Ab Initio No Core Full Configuration approach to the structure of light nuclei

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SciDAC project – UNEDF

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

http://www.unedf.org

INCITE award – Computational Nuclear Structure

PI: David Dean (ORNL)

PetaApps award

PIs: Jerry Draayer (LSU), Umit Catalyurek (OSU)
Masha Sosonkina, James Vary (ISU)

SciDAC/UNEDF – Uniform description of nuclear structure

SciDAC project – UNEDF http://www.unedf.org
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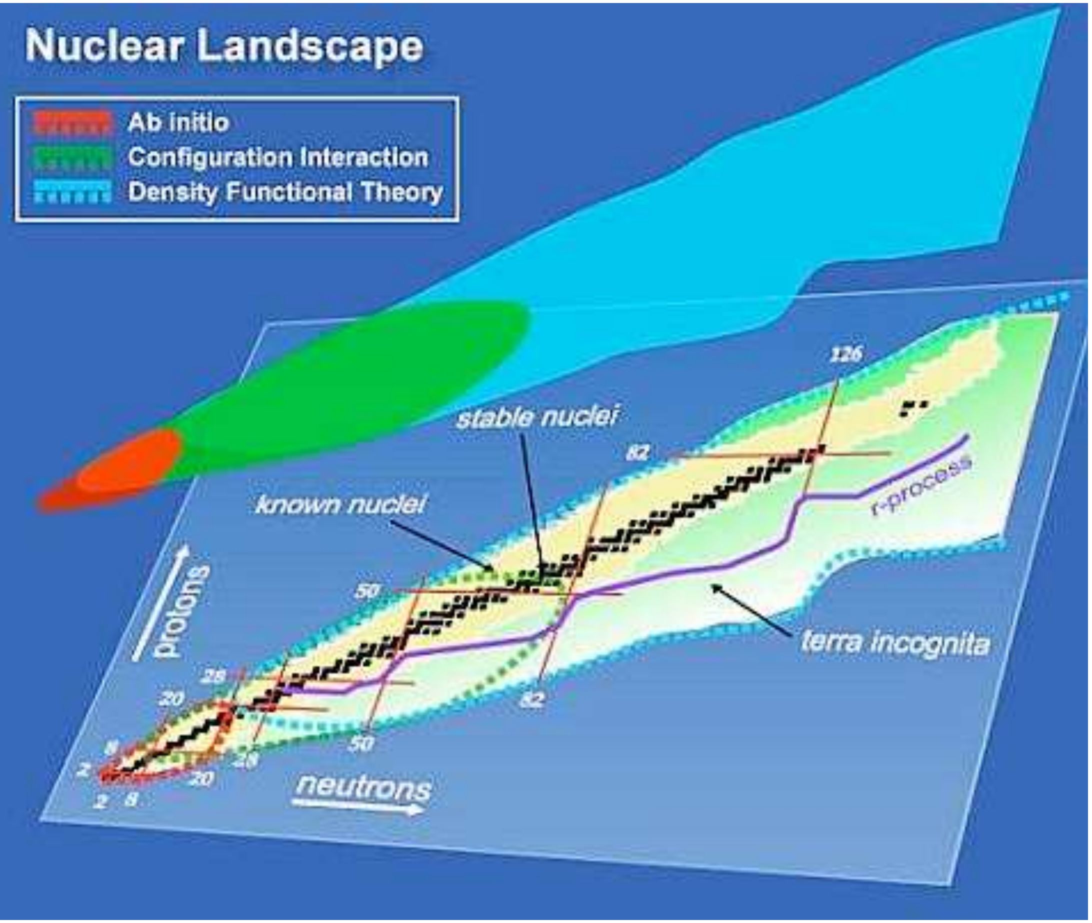

- Universal Nuclear Energy Density Functional theory that spans the entire mass table based on ab initio calculations for light nuclei
  - Coupled Cluster (Papenbrock *et al*, ORNL)
  - No-Core Configuration Interaction calculations numerical code: MFDn
  - Greens Function Monte Carlo (Pieper *et al*, ANL)

Ab initio nuclear structure calculations

Eigenvalue problem $\hat{\mathbf{H}}|\Psi\rangle = E|\Psi\rangle$ with Hamiltonian

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

- Self-bound quantum many-body problem, with $3A$ degrees of freedom in coordinate or momentum space
- Strong interactions, with both short-range and long-range pieces
- Multiple scales, from keV's to MeV's

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Configuration Interaction Methods

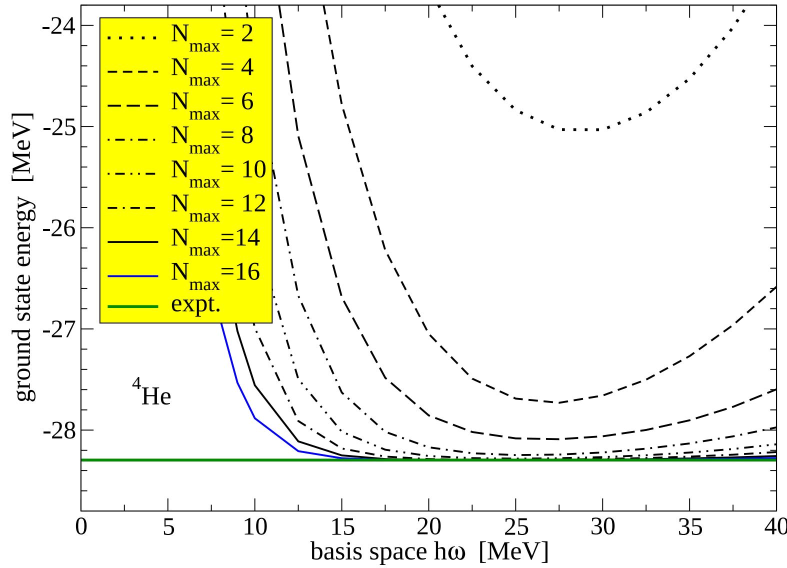
- Expand wave function in basis states $|\Psi\rangle = \sum a_i |\psi_i\rangle$
- Express Hamiltonian in basis $\langle\psi_j|\hat{\mathbf{H}}|\psi_i\rangle = H_{ij}$
- Diagonalize Hamiltonian matrix H_{ij}
- Complete basis $\longrightarrow$ exact result
  - caveat: complete basis is infinite dimensional

- 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

Configuration Interaction Methods

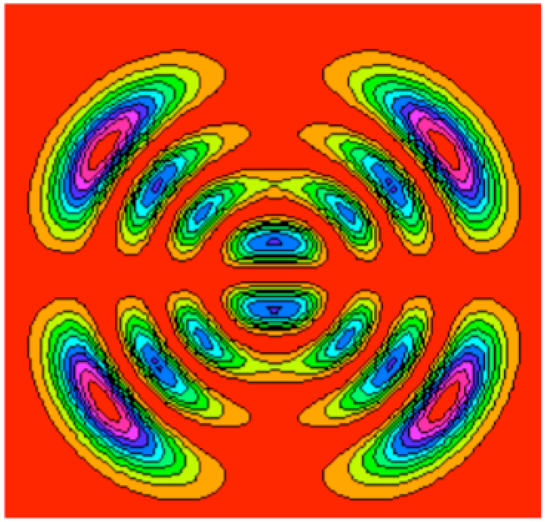
- Expand wave function in basis states $|\Psi\rangle = \sum a_i|\psi_i\rangle$
- Express Hamiltonian in basis $\langle\psi_j|\hat{\mathbf{H}}|\psi_i\rangle = H_{ij}$
- Diagonalize Hamiltonian matrix H_{ij}
- Variational: for any finite truncation of the basis space, eigenvalue is an upper bound for the ground state energy
- Smooth approach to asymptotic value with increasing basis space: No-Core Full Configuration calculation
- Convergence: independence of N_{max} and H.O. basis $\hbar\omega$
  - different methods (NCFC, CC, GFMC, ...) using the same interaction should give same results within numerical errors



