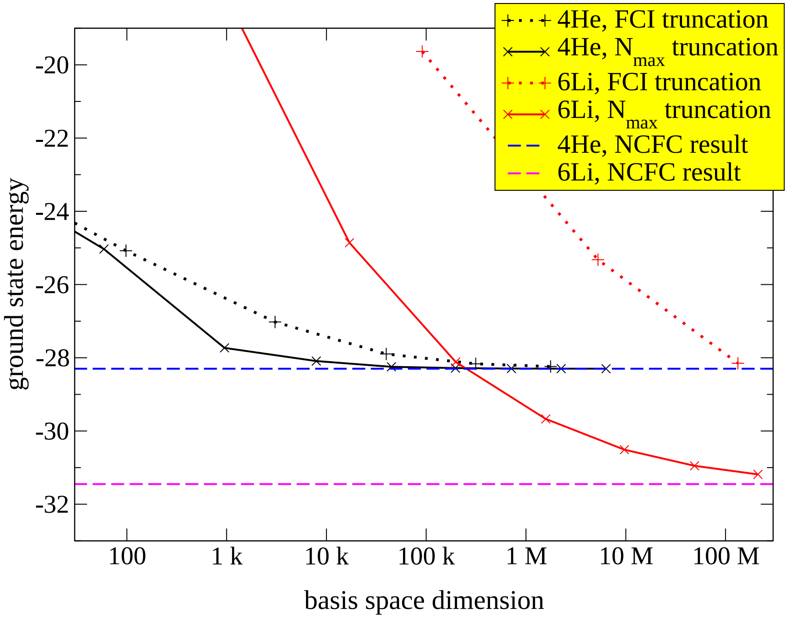
$$\hat{\mathbf{J}}_z|\psi\rangle \quad = \quad M|\psi\rangle \quad = \sum_{i=1}^{A} m_i|\psi\rangle$$

- Alternatives: LS-scheme, Total-J-scheme, Symplectic basis, ...

Truncation Schemes

- $N_{\max}$ truncation
  - truncation on the total number of H.O. oscillator quanta above minimal configuration for that nucleus
  - allows for exact seperation of Center-of-Mass motion and intrinsic motion





- Alternative truncation schemes
  - FCI – Full Configuration Interaction – truncation on single-particle basis only
  - Importance Sampling, Monte Carlo Sampling, Symplectic, . . .

Intermezzo: Center-of-Mass excitations

- Use single-particle coordinates, not relative (Jacobi) coordinates
  - straightforward to extend to many particles
  - have to seperate Center-of-Mass motion from intrinsic motion
- Add Lagrange multiplier to Hamiltonian

$$\hat{\mathbf{H}}_{\text{rel}} \quad \longrightarrow \quad \hat{\mathbf{H}}_{\text{rel}} + \Lambda_{CM}\left(\hat{\mathbf{H}}_{CM}^{H.O.} - \frac{3}{2}\,\hbar\omega\right)$$

with $\hat{\mathbf{H}}_{\text{rel}} = T_{\text{rel}} + V_{\text{rel}}$ the relative Hamiltonian

  - seperates CM excitations from CM ground state $|\Phi_{CM}\rangle$
  - Center-of-Mass wave function factorizes for H.O. basis functions in combination with N_{max} truncation

$$\begin{aligned} |\Psi_{\text{total}}\rangle &= |\phi_1\rangle \otimes \ldots \otimes |\phi_A\rangle \\ &= |\Phi_{\text{Center-of-Mass}}\rangle \otimes |\Psi_{\text{intrinsic}}\rangle \end{aligned}$$

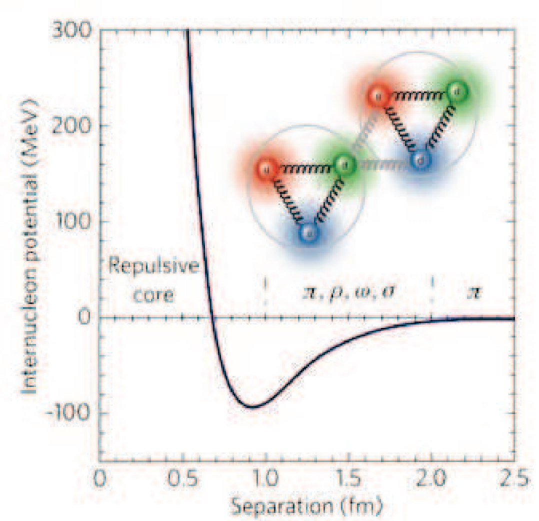
where

$$\hat{\mathbf{H}}_{\text{rel}}|\Psi_{\text{j, intrinsic}}\rangle = E_{\text{j}}|\Psi_{\text{j, intrinsic}}\rangle$$

Configuration Interaction Methods

- Expand wave function in basis states $|\Psi\rangle = \sum a_i |\psi_i\rangle$
- Express Hamiltonian in basis $\langle\psi_j|\hat{\mathbf{H}}|\psi_i\rangle = H_{ij}$

$$\hat{\mathbf{H}} = \hat{\mathbf{T}}_{\text{rel}} + \Lambda_{CM}\left(\hat{\mathbf{H}}^{H.O.}_{CM} - \frac{3}{2}\hbar\omega\right) + \sum_{i<j} V_{ij} + \sum_{i<j<k} V_{ijk} + \ldots$$

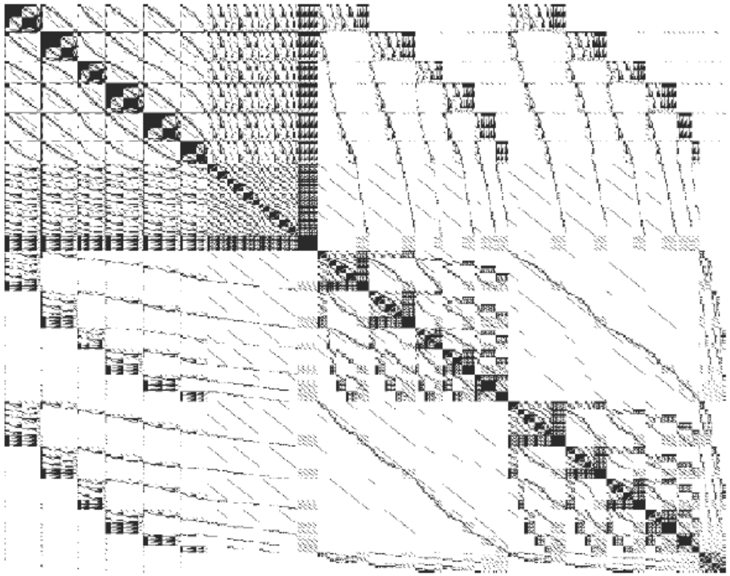


- Pick your favorite potential
  - Argonne potentials: AV8, AV18 (plus Illinois NNN interactions)
  - Bonn potentials
  - Chiral NN interactions (plus chiral NNN interactions)
  - ...
  - JISP16 (phenomenological NN potential)
  - ...

Configuration Interaction Methods

- Expand wave function in basis states $|\Psi\rangle = \sum a_i |\psi_i\rangle$
- Express Hamiltonian in basis $\langle\psi_j|\hat{\mathbf{H}}|\psi_i\rangle = H_{ij}$
  - large sparse symmetric matrix

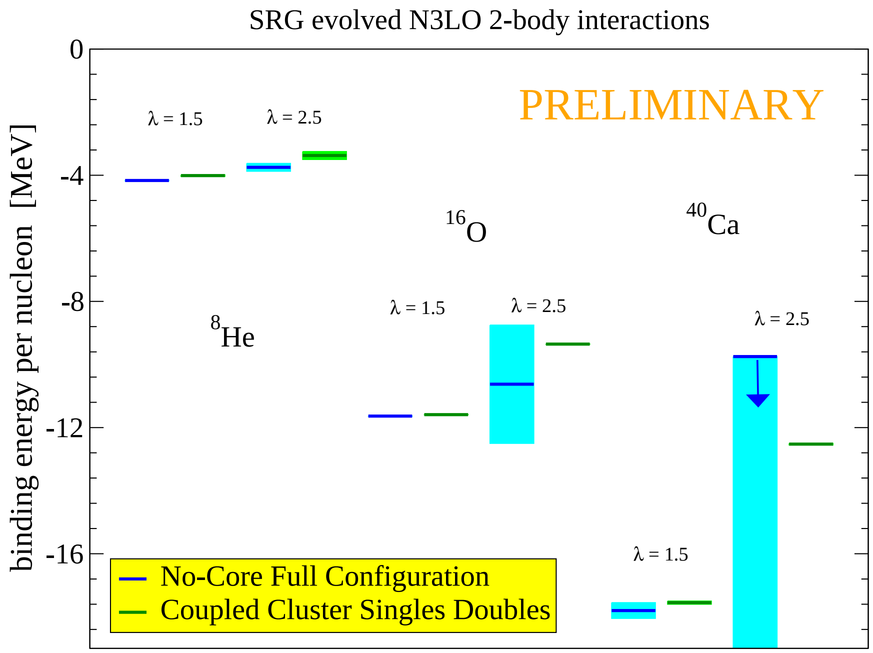
Sparsity Structure for ^{6}Li



- Obtain lowest eigenvalues using Lanczos algorithm
  - Eigenvalues: bound state spectrum
  - Eigenvectors: nuclear wavefunctions
- Use wavefunctions to calculate observables
- Challenge: eliminate dependence on basis space truncation

CI calculation – convergence

- Expand wave function in basis states $|\Psi\rangle = \sum a_i |\psi_i\rangle$
- Express Hamiltonian in basis $\langle\psi_j|\hat{\mathbf{H}}|\psi_i\rangle = H_{ij}$
- Diagonalize sparse real symmetric matrix H_{ij}
- Variational: for any finite truncation of the basis space, eigenvalue is an upper bound for the ground state energy
- Smooth approach to asymptotic value with increasing basis space
  $\Longrightarrow$ extrapolation
  to infinite basis
- Convergence: independence of basis space parameters
  - different methods
    (NCFC, CC, GFMC, DME, ...)
    using the same interaction should give same results within numerical errors



Intermezzo: Extrapolation Techniques

Challenge: achieve numerical convergence for no-core Full Configuation calculations using finite model space calculations

- Perform a series of calculations with increasing N_{max} truncation (while keeping everything else fixed)
- Extrapolate to infinite model space $\longrightarrow$ exact results
  - binding energy: exponential in N_{max}

$$E^{N}_{\text{binding}} = E^{\infty}_{\text{binding}} + a_1 \exp(-a_2 N_{\text{max}})$$

  - use 3 or 4 consecutive N_{max} values to determine $E^{\infty}_{\text{binding}}$
  - use $\hbar\omega$ and N_{max} dependence to estimate numerical error bars

    Maris, Shirokov, Vary, Phys. Rev. C79, 014308 (2009)
  - need at least $N_{\text{max}} = 8$ for meaningfull extrapolations

Intermezzo: Extrapolation Techniques

Challenge: achieve numerical convergence for no-core Full Configuation calculations using finite model space calculations

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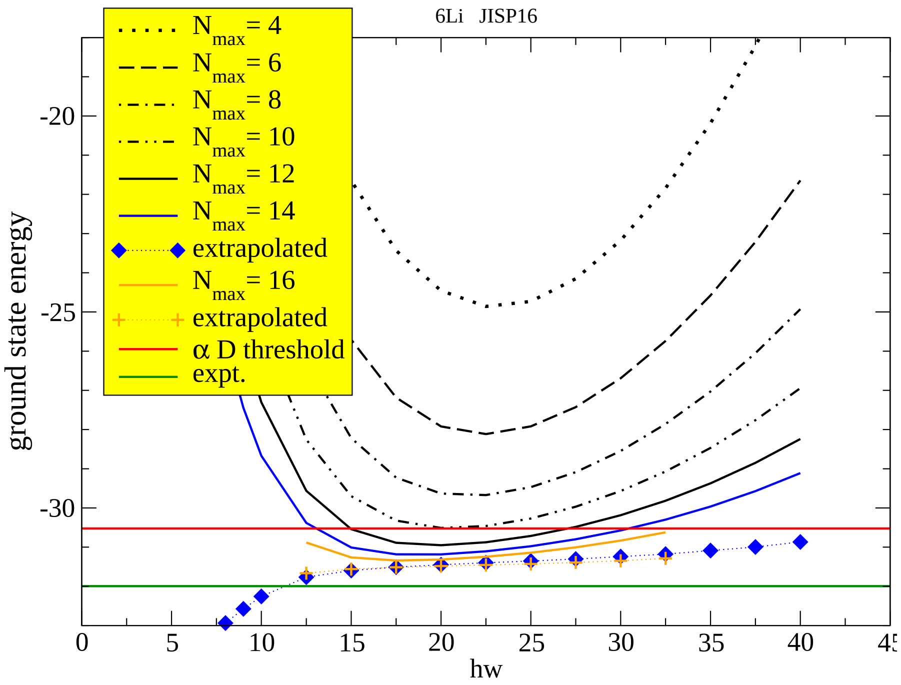
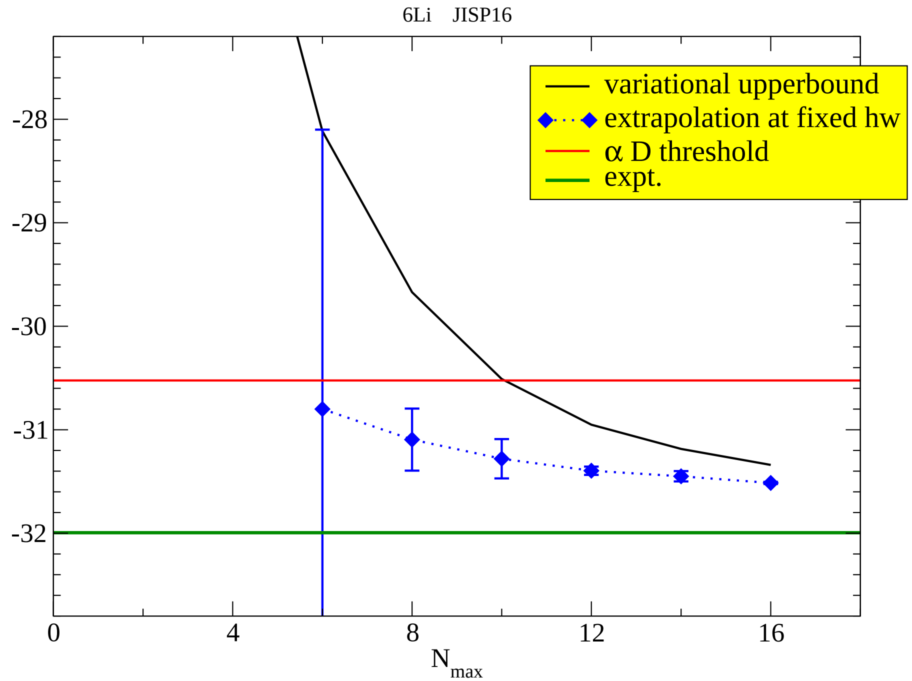
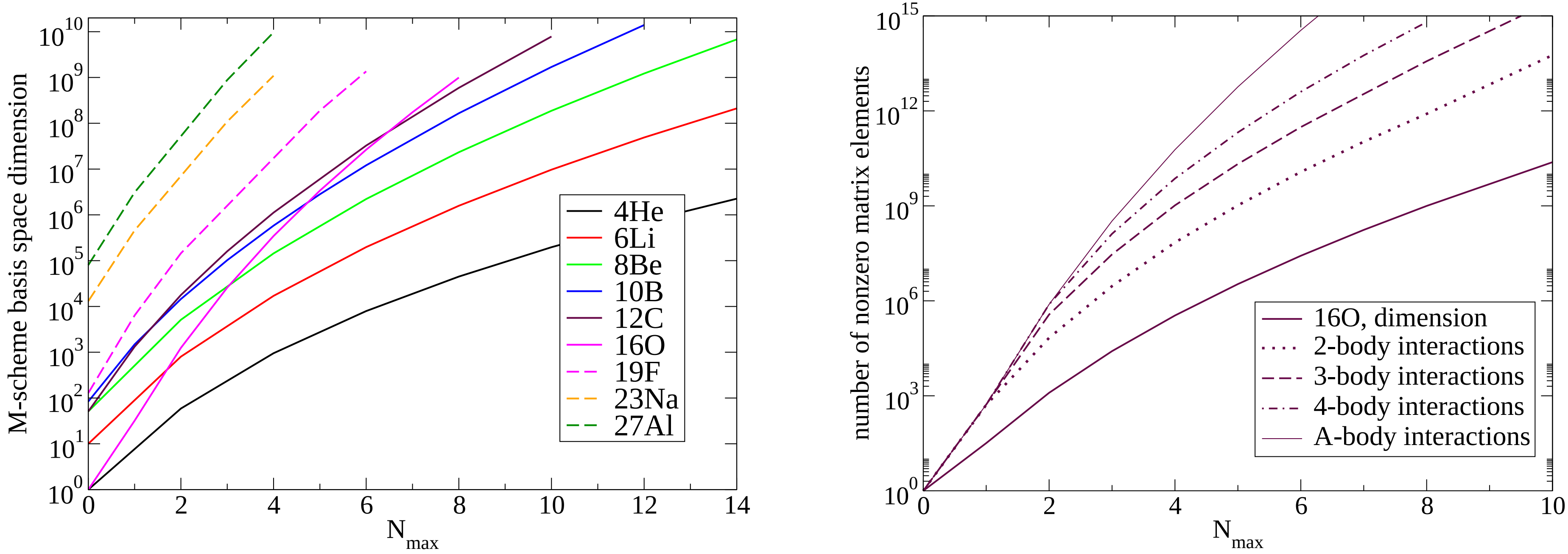