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 $|\phi\rangle$

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



sample harmonic oscillator basis function

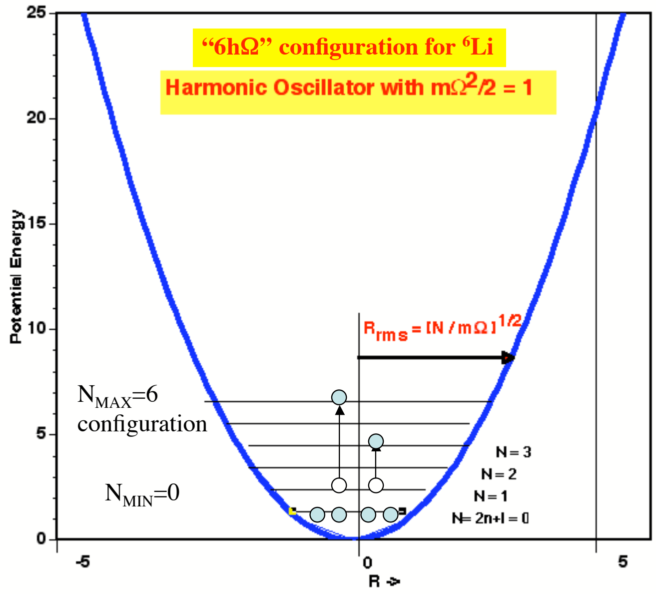
  - single-particle basis states
    eigenstates of SU(2) operators
    $\hat{\mathbf{L}}^2$, $\hat{\mathbf{S}}^2$, $\hat{\mathbf{J}}^2 = (\hat{\mathbf{L}} + \hat{\mathbf{S}})^2$, and $\hat{\mathbf{J}}_\mathbf{z}$
    w. quantum numbers $|\phi\rangle \;=\; |n, l, s, j, m\rangle$
  - radial wavefunctions: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

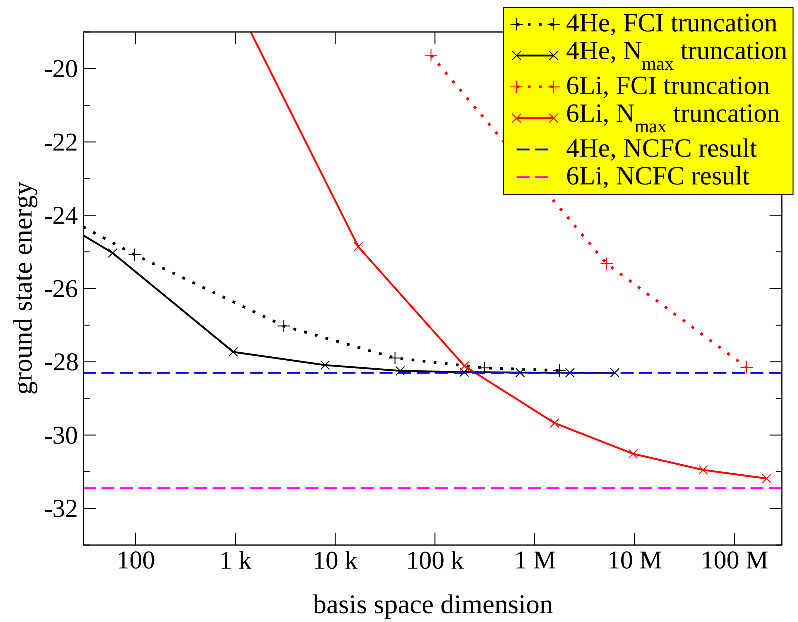
$$\hat{\mathbf{J}}_\mathbf{z}|\psi\rangle \quad = \quad M|\psi\rangle \quad = \sum_{i=1}^{A} m_i |\psi\rangle$$

- 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

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

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 $|\Psi\rangle = \sum a_i |\psi_i\rangle$
  - Slater Determinants of single-particle states
  - $N_{\max}$ truncation on total number of H.O. quanta
- Express Hamiltonian in basis $\langle \psi_j | \hat{\mathbf{H}} | \psi_i \rangle = H_{ij}$

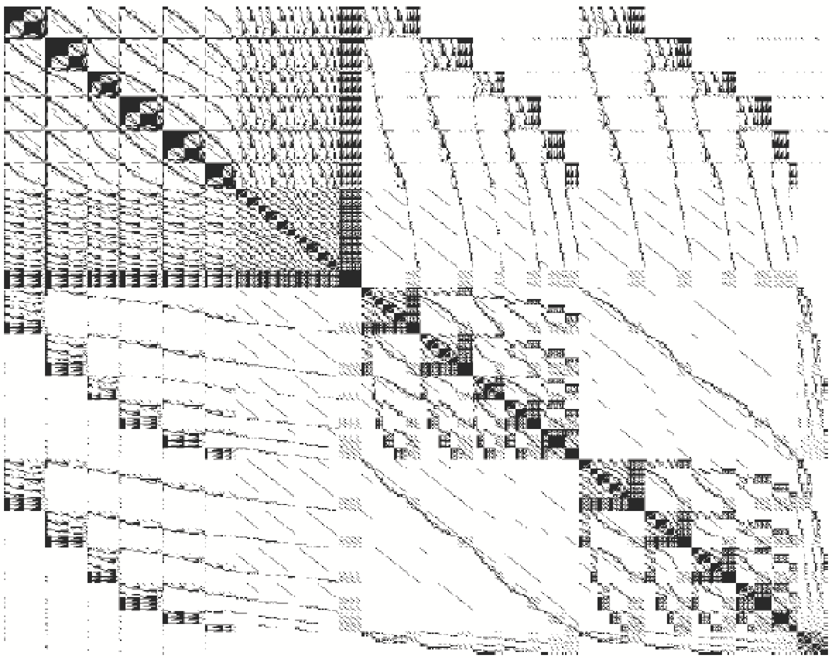
$$\hat{\mathbf{H}} = \hat{\mathbf{T}}_{\text{rel}} + \Lambda_{CM} \left(\hat{\mathbf{H}}_{CM}^{H.O.} - \frac{3}{2} \big(\sum_i m_i \big) \, \omega \right) + \sum_{i<j} V_{ij} + \sum_{i<j<k} V_{ijk} + \ldots$$

  - 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 $|\Psi\rangle = \sum a_i |\psi_i\rangle$
  - Slater Determinants of single-particle states
  - $N_{\max}$ truncation on total number of H.O. quanta
- Express Hamiltonian in basis $\langle\psi_j|\hat{\mathbf{H}}|\psi_i\rangle = H_{ij}$
  - large sparse symmetric matrix

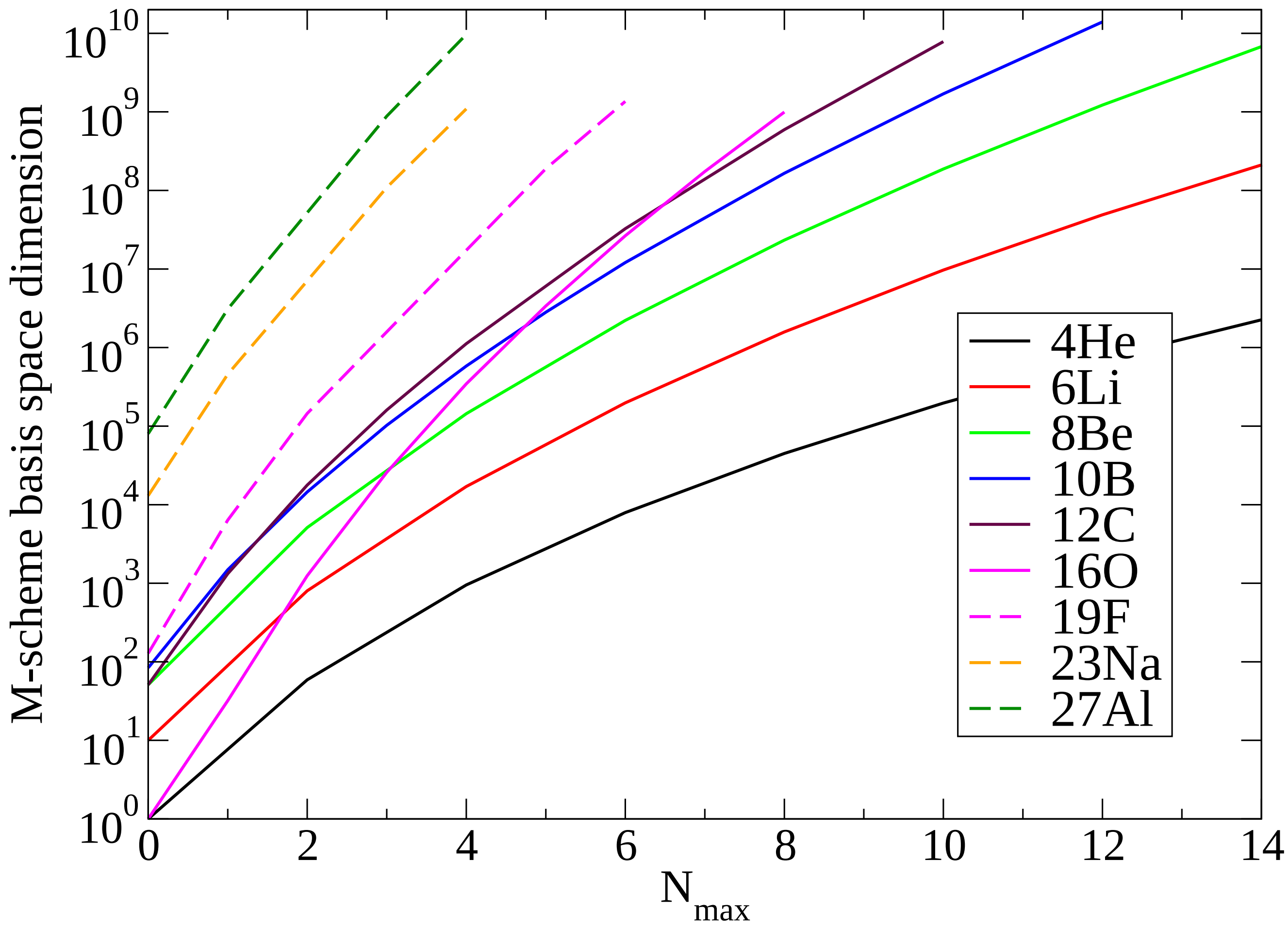
Sparsity Structure for ^{6}Li



- Obtain lowest eigenvalues using Lanczos algorithm
  - Eigenvalues: bound state spectrum
  - Eigenvectors: nuclear wavefunctions

CI calculations – main challenge

Single most important computational issue:
exponential increase of dimensionality with increasing H.O. levels



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)

Intermezzo: Extrapolation Techniques

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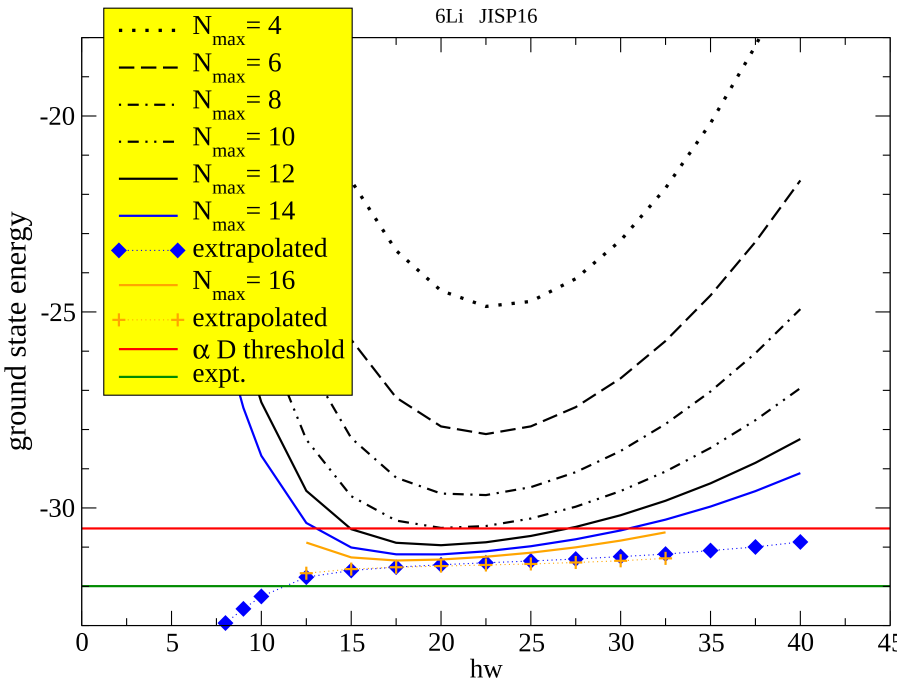
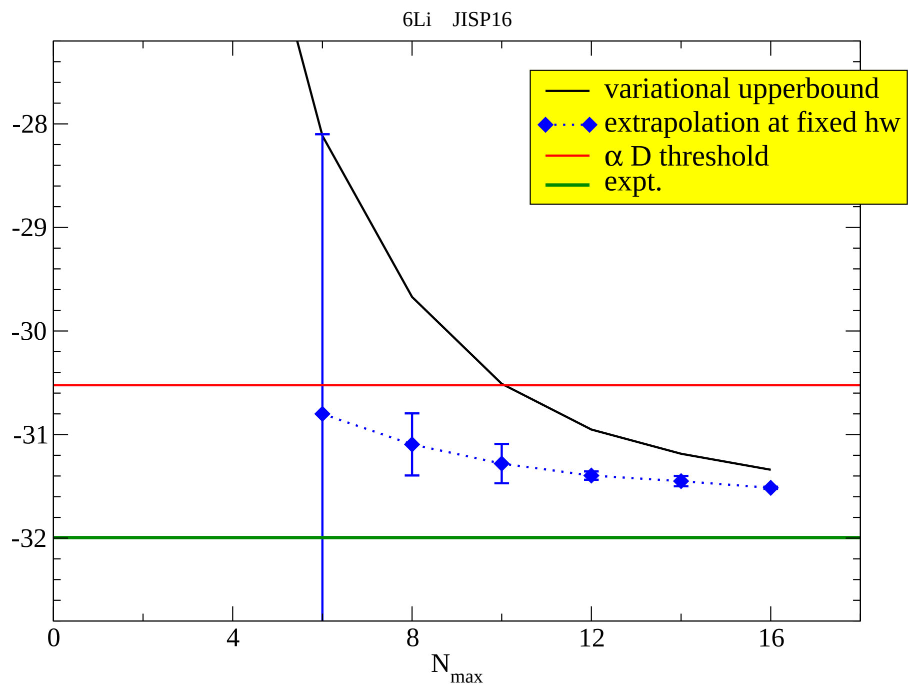




Intermezzo: Bare vs. Renormalized Hamiltonians

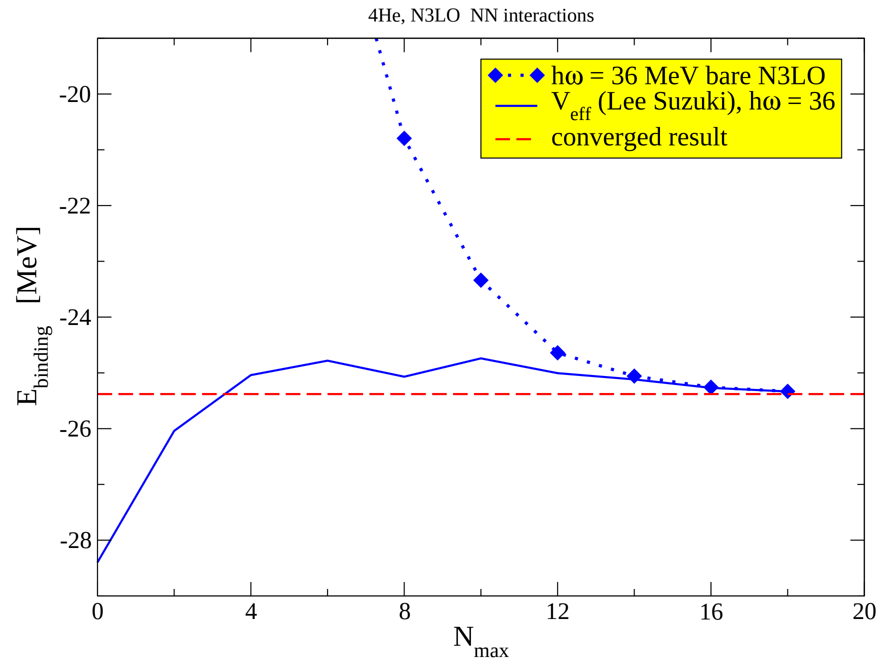
Challenge: achieve numerical convergence for no-core Full Configuation calculations using finite model space calculations