CI calculations – main challenges

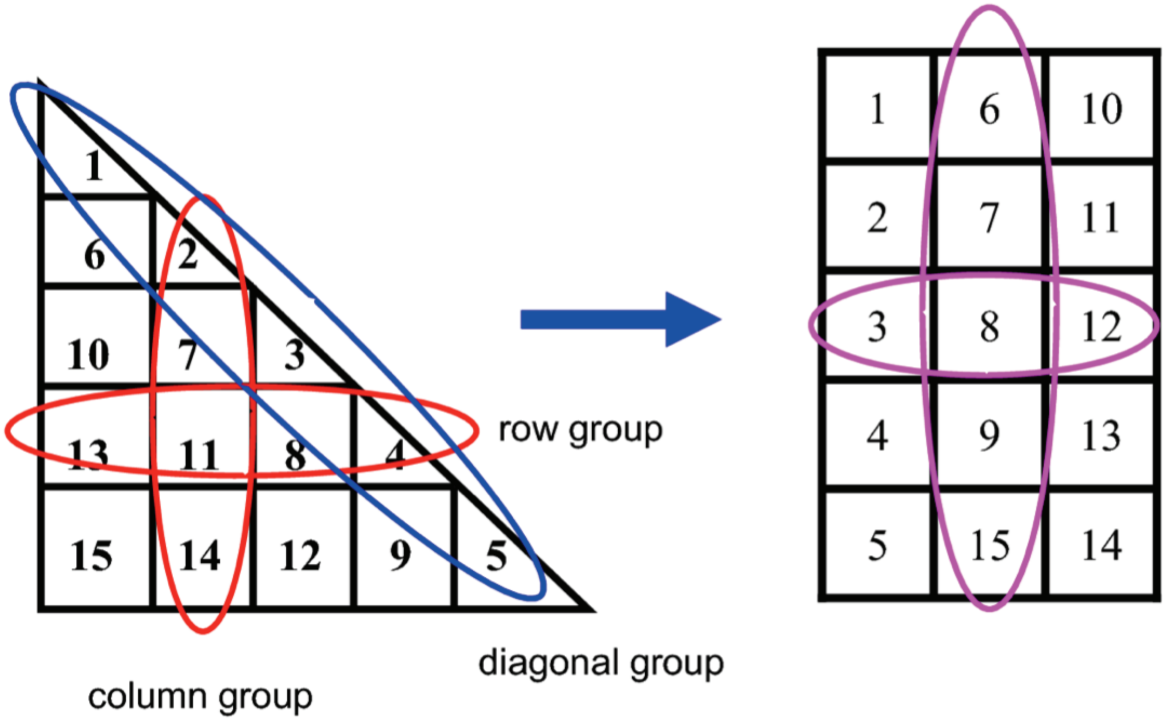


- Single most important computational issue:
  exponential increase of dimensionality with increasing H.O. levels
- Additional computational issue:
  sparseness of matrix / number of nonzero matrix elements

High-performance computing

- Hardware
  - individual desk- and lap-tops
  - local linux clusters
  - NERSC (DOE)
    - 10,000,000 CPU hours for ISU collaboration
  - Leadership Computing Facilities (DOE)
    INCITE award – Computational Nuclear Structure (PI: J. Vary, ISU)
    - 28,000,000 CPU hours on Cray XT5 at ORNL
    - 15,000,000 CPU hours on IBM BlueGene/P at ANL
  - grand challenge award at Livermore (Jurgenson, Navratil, Ormand)
  - applied for CPU time at NCSA (NSF) – Blue Waters (IBM)
- Software
  - Lanczos algorithm – iterative method
    to find lowest eigenvalues and eigenvectors of sparse matrix
  - implemented in Many Fermion Dynamics
    - parallel F90/MPI/OpenMP CI code for nuclear physics

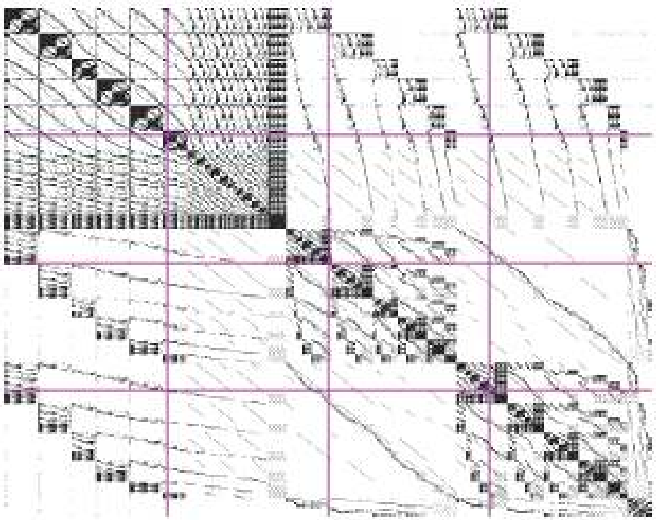
MFDn – 2-dimensional distribution of matrix

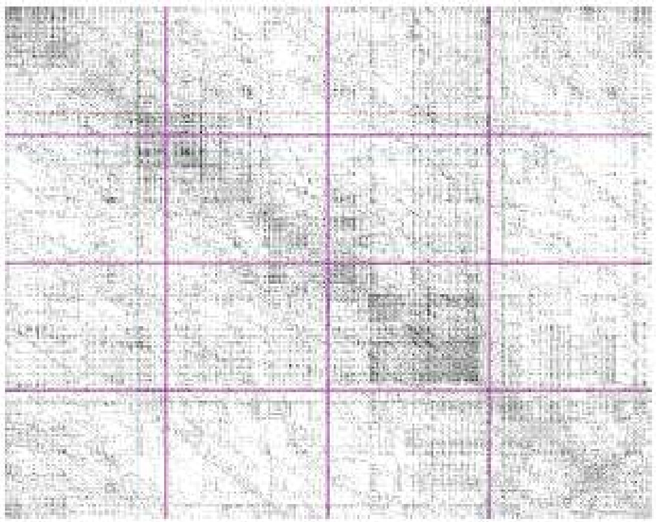


- Real symmetric matrix: store only lower (or upper) triangle
- Store Lanczos vectors distributed over all processors
- In principle, we can deal with arbitrary large vectors
  even if we cannot store an entire vector on a single processor
  - largest dimension: 8 billion, 32 GB / vector in single precision

MFDn – load-balancing

- Lexico-graphical enumeration of basis states on d procs
- Round-robin distribution of basis states over d procs





- Almost perfect load balancing
- However, no (apparent) structure in sparse matrix
  - multi-level blocking scheme to locate nonzero's (Sternberg 2008)

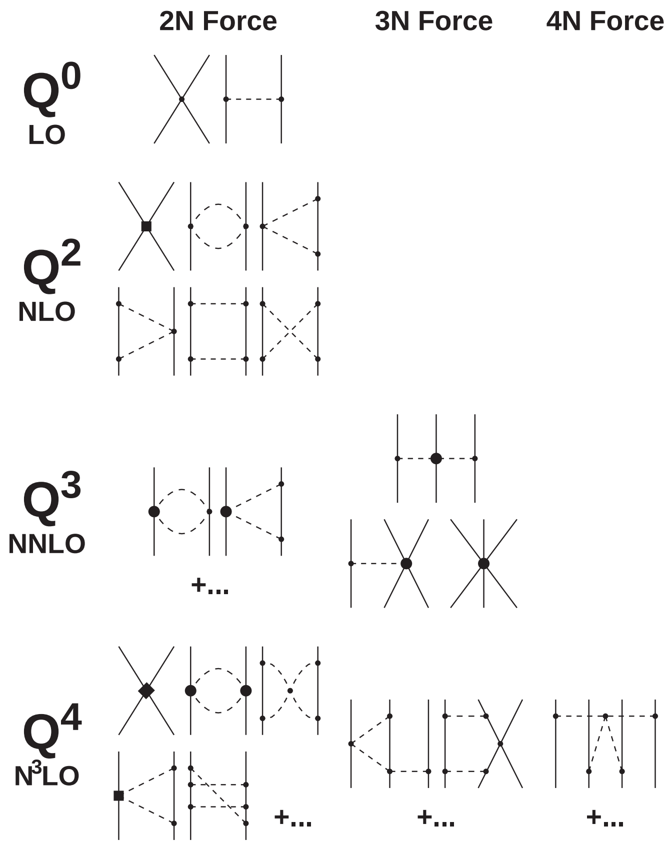
Under development: distribute groupds of basis states over d procs in order to retain part of the natural structure of the matrix

Strong force between nucleons

- Strong interaction in principle calculable from QCD
- Use chiral perturbation theory to obtain effective A-body interaction from QCD   Entem and Machleidt, Phys. Rev. C**68**, 041001 (2003)
  - controlled power series expansion in Q/Λ_χ with $\Lambda_\chi \sim 1$ GeV
  - natural hierarchy for many-body forces

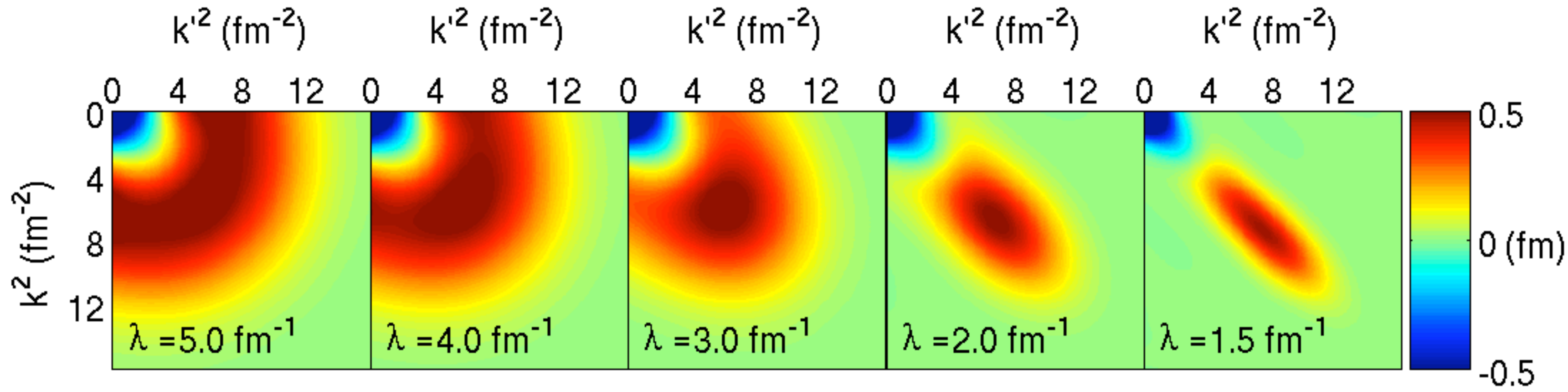
$$V_{NN} \gg V_{NNN} \gg V_{NNNN}$$

  - in principle no free parameters
    - in practice a few undetermined parameters
  - renormalization necessary
    - Lee–Suzuki–Okamoto
    - Similarity Renormalization Group



Similarity Renormalization Group – NN interaction

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

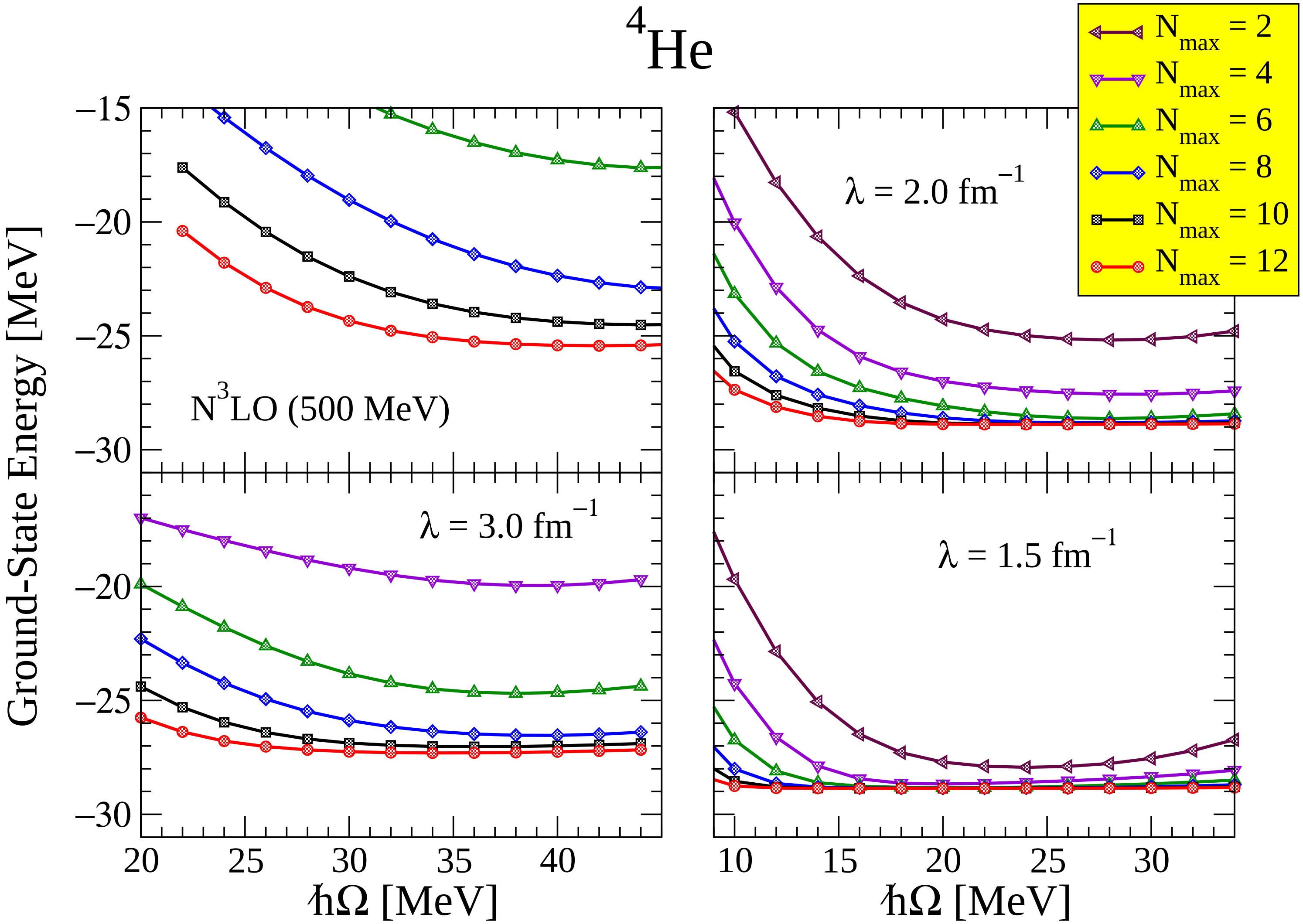


  - drives interaction towards band-diagonal structure
  - SRG shifts strength between 2-body and many-body forces
- Initial chiral EFT Hamiltonian
  power-counting hierarchy A-body forces

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

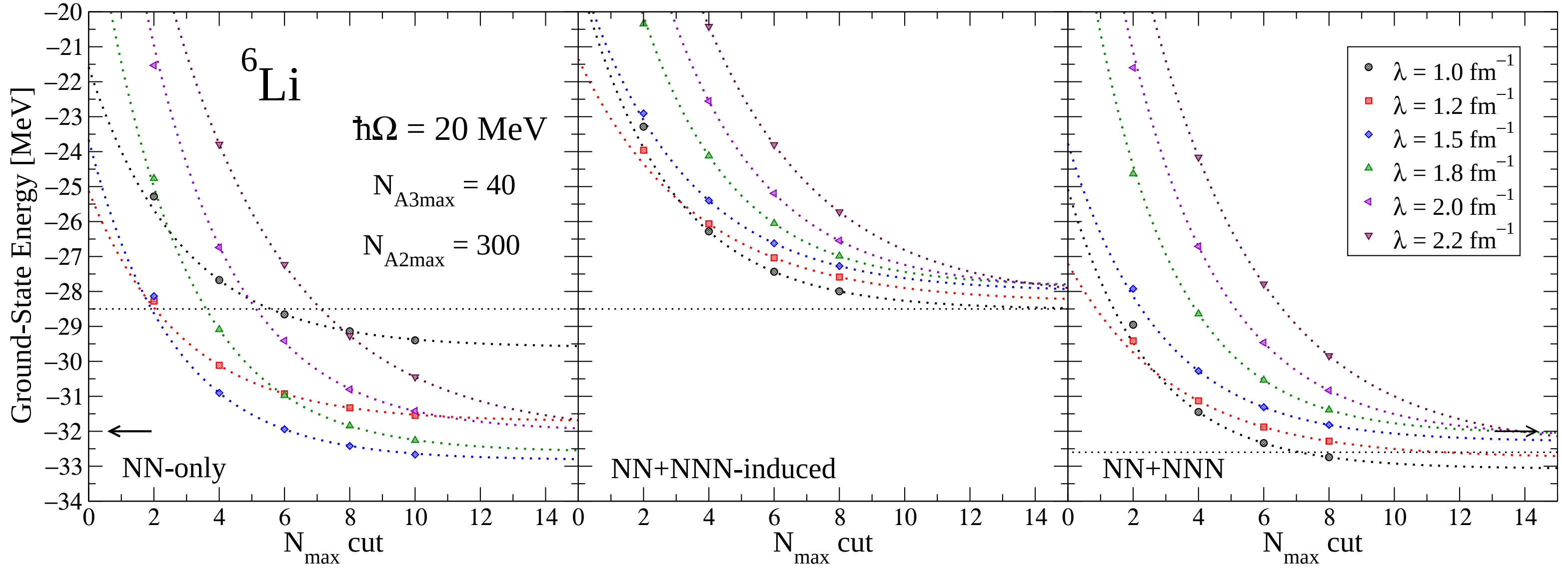
  - key issue: preserve hierarchy of many-body forces

Improve convergence rate by applying SRG to N3LO



Bogner, Furnstahl, Maris, Perry, Schwenk, Vary, NPA801, 21 (2008), arXiv:0708.3754

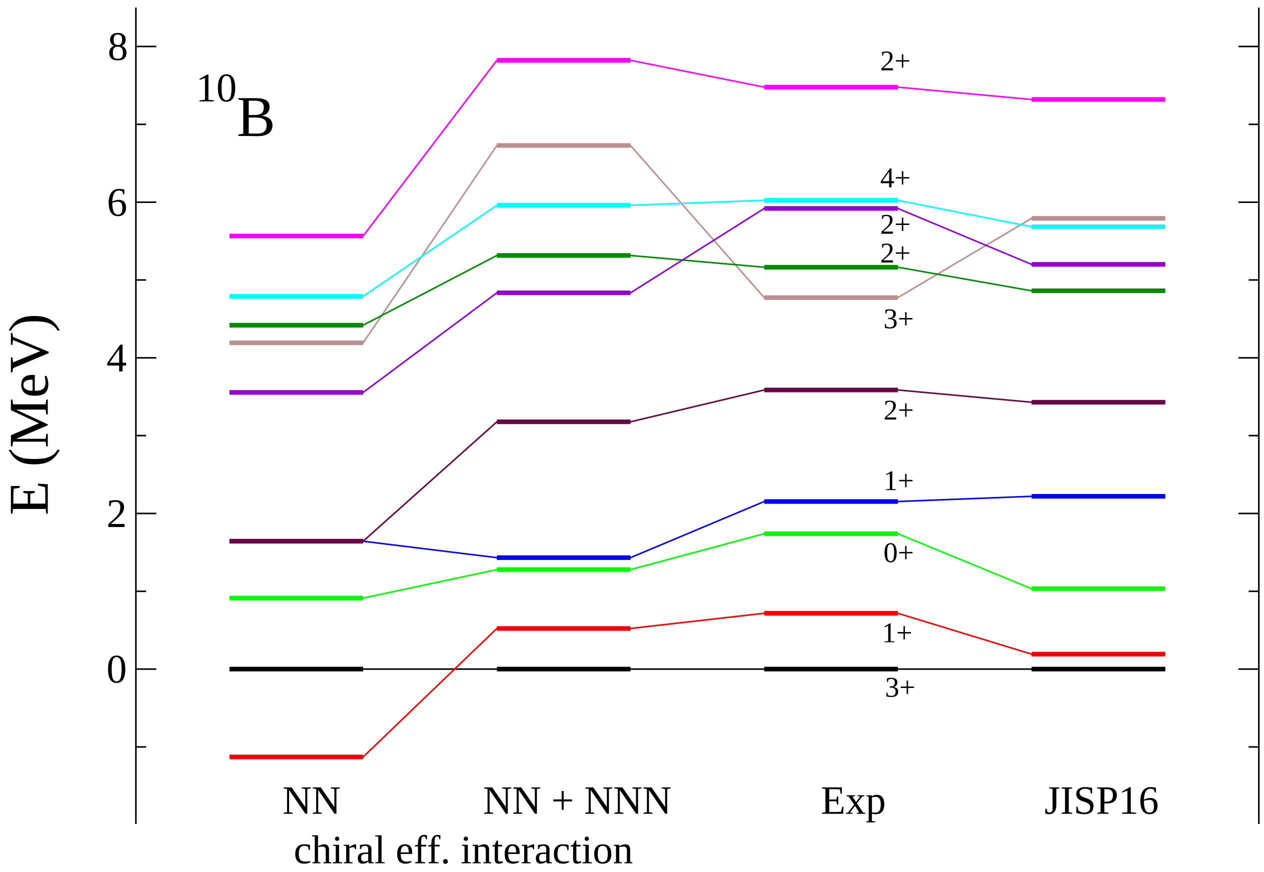
Effect of three-body forces



(Jurgenson, Navratil, Furnstahl, PRC83, 034301 (2011), arXiv:1011.4085)

- Induced 3NF significantly reduce dependence on SRG parameter
- N2LO 3NF
  - binding energy in agreement with experiment
  - may need induced 4NF?
- Calculations for $A = 7$ to 12 in progress (LLNL)

Do we really need 3-body interactions?



Spectrum of ^{10}B

with chiral 2- and 3-body forces at $N_{\text{max}} = 6$

nonlocal 2-body interaction JISP16 at $N_{\text{max}} = 8$

Vary, Maris, Negoita, Navratil, Gueorguiev, Ormand, Nogga, Shirokov, and Stoica, in “Exotic Nuclei and Nuclear/Particle Astrophysic (II)”, AIP Conf. Proc. 972, 49 (2008); N3LO+3NF from Navratil, Gueorguiev, Vary, Ormand, and Nogga, PRL 99, 042501 (2007); for JISP16 see Shirokov, Vary, Mazur, Weber, PLB **644**, 33 (2007)

Phenomeological NN interaction: JISP16

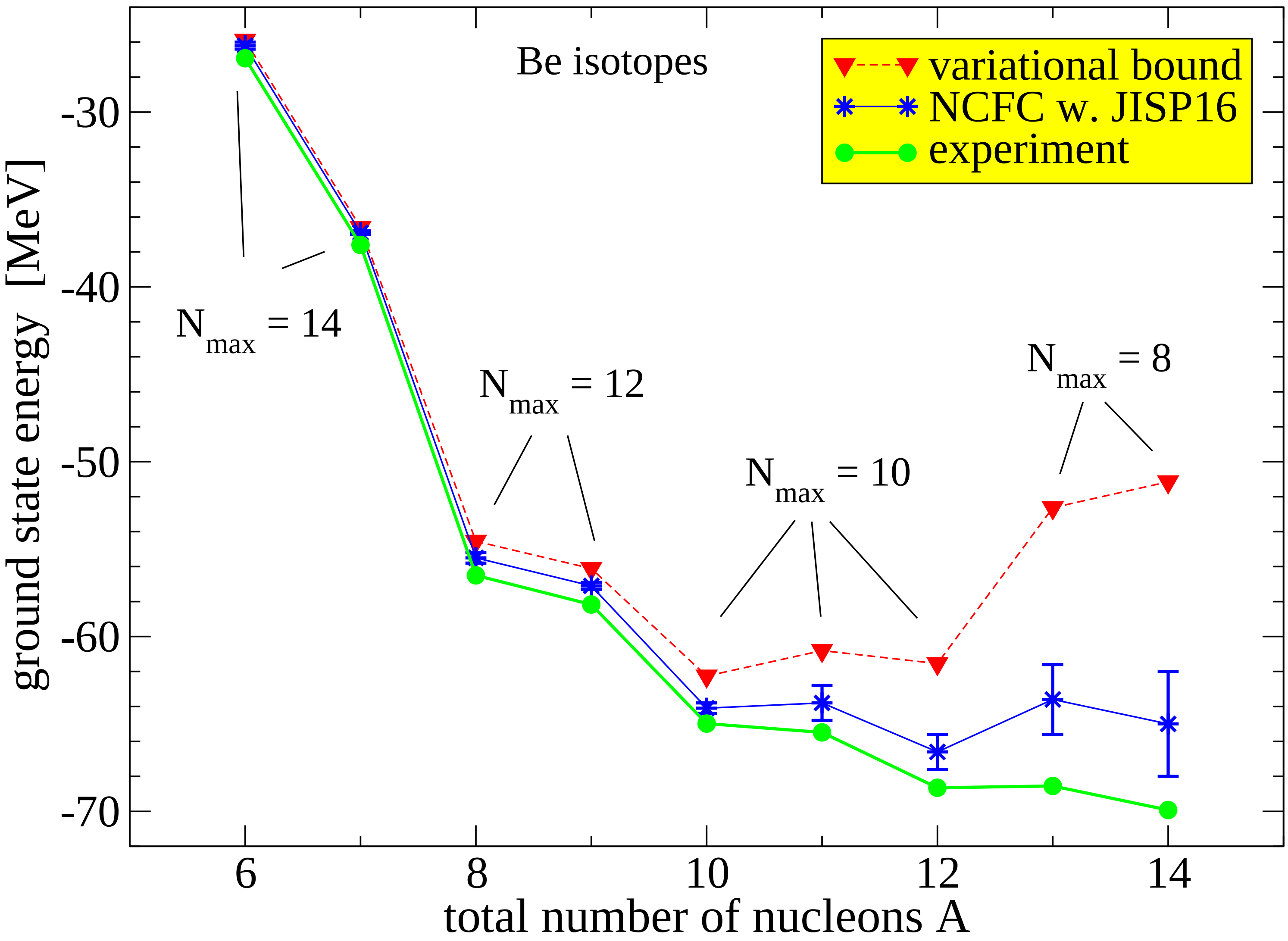
A.M. Shirokov, J.P. Vary, A.I. Mazur, T.A. Weber, PLB **644**, 33 (2007)