- Extrapolate to infinite model space $\longrightarrow$ exact results
- Renormalize interaction $\longrightarrow$ effective interaction V_{eff}
  - can improve quality of results in small model spaces
- Caveats
  - induces many-body forces
    - induced 3-body forces are often neglected
    - induced 4-, 5-, ..., A-body forces are always neglected
  - variational principle applicable to renormalized Hamiltonian not to original (bare) Hamiltonian
  - often complicates extrapolation to asymptotic values
  - need to renormalize operators as well

Intermezzo: Bare vs. Renormalized Hamiltonians

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

- Extrapolate to infinite model space $\longrightarrow$ exact results
- Renormalize interaction $\longrightarrow$ effective interaction V_{eff}
- Commonly used in No Core Shell Model calculations: Lee–Suzuki Renormalization
  - different V_{eff} for each nucleus and each model space
  - disadvantages
    - no variational principle
    - approach to continuum limit non-monotonic



Intermezzo: Bare vs. Renormalized Hamiltonians

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

- Extrapolate to infinite model space $\longrightarrow$ exact results
- Renormalize interaction $\longrightarrow$ effective interaction V_{eff}
- Commonly used in No Core Shell Model calculations:
  Lee–Suzuki Renormalization
- SRG: Similarity transformations
  applied to the free-space Hamiltonian
  - same renormalized Ham. for all nuclei and model spaces
  - variational principle applicable to renormalized Hamiltonian
  - smooth approach to continuum limit
  - currently working on renormalized operators (OSU group)
- Other methods: $V_{\text{low }k}$, V_{UCOM}

Nuclear interaction

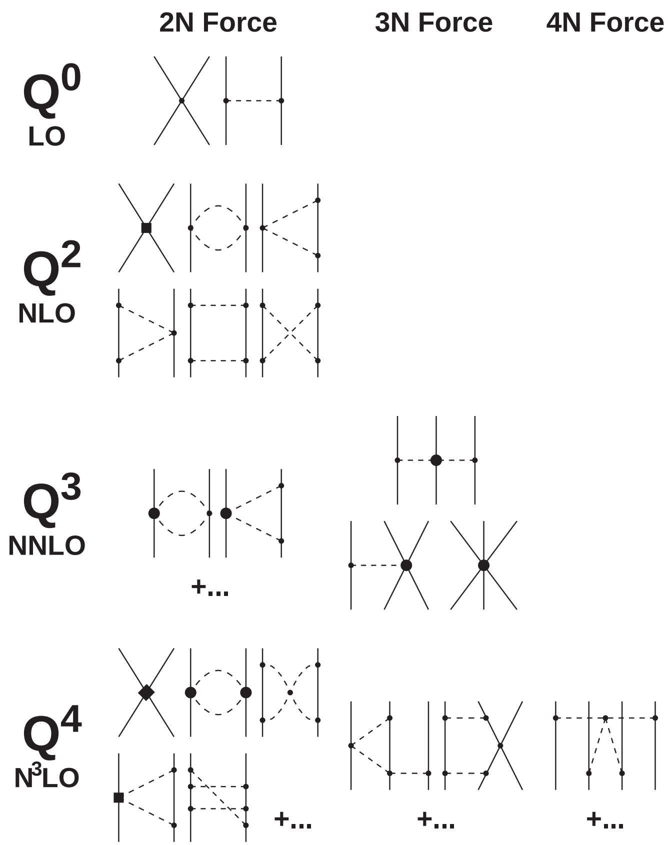
Strong force between nucleons not well known . . .

. . . but should be 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

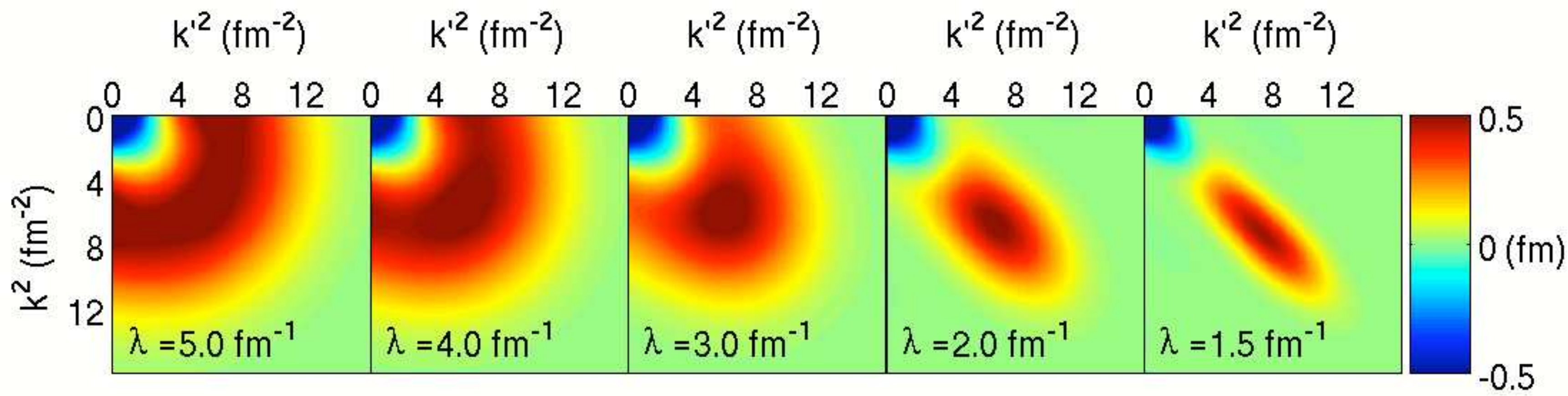
$$V_{NN} \gg V_{NNN} \gg V_{NNNN}$$

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



Similarity Renormalization Group – NN interaction

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



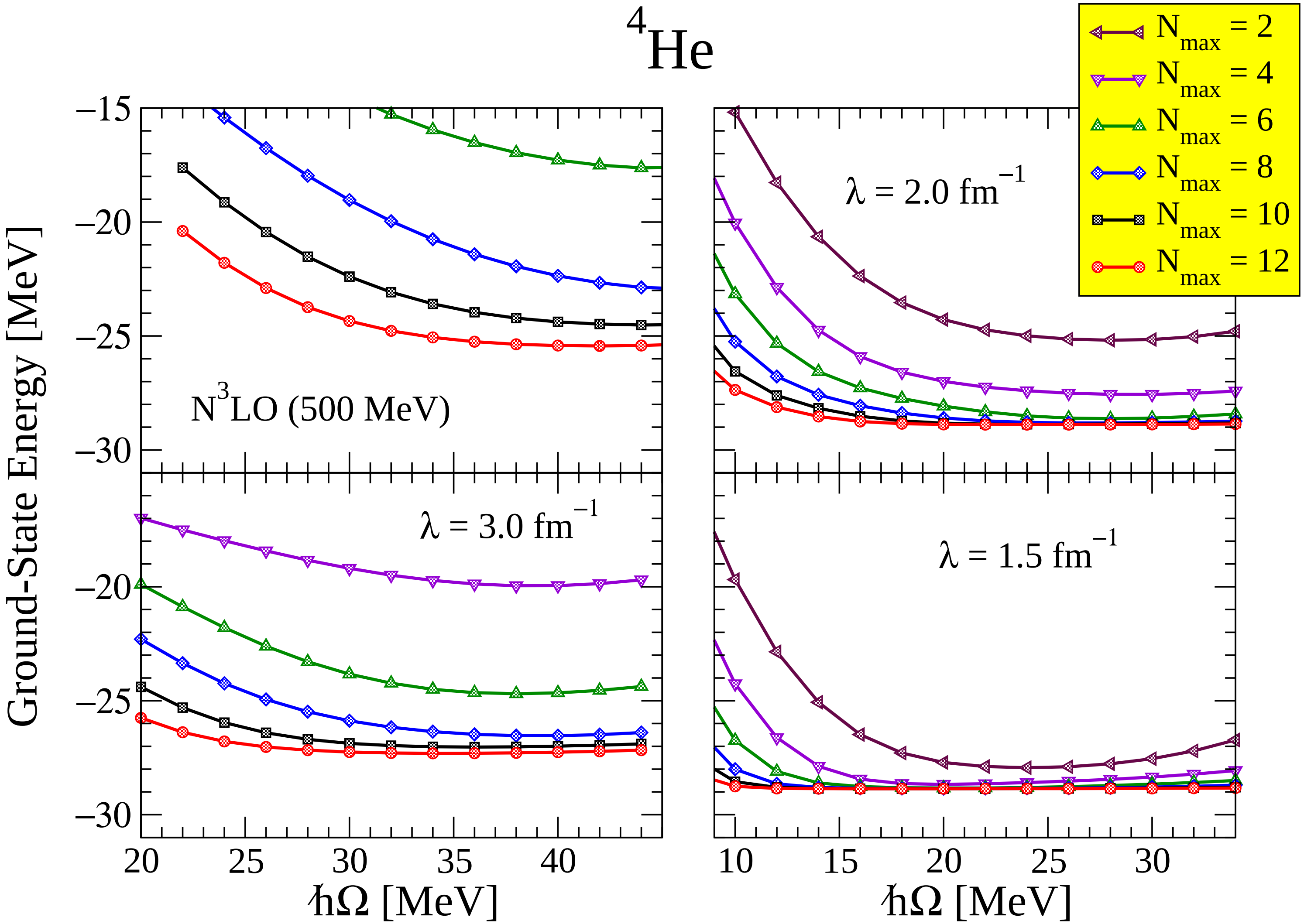
  - drives interaction towards band-diagonal structure
  - SRG shifts strength between 2-body and many-body forces

- 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

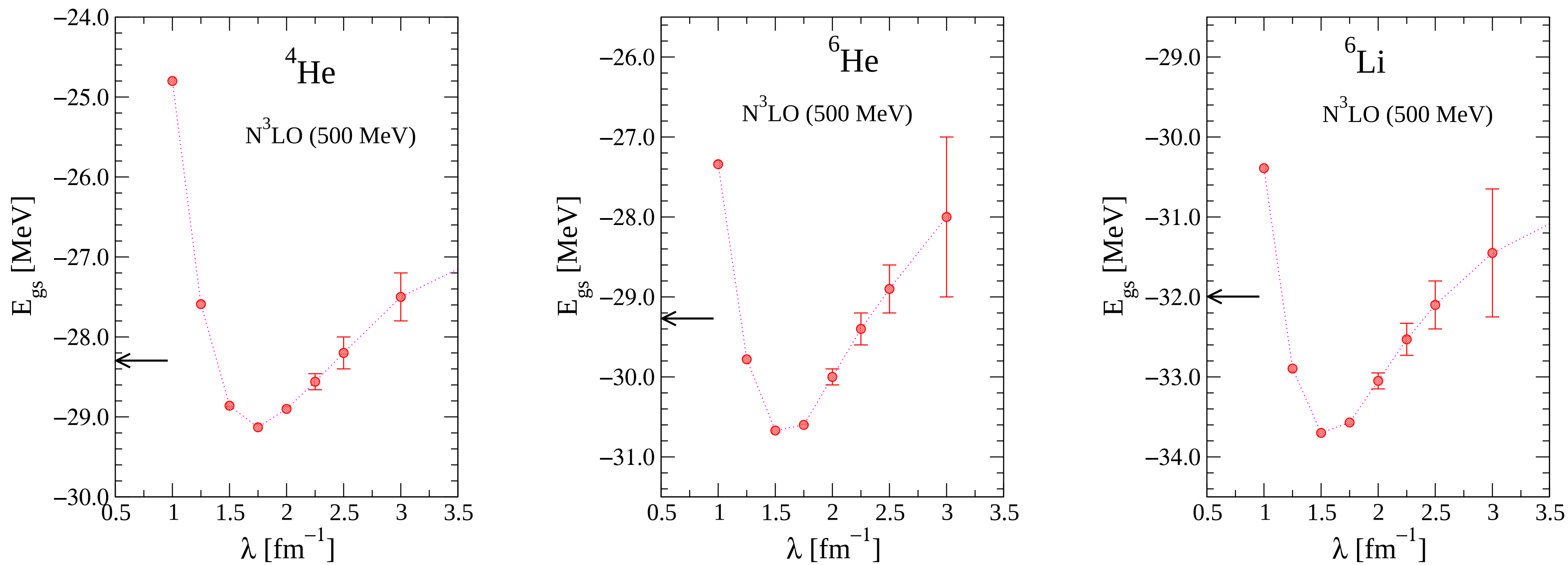
Improve convergence rate by applying SRG to N3LO



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

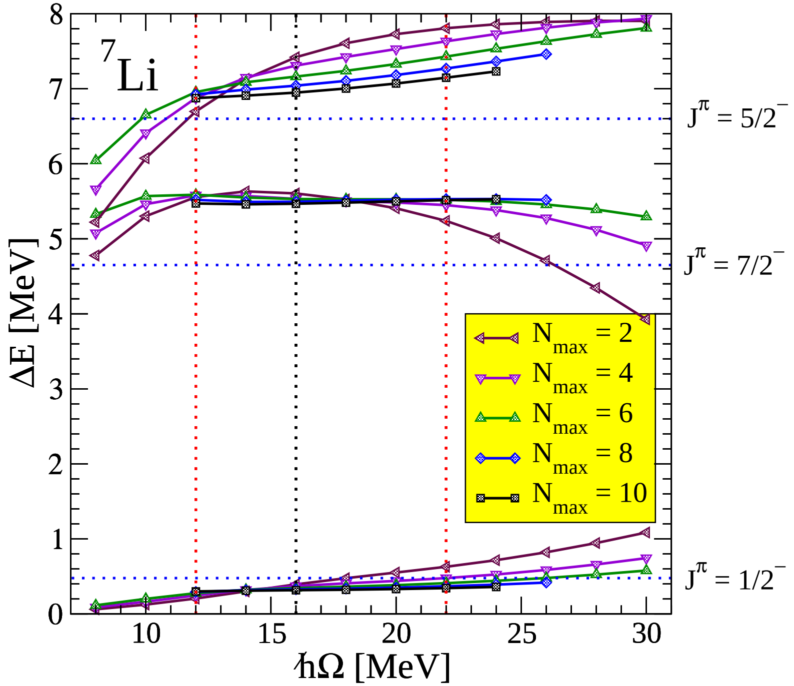
Results with SRG-evolved N3LO NN interaction

- Convergence rate significantly improved by SRG evolution
- Net contribution of many-body body forces remain "natural" down to $\lambda \approx 1.2 \sim 1.5\ \mathrm{fm}^{-1}$