J-matrix Inverse Scattering Potential tuned up to ^{16}O

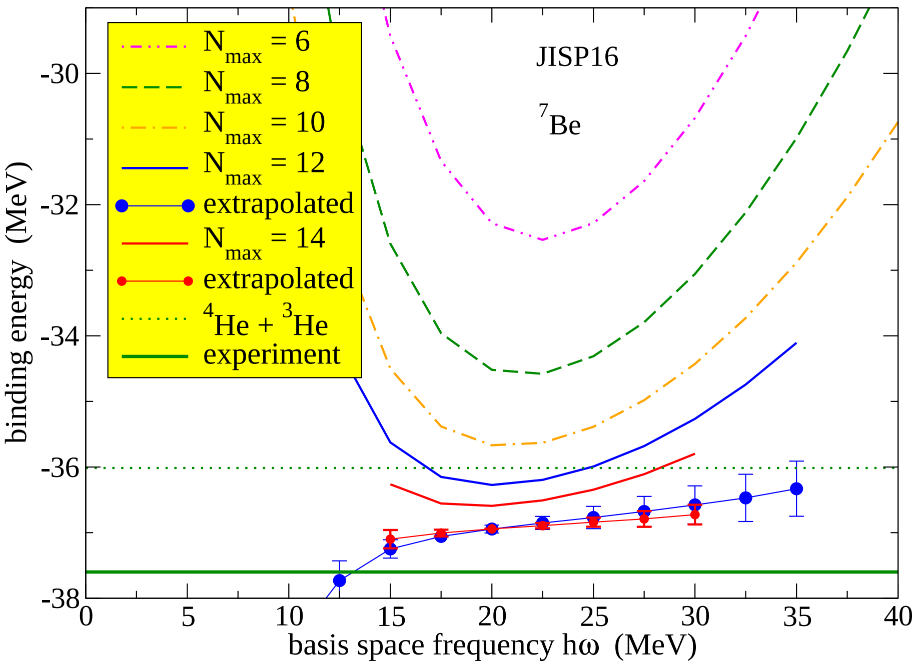
- finite rank seperable potential in H.O. representation
- fitted to available NN scattering data
- use unitary transformations to tune off-shell interaction to
  - binding energy of ^{3}He
  - low-lying spectrum of ^{6}Li (JISP6, precursor to JISP16)
  - binding energy of ^{16}O
- good fit to a range of light nuclear properties
- very soft potential compared to other NN potentials
- nonlocal potential (by construction)
- details available at

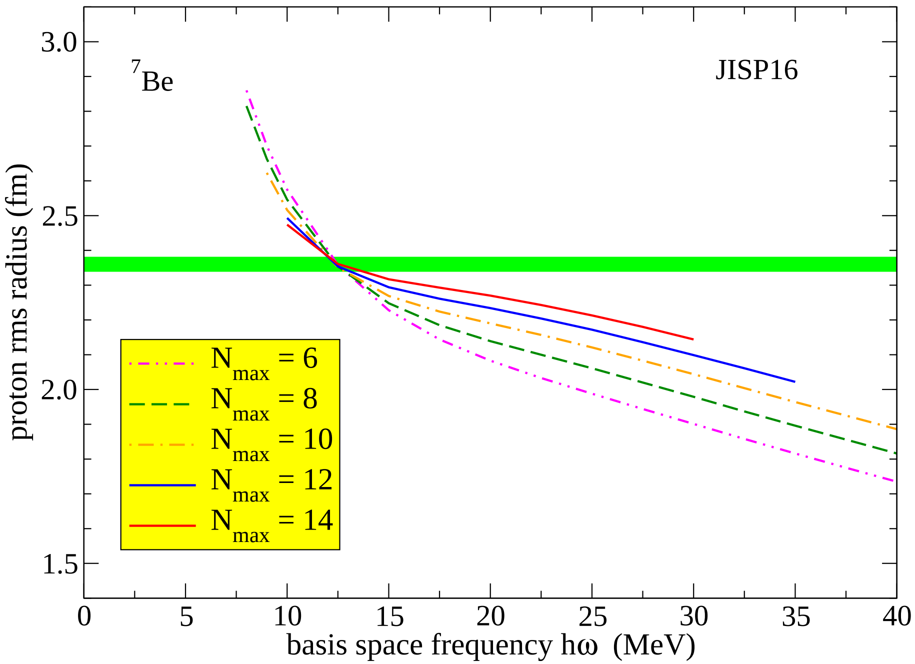
  `http://nuclear.physics.iastate.edu/`

Ground state energy Be-isotopes with JISP16



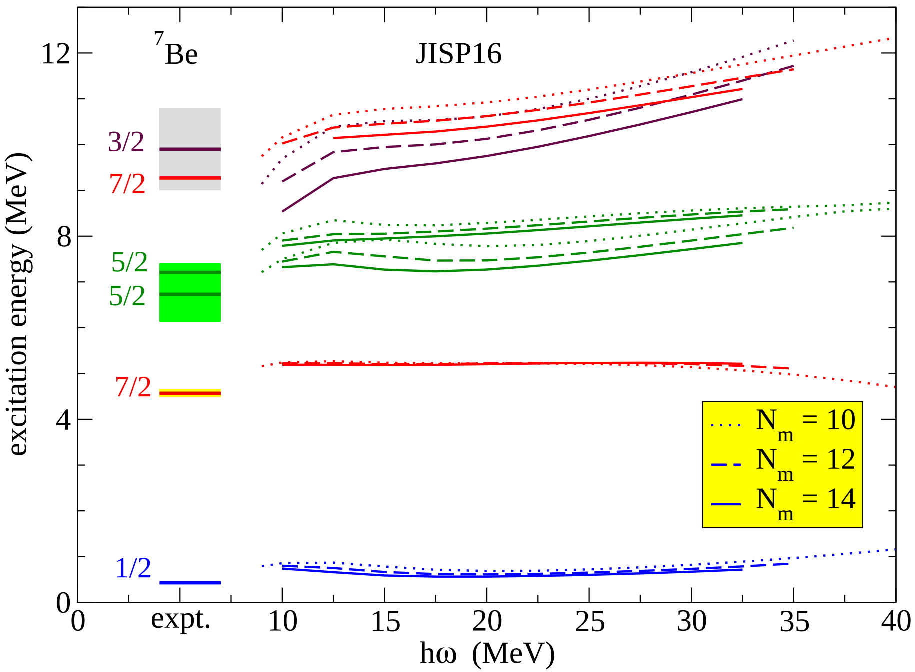
7Be – Ground state properties

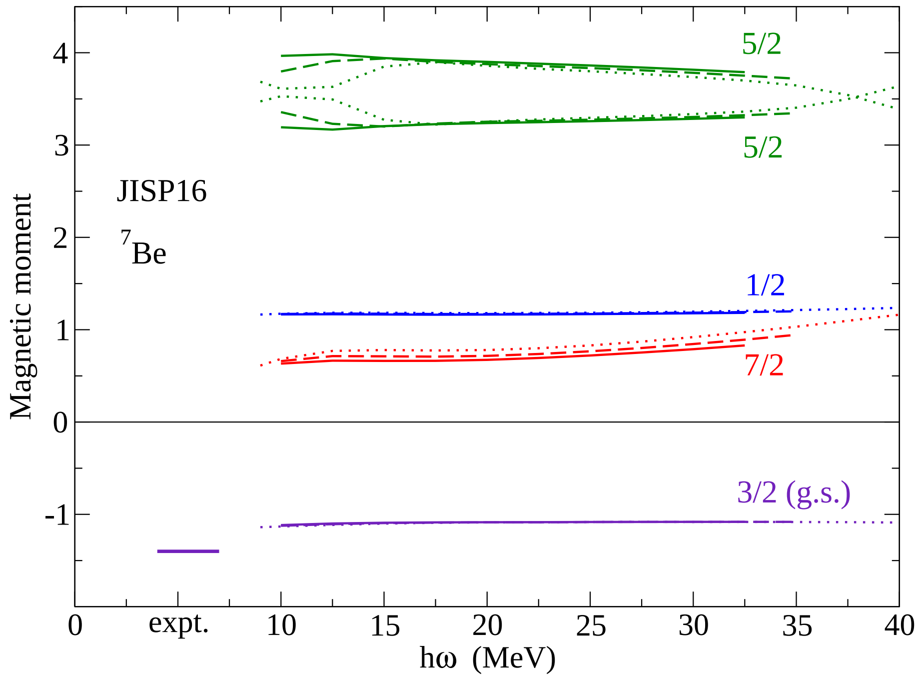




- Binding energy converges monotonically, with optimal H.O. freuqency around $\hbar\omega = 20$ MeV to 25 MeV
- Ground state about 0.7 MeV underbound with JISP16
- Proton point radius does not converge monotonically

7Be – Excited states



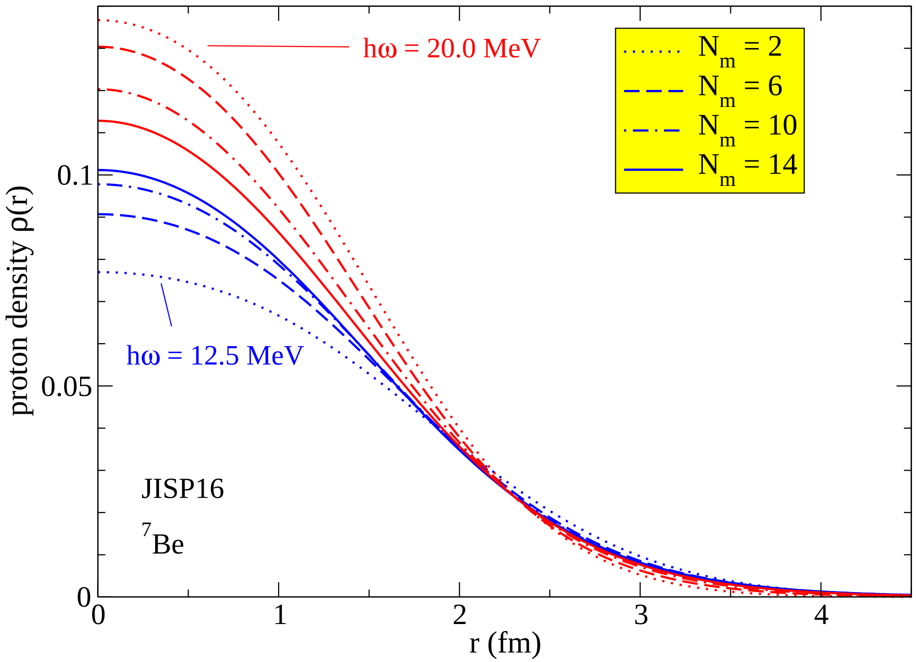


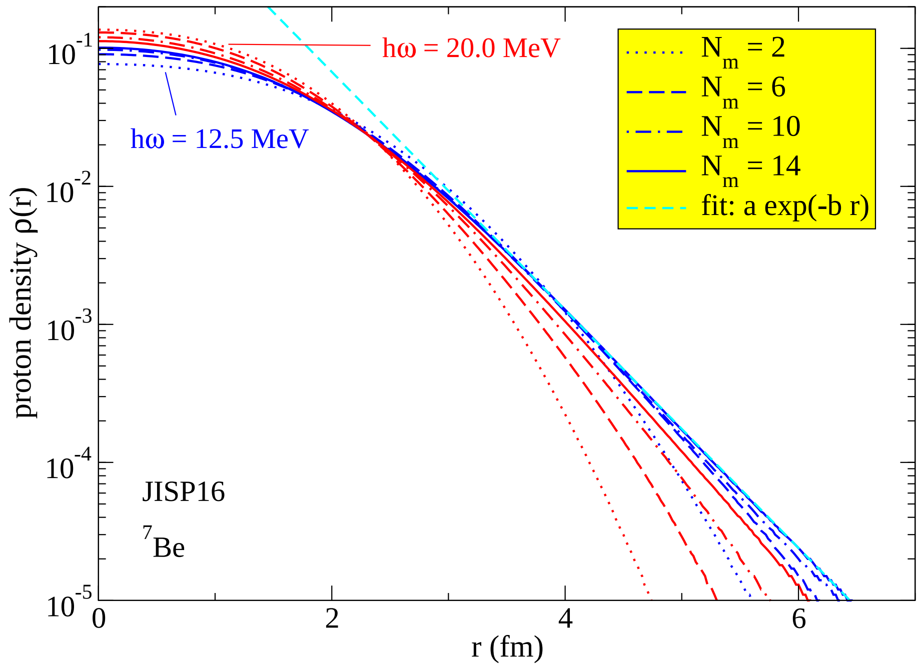
- Excitation energy of narrow states
  - converge rapidly
  - agree with experiments
- Broad resonances depend $\hbar\omega$
- Magnetic moments well converged
  - 2-body currents needed for agreement with data (meson-exchange currents)

7Be – Proton density

- Intrinsic density – center-of-mass motion taken out

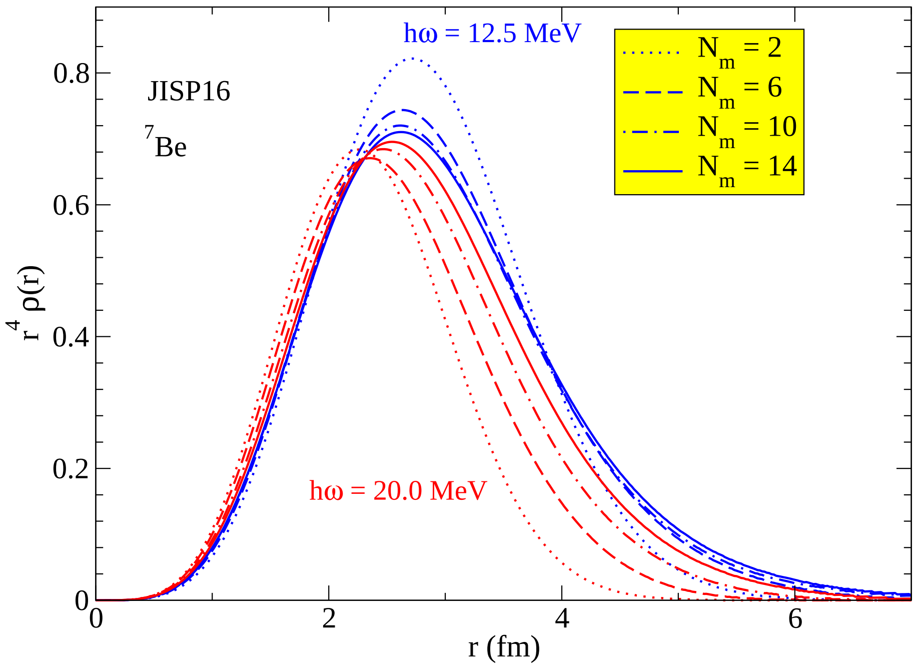
w. Cockrell, PhD student ISU

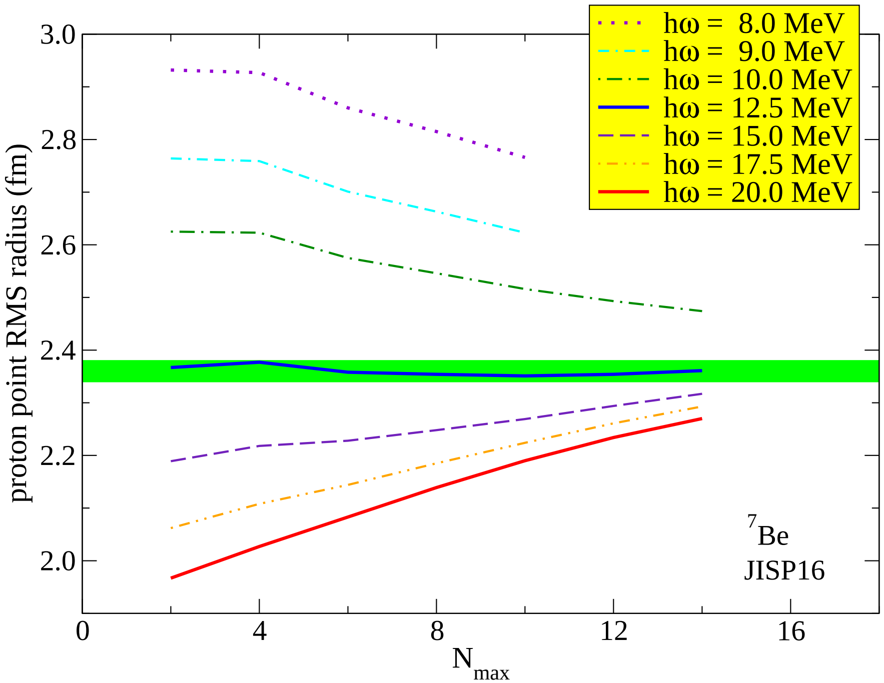




- Slow build up of asymptotic tail of wavefunction
- Proton density appears to converge more rapidly at $\hbar\omega = 12.5$ MeV than at 20 MeV because long-range part of wavefunction is better represented with smaller H.O. parameter

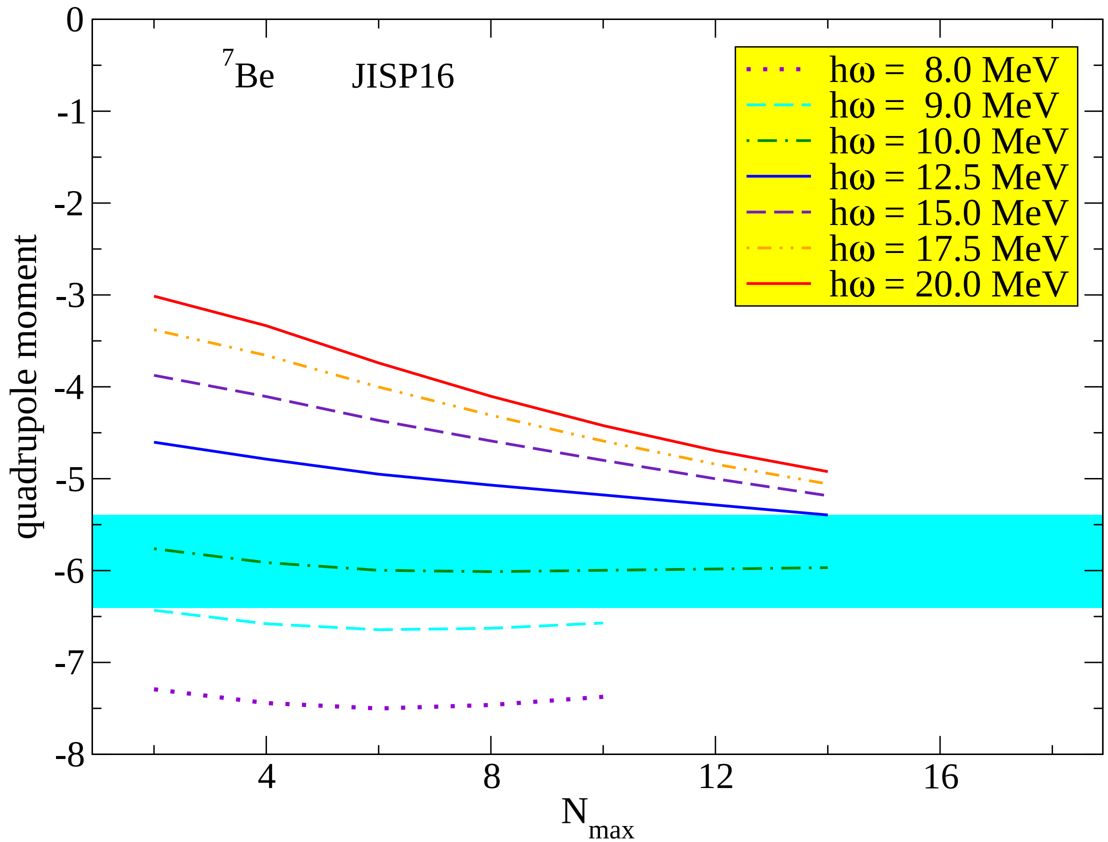
7Be – Proton radius





- Calculation one-body observables $\langle i|\mathcal{O}|j\rangle \sim \int \mathcal{O}(r)\, r^2\, \rho_{ij}(r)\, dr$
- RMS radius: $\mathcal{O}(r) = r^2$
- Slow convergence of RMS radius due to slow build up of asymptotic tail
- Ground state RMS radius in agreement with data

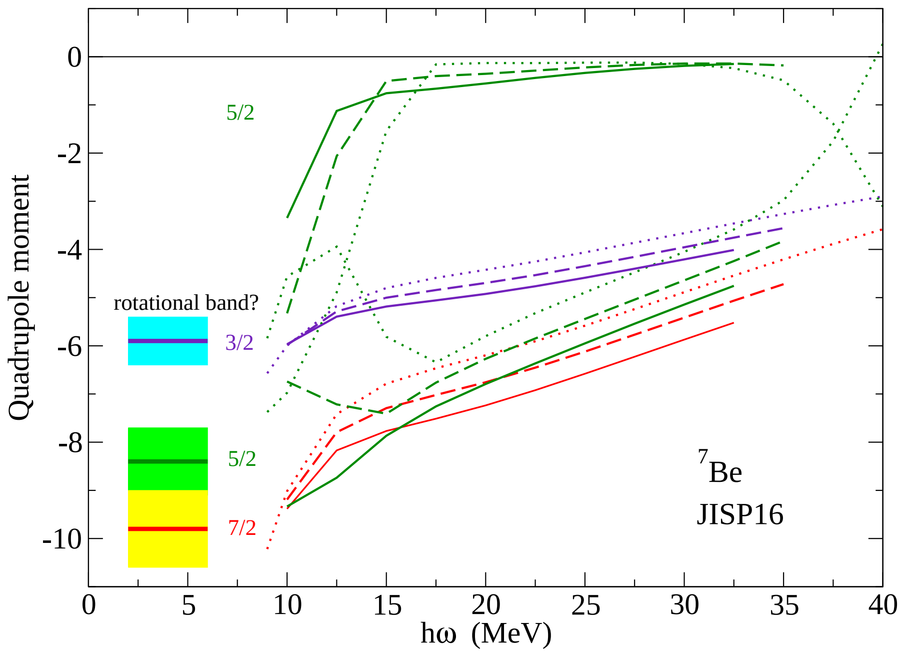
7Be – Quadrupole moment

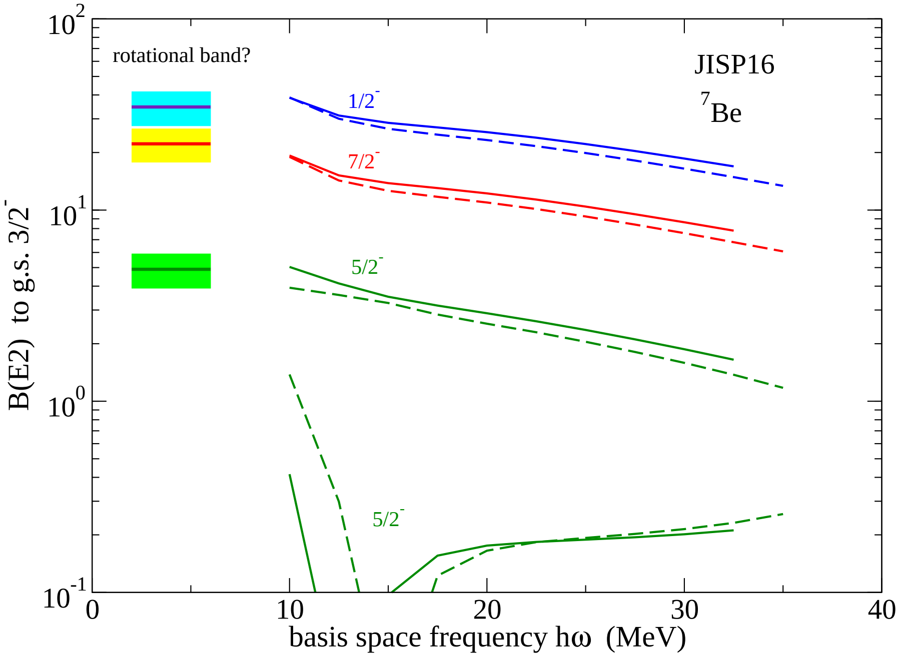


- Ground state quadrupole moment in agreement with data
- Optimal basis space around $\hbar\omega = 10$ MeV to 12 MeV
- Similar slow convergence for E2 transitions

7Be – Rotational band

E2 observables suggest rotational structure for $\frac{3}{2}$, $\frac{1}{2}$, $\frac{7}{2}$, $\frac{5}{2}$ states

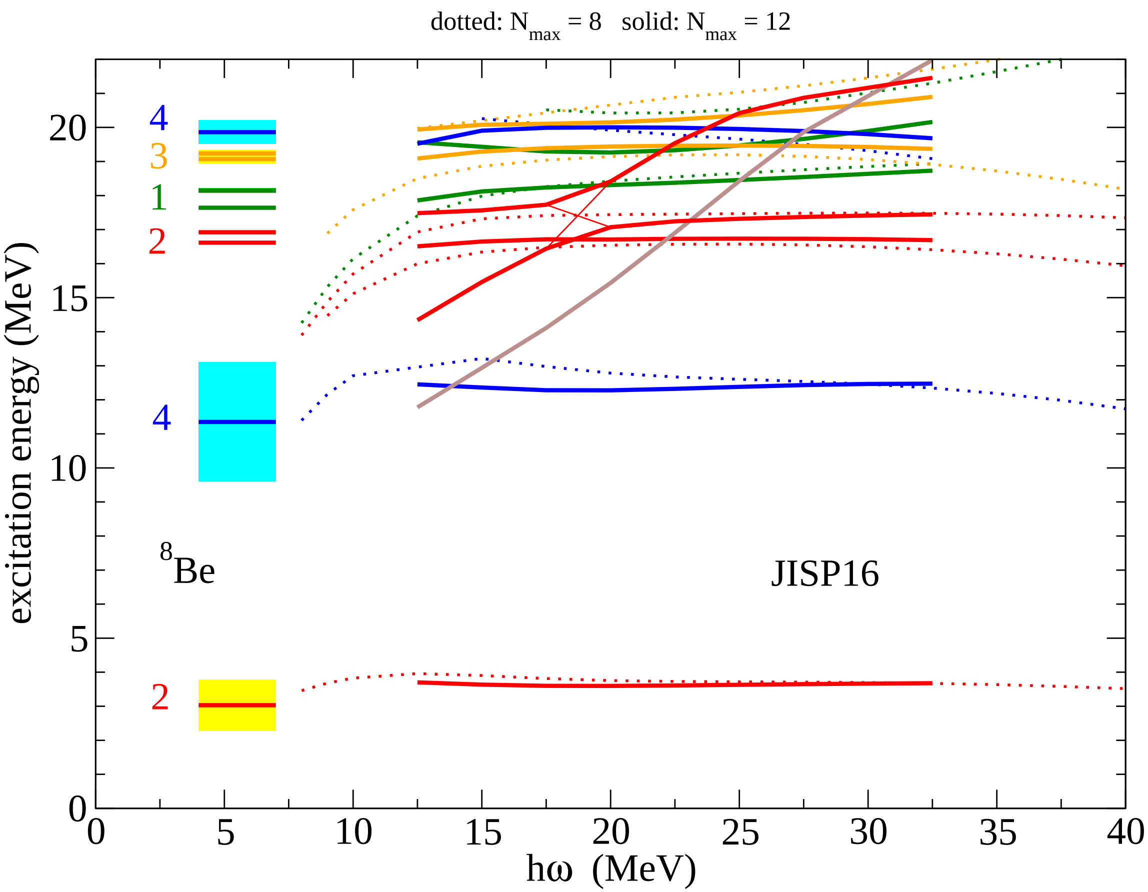




$$Q(J) = \frac{\frac{3}{4} - J(J+1)}{(J+1)(2J+3)} Q_0^{\frac{1}{2}}$$

$$B(E2; i \to f) = \frac{5}{16\pi} \left(Q_0^{\frac{1}{2}}\right)^2 \left(J_i, \frac{1}{2}; 2, 0 \middle| J_f, \frac{1}{2}\right)^2$$

8Be – Spectrum positive parity

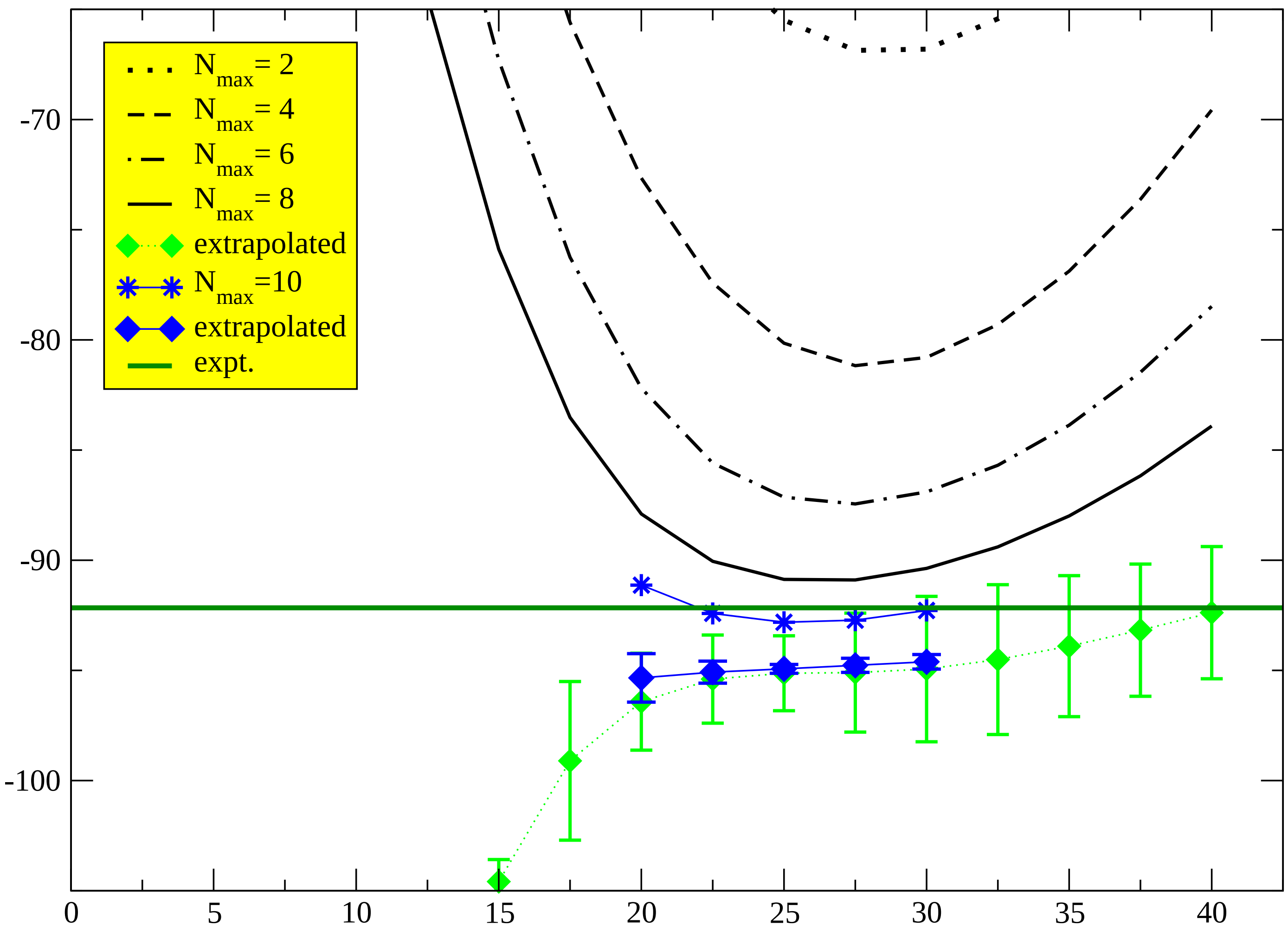


- Pairs of isospin 0 and 1 states with J = 2, 1, and 3
- Evidence of continuum states (J = 0 and 2) at $N_{\text{max}} = 12$
- Rotational band