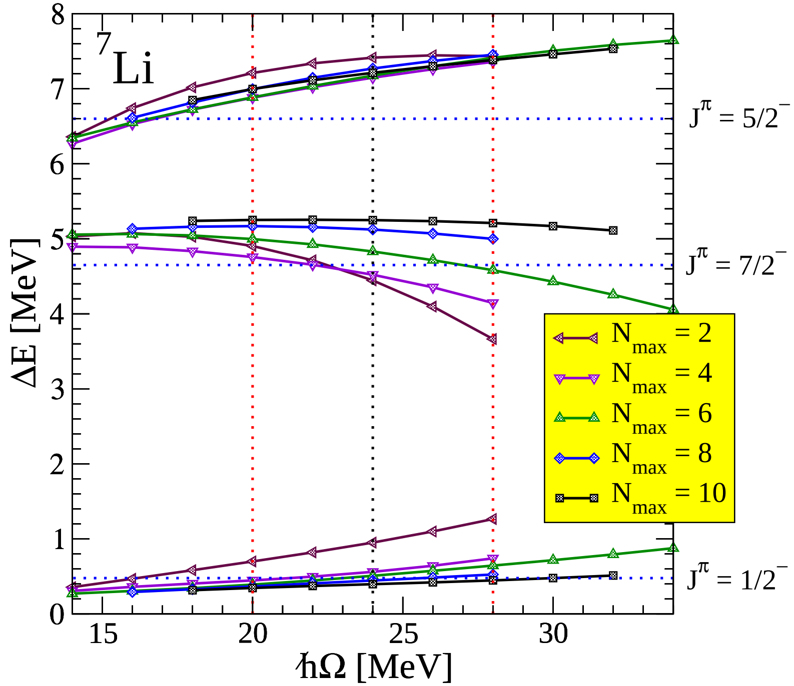


(Bogner, Furnstahl, Maris, Perry, Schwenk, Vary, NPA801, 21 (2008), arXiv:0708.3754)

Spectrum of 7Li with SRG-evolved N3LO NN interaction



$\lambda = 1.50$

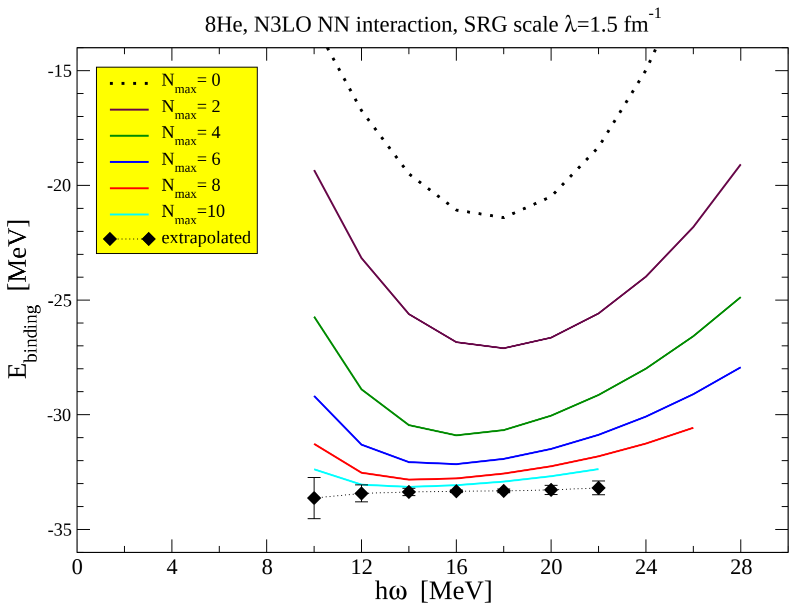


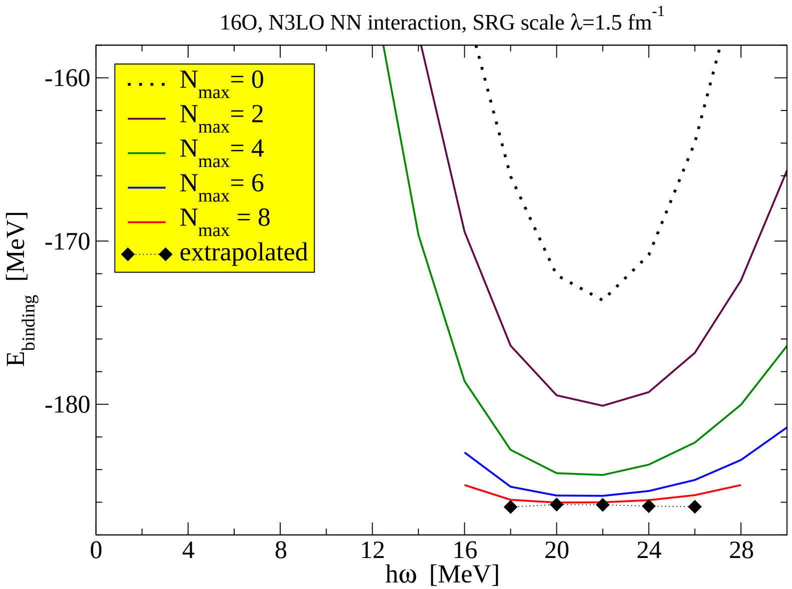
$\lambda = 2.50$

- Lowest two excited states well-converged
- Spectrum remarkebly insensitive to λ,
  despite difference in ground state energy of about 3 MeV

More results with SRG-evolved N3LO NN interaction

- Rapid convergence 8He, 12C, 16O, 40Ca at $\lambda = 1.5\ \mathrm{fm}^{-1}$
  - check between our results and Coupled Cluster (Dean *et al*)
- All overbound at $\lambda = 1.5\ \mathrm{fm}^{-1}$



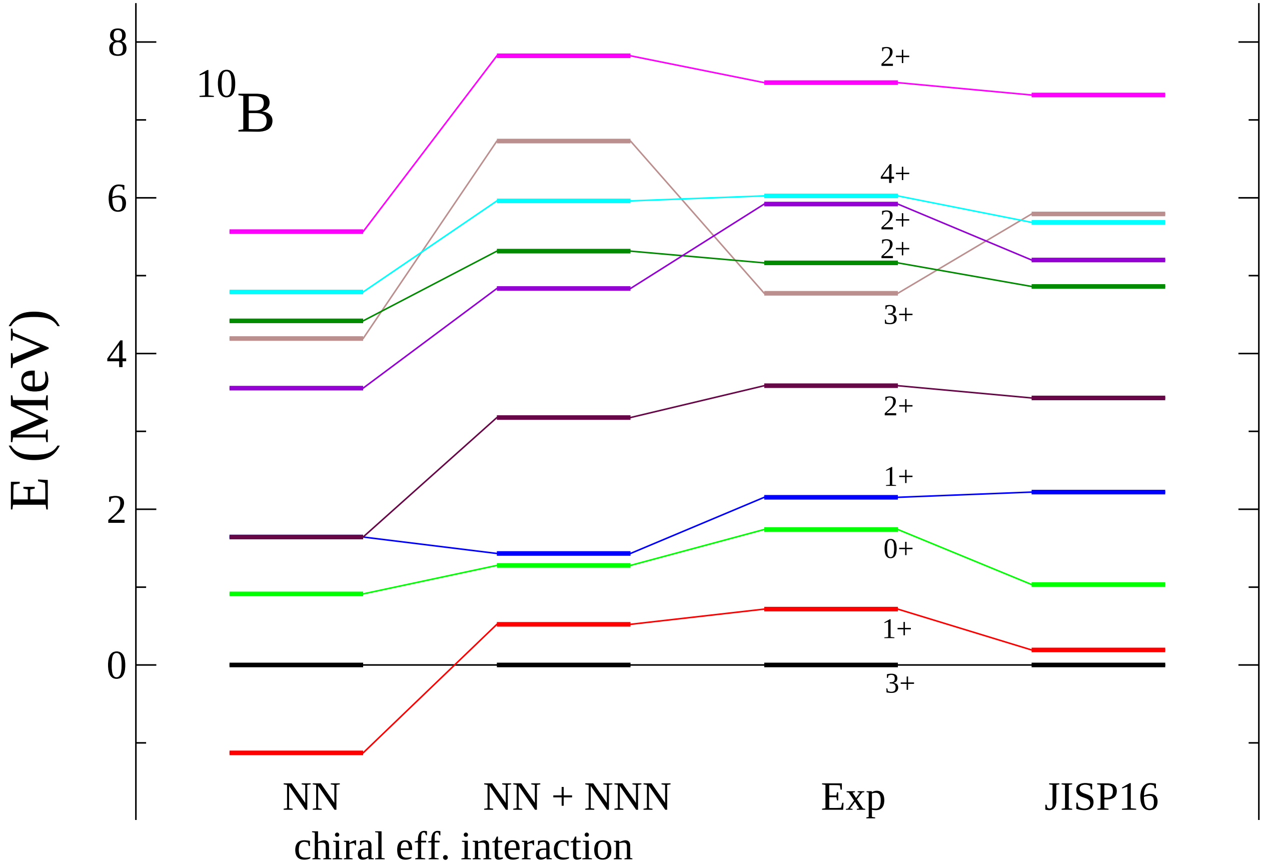


- Also overbound at $\lambda = 2.5\ \mathrm{fm}^{-1}$: 3-body forces necessary
- 3-body forces also necessary for spectra, . . .