	expt.	calc	rotor
E_4/E_2	3.75	3.40	3.33

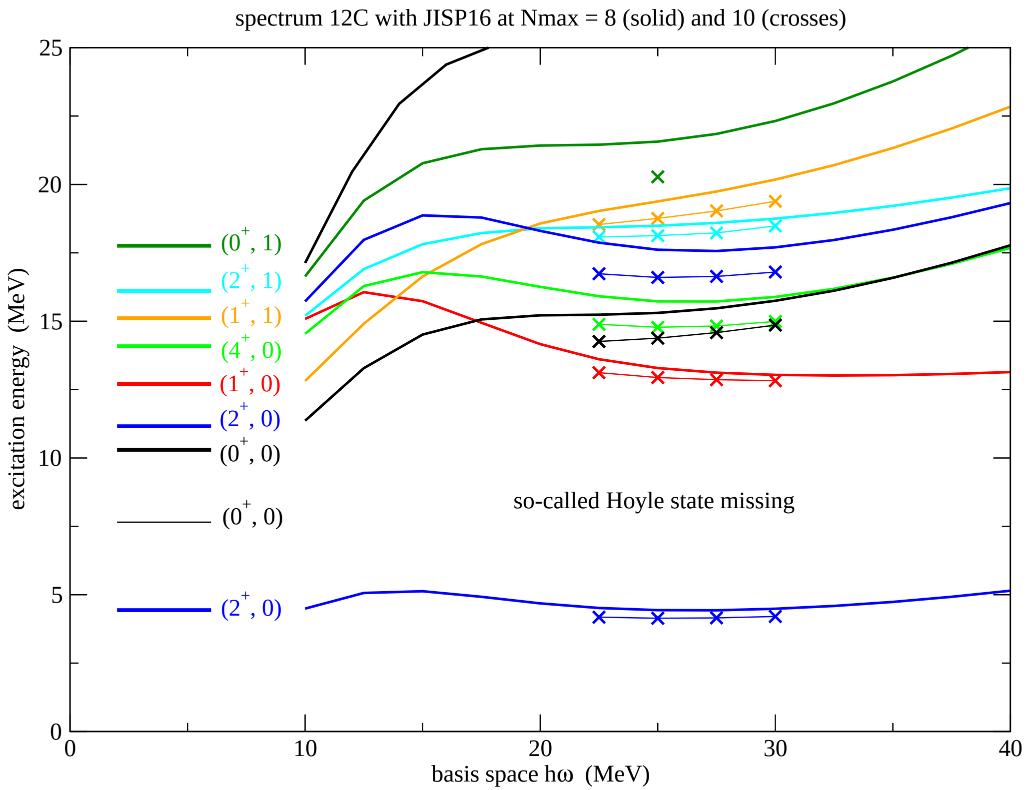
- Ground state above 2α threshold: radius not converged
- Quadrupole moments 2^+ and 4^+ not converged, nor B(E2)'s, but in qualitative agreement with rotational structure

Results with JISP16 for ^{12}C



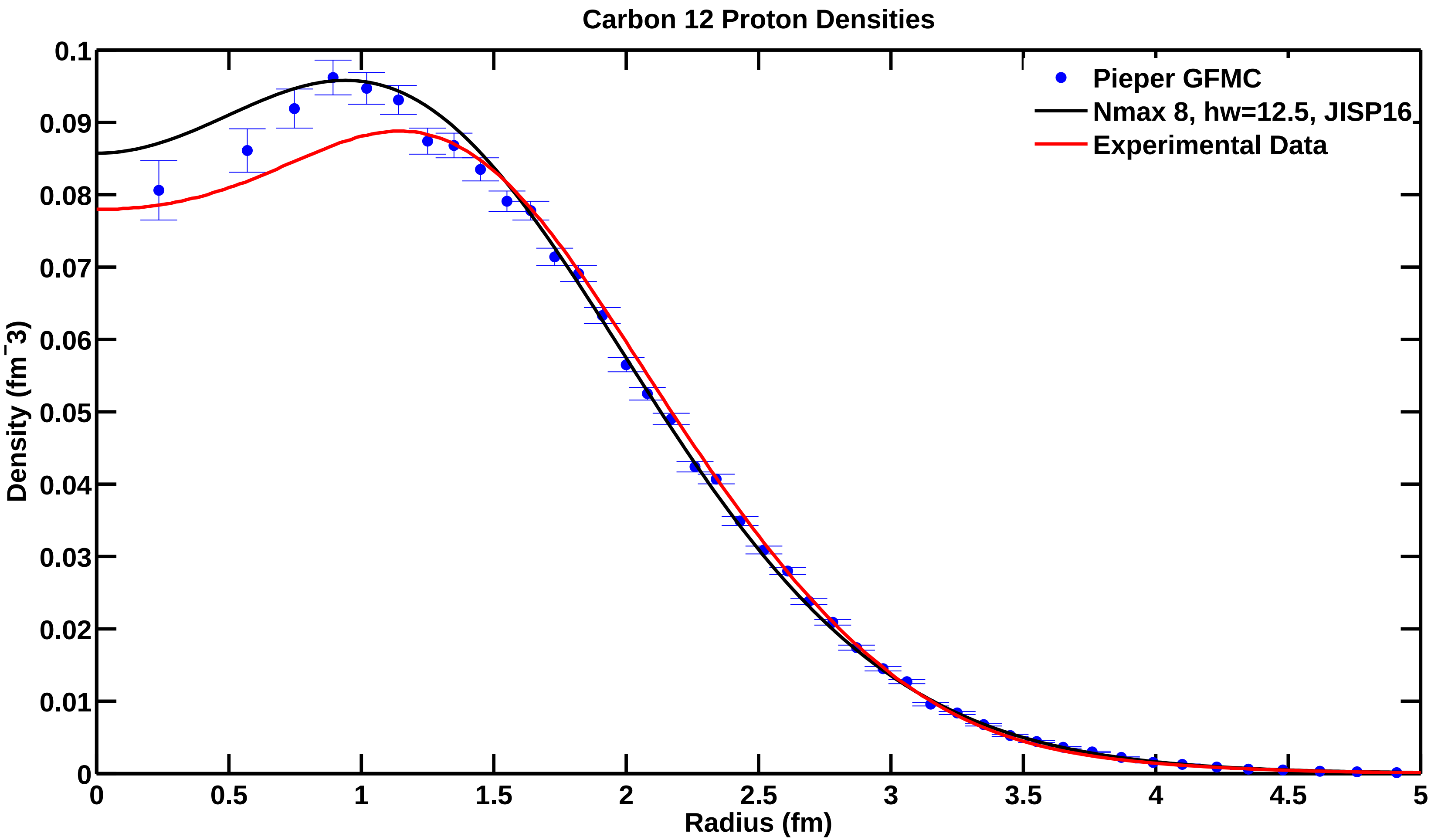
- Calculations for $N_{\text{max}} = 10$ underway (D = 8 billion) using 100,000 cores on JaguarPF (ORNL) under INCITE award

Spectrum of ^{12}C with JISP16 – work in progress



- Pos. parity states in agreement with data, except for Hoyle state
- Electromagnetic transitions in progress
  - rotational 2^+ and 4^+ states, significantly enhanced B(E2)
  - optimal basis $\hbar\omega$ for Q and B(E2) around $\hbar\omega = 12.5$ MeV
- Neutrino and pion scattering calculations in progress

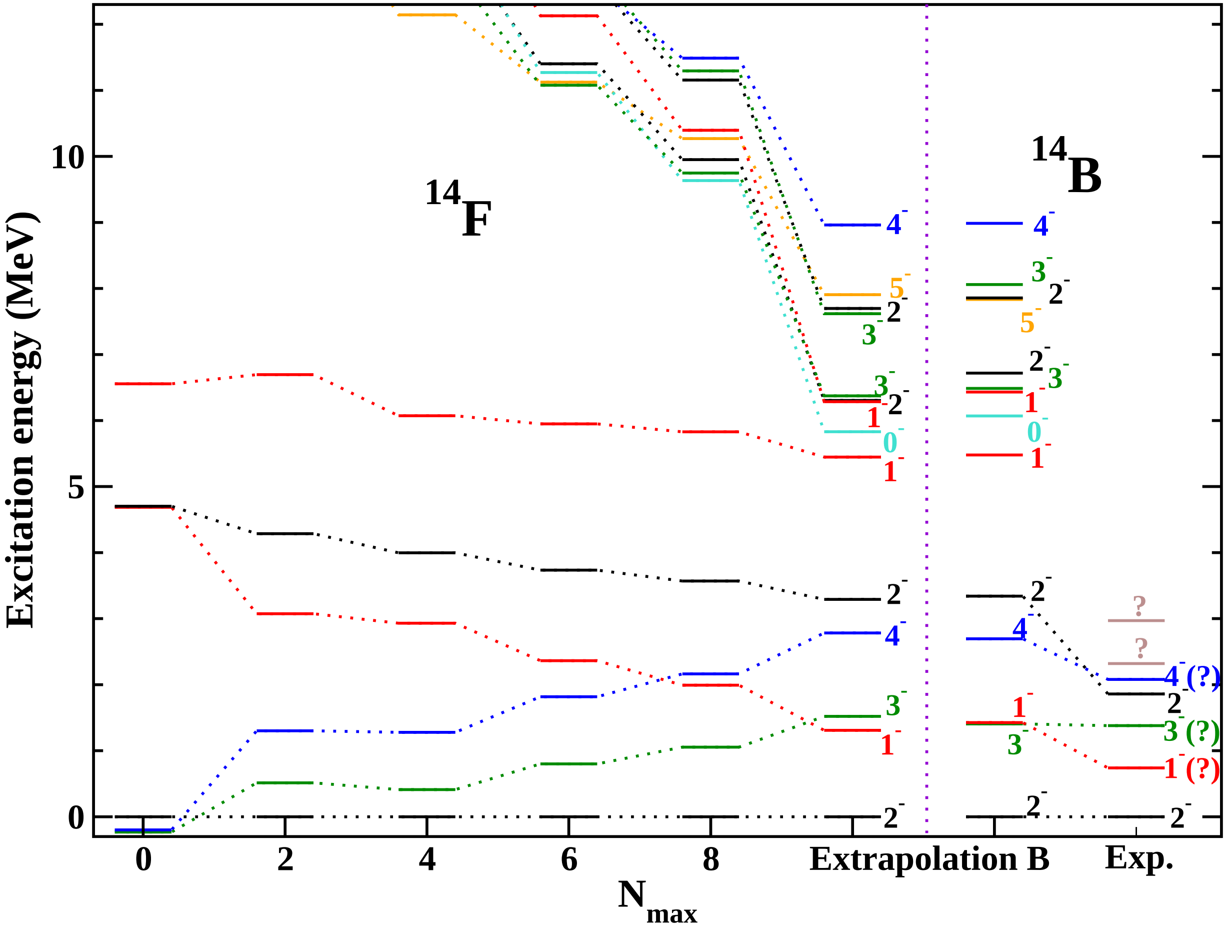
Density of ^{12}C with JISP16



- GFMC: AV18 + IL7, on BlueGene/P using 131,072 cores (INCITE)
  "More scalability, Less pain", Lusk, Pieper, and Butler, SciDAC review 17, 30 (2010)
- JISP16 density at $N_{\text{max}} = 8$, $\hbar\omega = 12.5$ MeV

Scientific Discovery – unstable nucleus ^{14}F

Maris, Shirokov, Vary, arXiv:0911.2281 [nucl-th], Phys. Rev. C81, 021301(R) (2010)



dimension $2 \cdot 10^9$
nonzero m.e. $2 \cdot 10^{12}$
runtime 2 to 3 hours on
7,626 quad-core nodes
on Jaguar (XT4)
(INCITE 2009)

- Predicted ground state energy: 72 ± 4 MeV (unstable)
- Mirror nucleus ^{14}B: 86 ± 4 MeV agrees with experiment 85.423 MeV

Predictions for ^{14}F confirmed by experiments at Texas A&M

Theory published PRC: Feb. 4, 2010

Physics Letters B 692 (2010) 307–311

Experiment published: Aug. 3, 2010

Contents lists available at ScienceDirect

Physics Letters B

www.elsevier.com/locate/physletb

First observation of ^{14}F

V.Z. Goldberg [a,*], B.T. Roeder [a], G.V. Rogachev [b], G.G. Chubarian [a], E.D. Johnson [b], C. Fu [c], A.A. Alharbi [a,1], M.L. Avila [b], A. Banu [a], M. McCleskey [a], J.P. Mitchell [b], E. Simmons [a], G. Tabacaru [a], L. Trache [a], R.E. Tribble [a]

[a] Cyclotron Institute, Texas A&M University, College Station, TX 77843-3366, USA
[b] Department of Physics, Florida State University, Tallahassee, FL 32306-4350, USA
[c] Indiana University, Bloomington, IN 47408, USA

NCFC predictions (JISP16) in close agreement with experiment

TAMU Cyclotron Institute

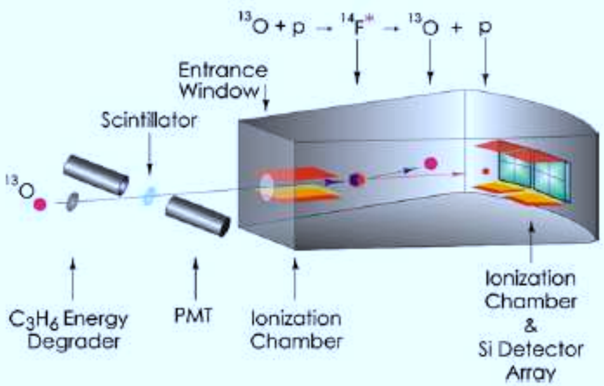


Fig. 1. (Color online.) The setup for the ^{14}F experiment. The "gray box" is the scattering chamber. See explanation in the text.