Navratil, Gueorguiev, Vary, Ormand, Nogga, PRL99, 014315 (2007)

- Next step: include NNN forces (LLNL group)

Results with chiral N3LO (3-body) and JISP16 (2-body)



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), Proceedings of the Carpathian Summer School of Physics 2007, AIP Conference Proceedings 972, 49 (2008)

Phenomeological NN interaction: JISP16

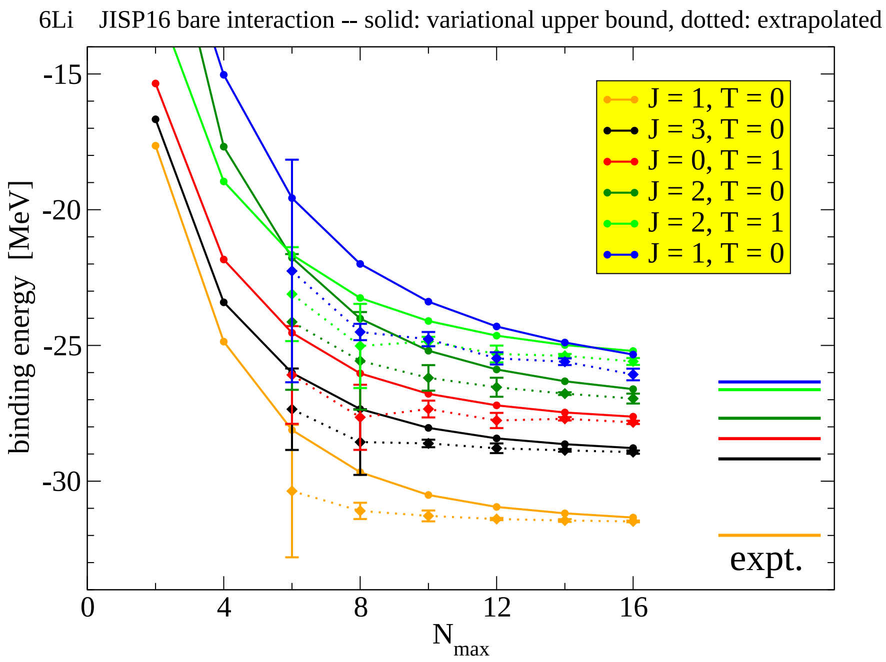
A.M. Shirokov, J.P. Vary, A.I. Mazur, T.A. Weber, PLB **644**, 33 (2007)

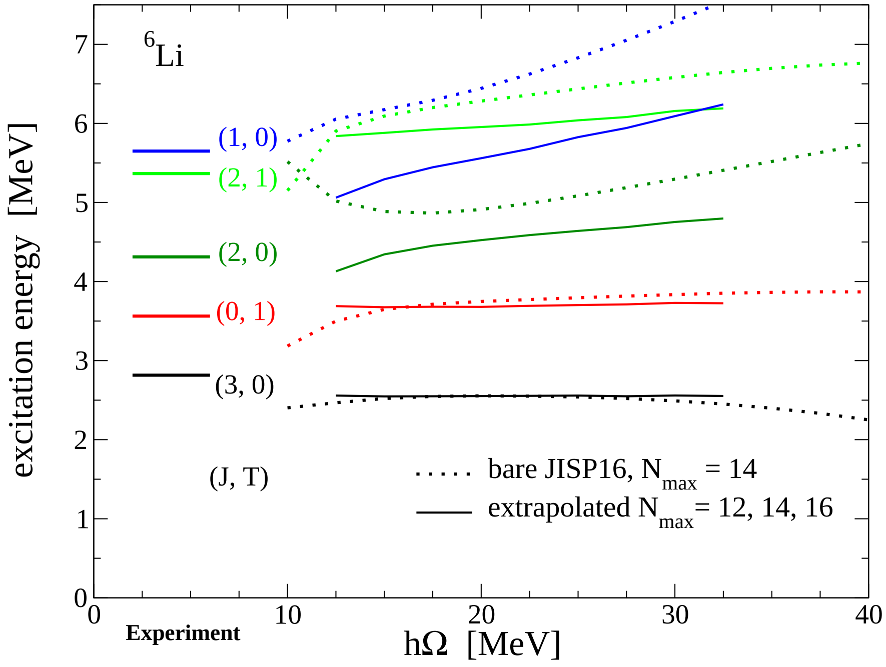
J-matrix Inverse Scattering Potential tuned up to ^{16}O

- 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/`

Results with JISP16 for ^{6}Li



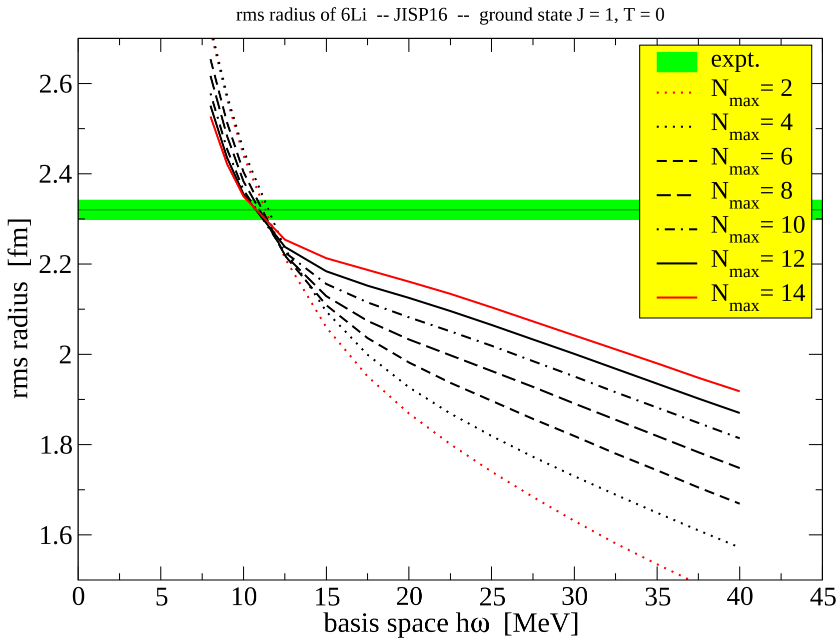


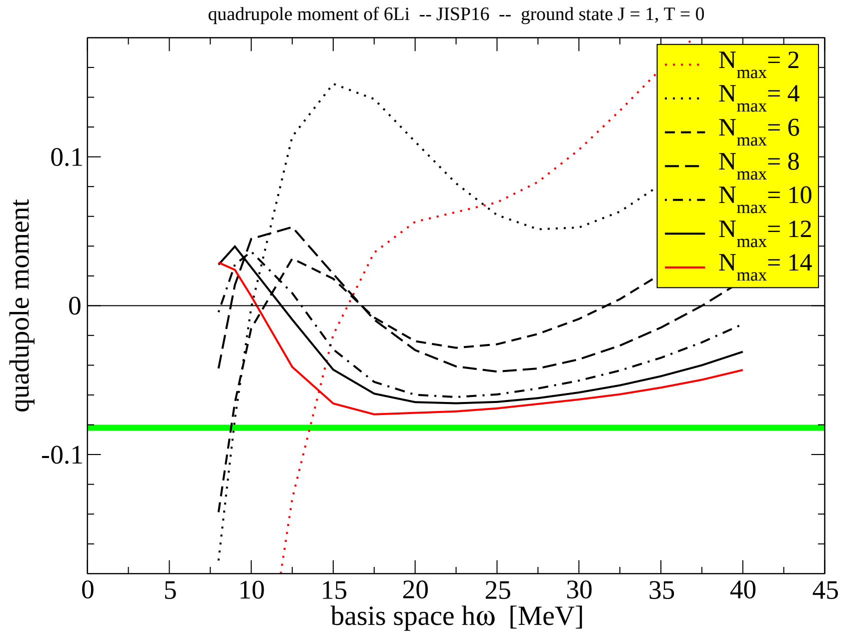
- Spectrum in good agreement with experimental data
  - in particular for narrow states
- Broad resonances $\leftrightarrow$ strong dependence on $\hbar\Omega$
  - agrees with inverse scattering analysis of α-nucleon states