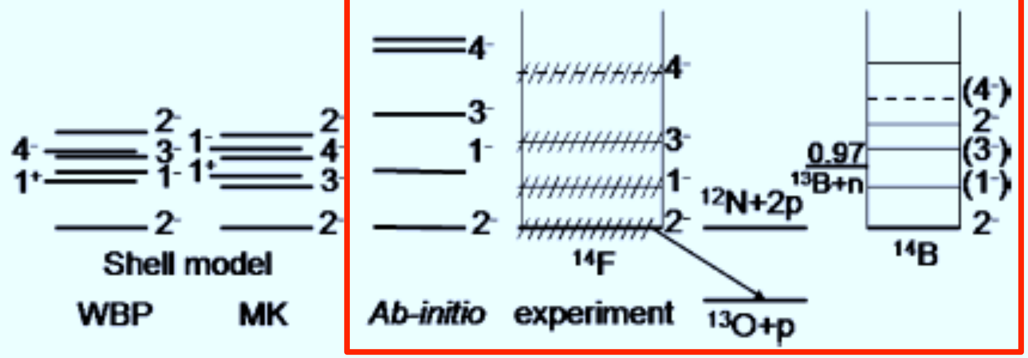
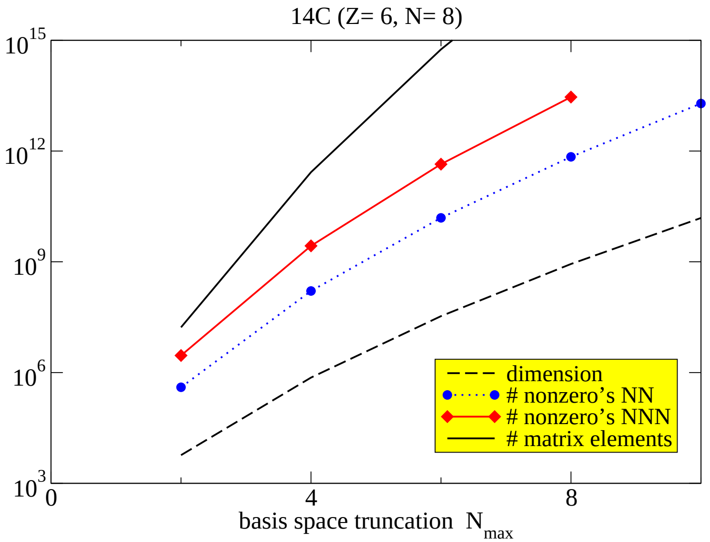
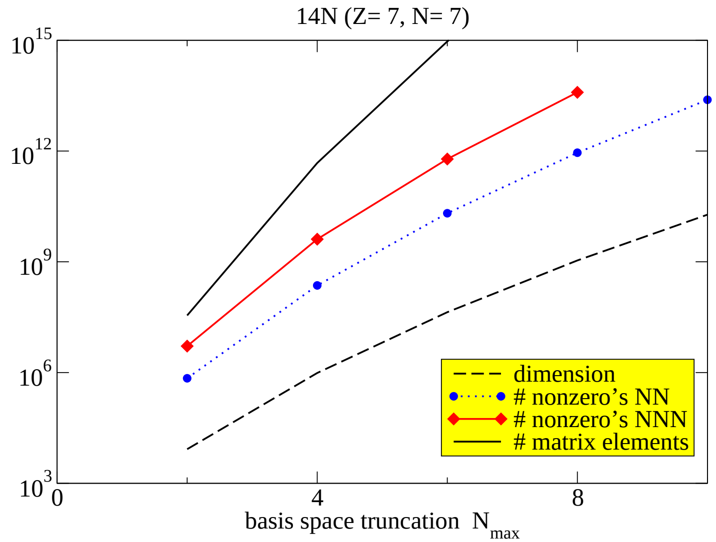


Fig. 6. ^{14}F level scheme from this work compared with shell-model calculations, *ab-initio* calculations [3] and the ^{14}B level scheme [16]. The shell model calculations were performed with the WBP [21] and MK [22] residual interactions using the code COSMO [23].

Petascale Early Science – Ab initio structure of Carbon-14



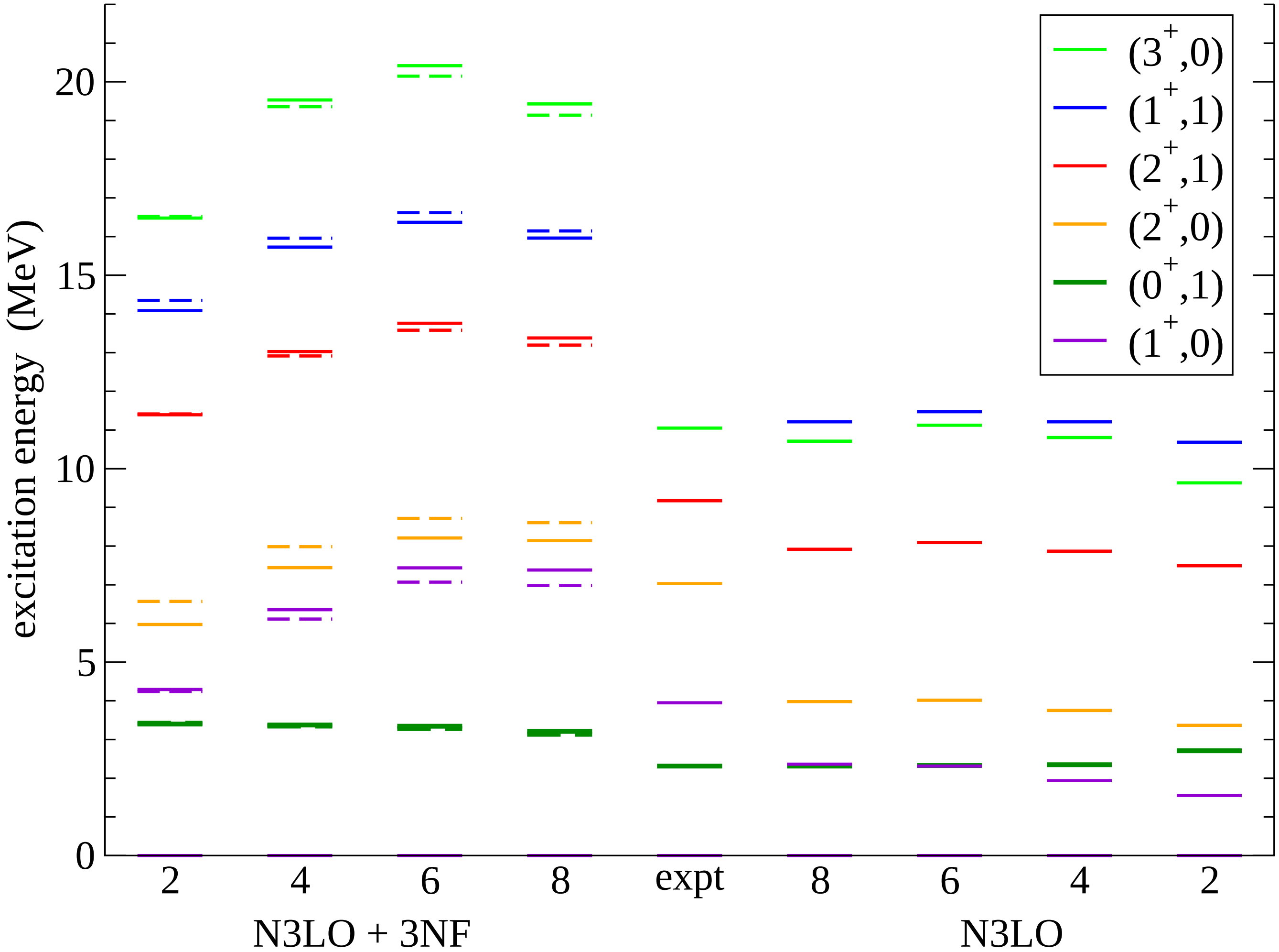


- Chiral effective 2-body plus 3-body interactions at $N_{\text{max}} = 8$
- Basis space dimension 1.1 billion
- Number of nonzero m.e. 39 trillion
- Memory to store matrix (CRF) 320 TB
- Total memory on JaguarPF 300 TB

ran on JaguarPF (XT5) using up to 36k 8GB processors (216k cores)
after additional code-development for partial "reconstruct-on-the-fly"

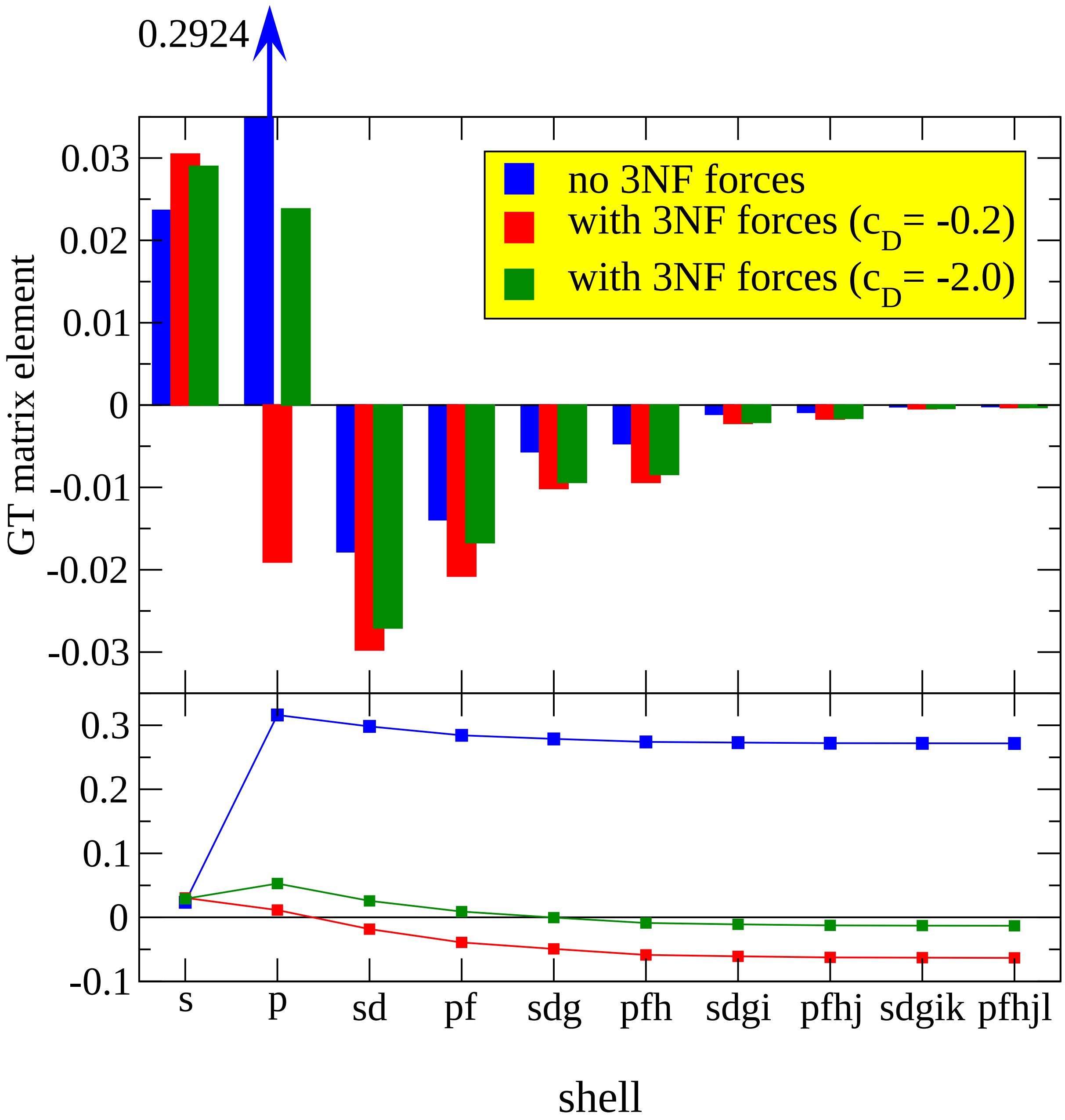
Ab initio structure of Carbon-14 and Nitrogen-14

Maris, Vary, Navratil, Ormand, Nam, Dean, arXiv:1101.5124 [nucl-th]



chiral 2-body plus 3-body forces (left) and 2-body forces only (right)

Origin of the anomalously long life-time of ^{14}C



- near-complete cancellations between dominant contributions within p-shell
- very sensitive to details

Maris, Vary, Navratil, Ormand, Nam, Dean, arXiv:1101.5124 [nucl-th]

Neutrons in a trap: Why

- Validate ab-initio DFT approaches
  against microscopic ab-initio calculations
  - compare Density Matrix Expansion
    and ab-initio NCFC calculations
    - using the same interaction
    - calculating the same observables for the same systems
- Construct Universal Nuclear Energy Density Fuctional
  consistent with ab-initio calculations
- Theoretical ’laboratory’ to explore
  - properties of different nuclear interactions
  - effect of density and gradient
    on nuclear properties for different interactions
- Model for neutron-rich systems
  in particular those with closed shell protons (Oxygen, Calcium)

Essential in order to make meaningful comparison with other methods:
quantify dependence on basis space truncation parameters

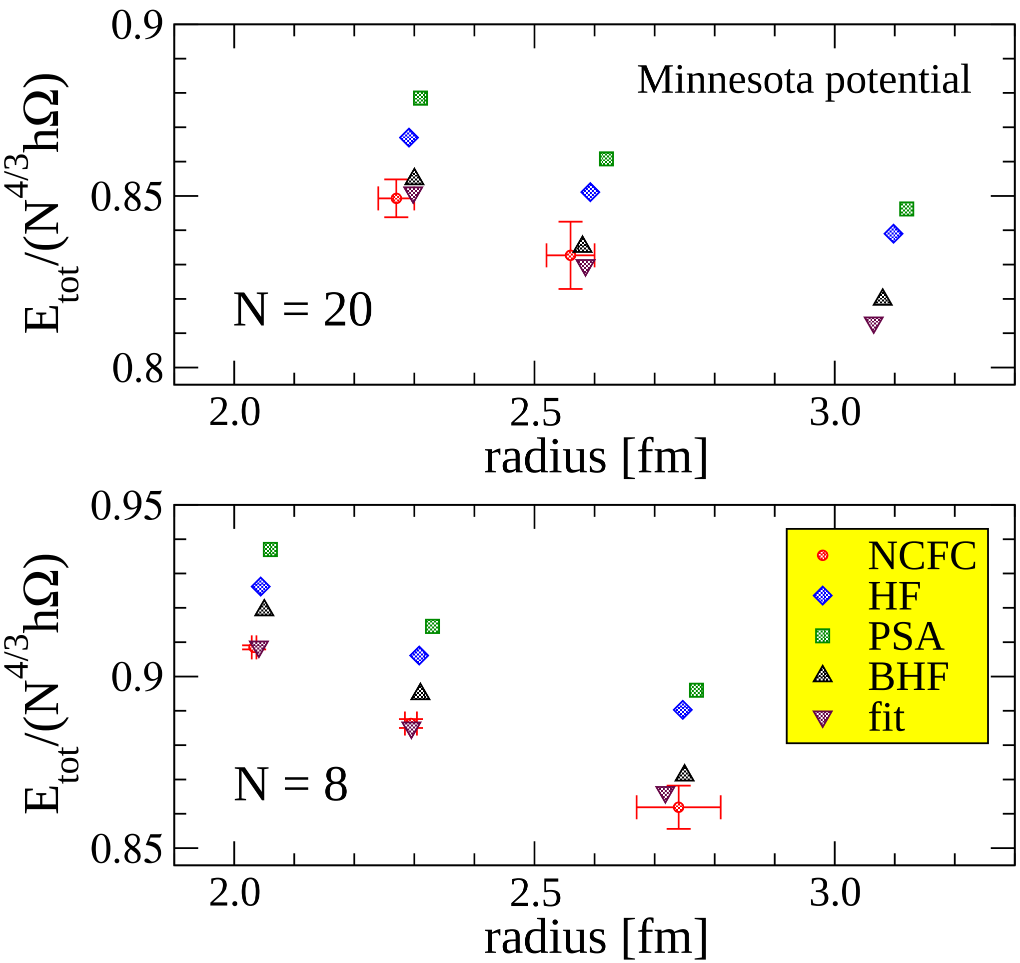
Validating ab-initio DME/DFT calculations

Bogner, Furnstahl, Kortelainen, Maris, Stoistov, Vary, in preparation

- Simple model for interaction
  - Minnesota potential
- Ab-initio NCFC calculations for neutrons in H.O. potential
  - including numerical error estimates on all ’observables’
- DFT using same NN interaction as NCFC
  - Hartree–Fock
  - Density Matrix Expansion, Hartree–Fock
  - Density Matrix Expansion, Brueckner–Hartree–Fock
- DFT fit to NCFC results
- Comparison for 8, 14, and 20 neutrons
  - total and internal energy per neutron
  - rms radius
  - form factor $F(q)$

Minnesota potential – Total energy vs. radius

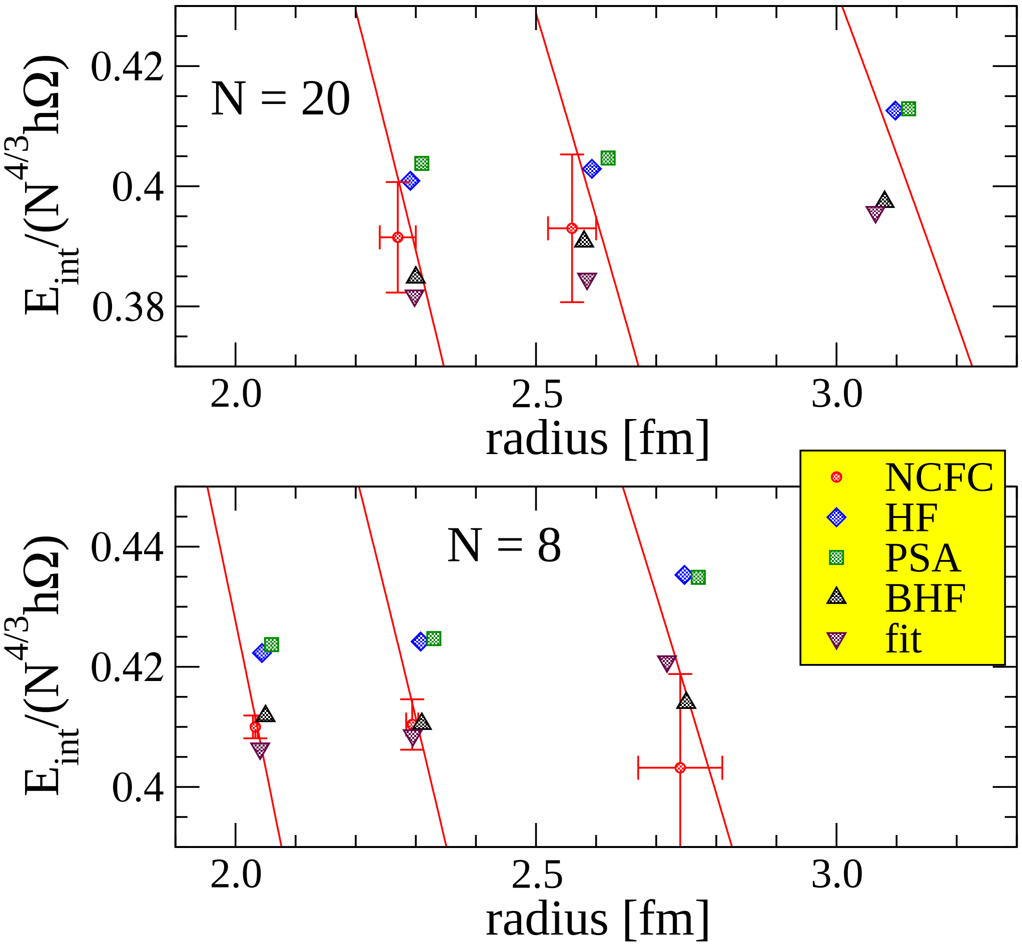
Bogner, Kortelainen, Furnstahl, Stoistov, Vary, PM, work in progress



- Neither HF nor DME/PSA HF in agreement with NCFC
- DME BHF close to NCFC results often within error estimates
- Fit with volume term and surface term can reproduce NCFC data

Internal energy vs. radius

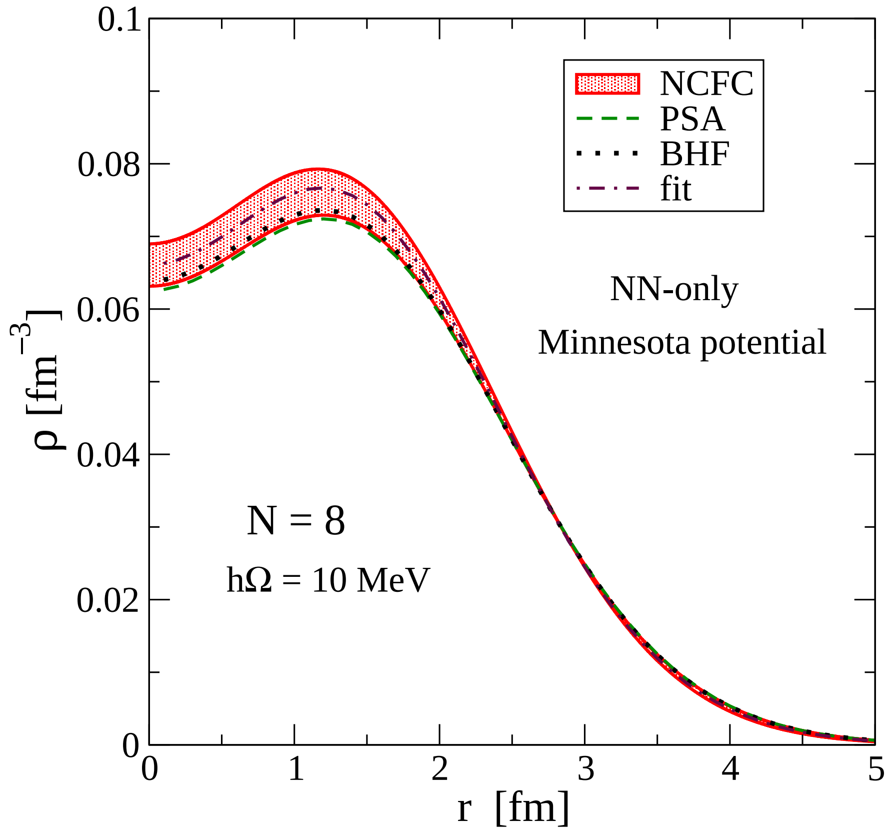
Variational upper bound on combination $E_{\text{int}} + \frac{1}{2} N\, m\, \Omega^2 r^2$

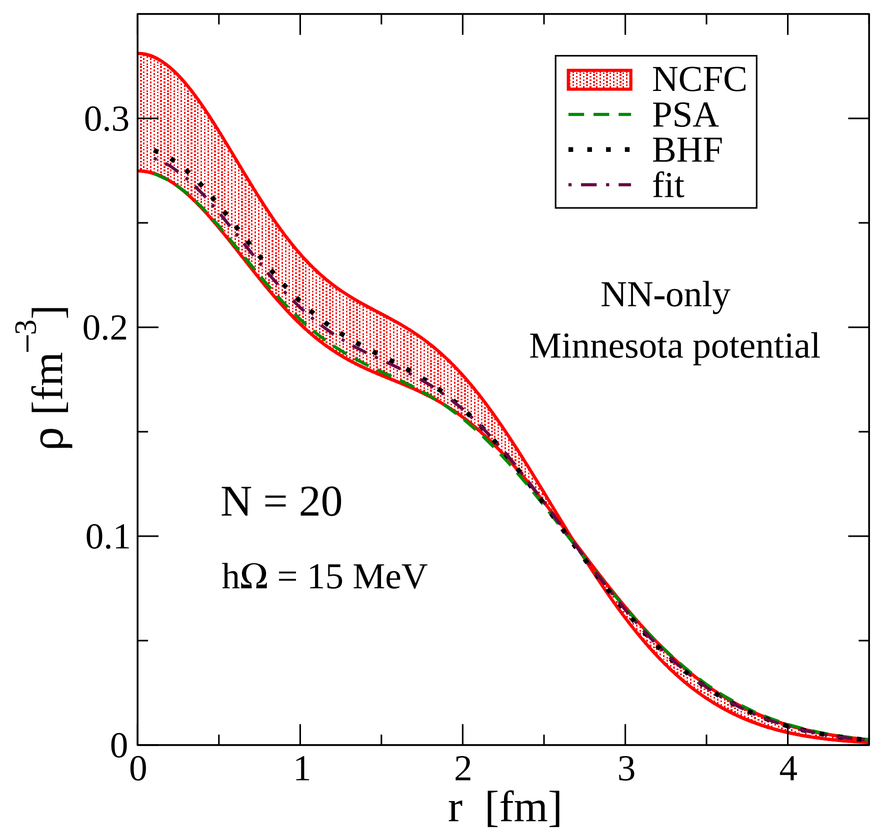


- Neither HF nor DME/PSA HF within variational bound
- DME BHF close to NCFC results often within error estimates and within bounds
- Fit with volume term and surface term can reproduce NCFC data

Minnesota potential – density

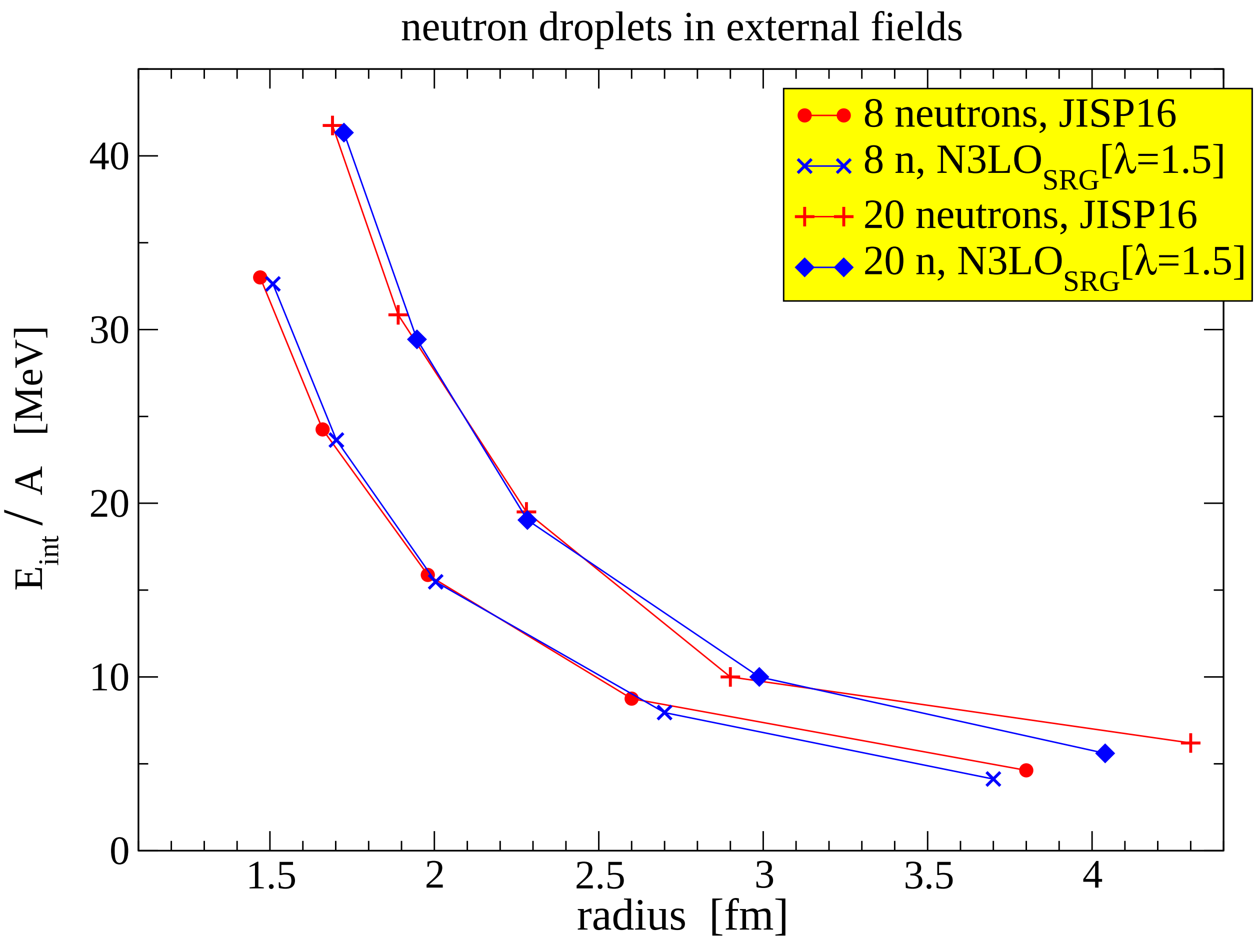
Bogner, Kortelainen, Furnstahl, Stoistov, Vary, PM, work in progress





- Agreement between DME/DFT calculations and NCFC
- Density profile dominated by H.O. external field modefied by NN interaction

E_{int} *vs. radius – more realistic potentials*



Results virtually identical for N3LO$(\lambda = 1.5)$ and JISP16
despite different results for nuclei (e.g. 186 vs. 144 MeV for ^{16}O)

presented at JUSTIPEN–EFES–Hokudai–UNEDF workshop, 2008, Hokkaido, Japan

Conclusions

- MFDn: Scalable and load-balanced CI code for nuclear structure
  - new version under development, has run on 200k+ cores on Jaguar (ORNL) enabling largest model-space calculations
- Significant benefits from collaboration between nuclear physicists, applied mathematicians, and computer scientists
- JISP16, nonlocal phenomenological 2-body interaction
  - good description of light nuclei (more than just energies!)
  - rapid convergence
  - prediction of new isotope, ^{14}F
- Understanding of the anomalously large lifetime of ^{14}C
- Validation of DFT/DME calculations (in progress)
- Main challenge: construction and diagonalization of extremely large (D > 1 billion) sparse matrices
- Future developments: Taming the scale explosion