    Shirokov, Mazur, Vary, Mazur, PRD79, 014610 (2009)
  - numerical error under investigation

Results with JISP16 for ^{6}Li

Ground state $\langle r^2 \rangle$ and Q

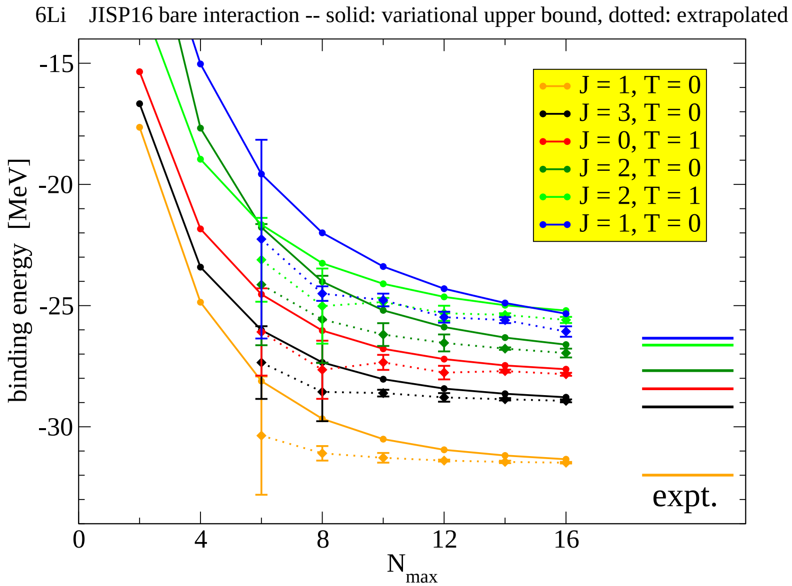


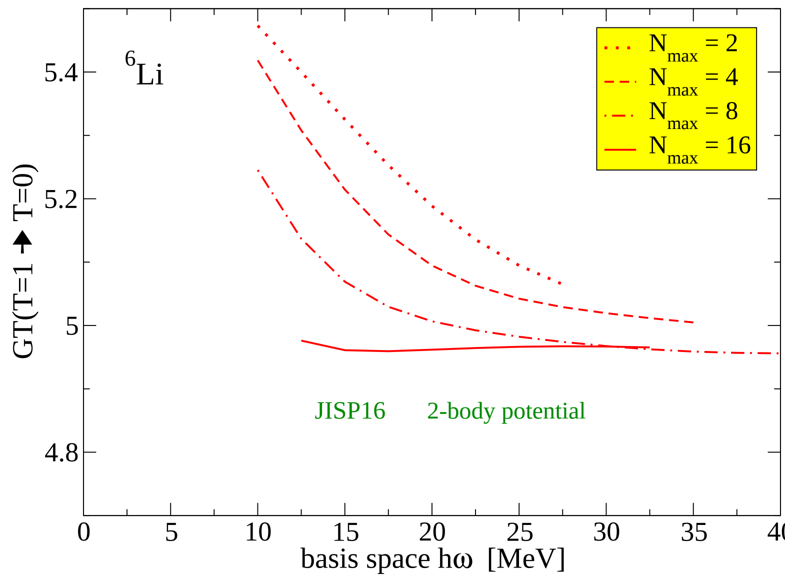


- Quadrupole moment Q agrees with data within uncertainties
- RMS charge radius in the right ballpark
- Not very well converged:
  - need realistic basis function

Negoita, PhD work in progress

Gamov–Teller transition in ^{6}Li and ^{6}He





Calculation within ^{6}Li good approximation for ^{6}He$(0^+,1) \to {}^6$Li$(1^+,0)$

- Corrections due to meson-exchange currents small

within ^{6}Li	^{6}He$(0^+,1) \to {}^6$Li$(1^+,0)$	including MEC corrections	expt.
4.96	4.95	4.83(3)	4.71

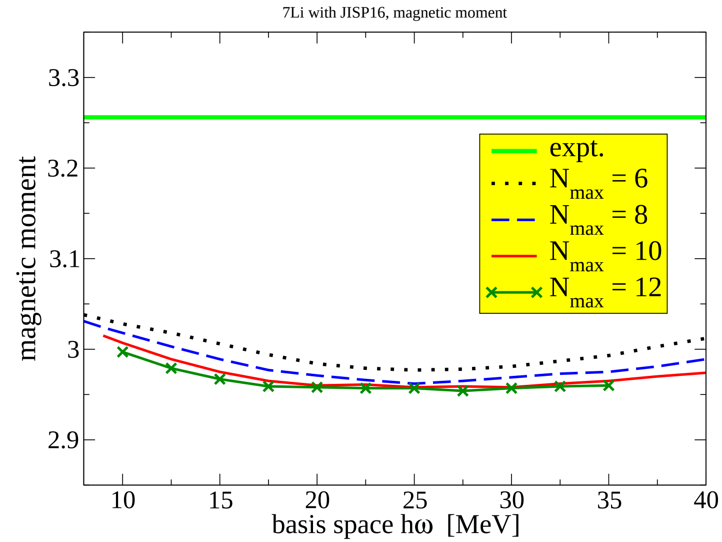
Vaintraub, Barnea, Gazit, arXiv:0903.1048 [nucl-th]

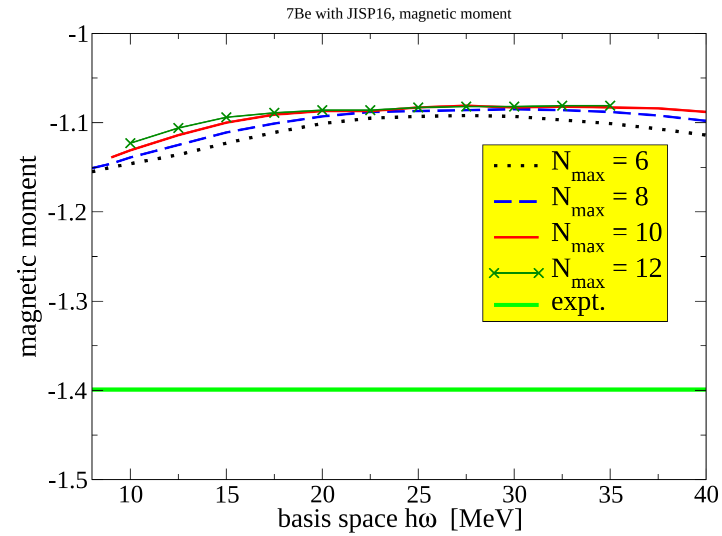
- Excellent agreement between JISP16 results and expereriment

Results with JISP16 for ^{7}Li and ^{7}Be – magnetic moments

	expt.	$N_{\text{max}} = 12$ at $\hbar\omega = 20$ MeV	
^{7}Li, E	39.270	-38.58(4)	extrapolated
^{7}Li, r_p	2.27(2)	2.07	
^{7}Li, μ	+3.256	+2.96(1)	converged
^{7}Li, $\mathcal{Q}$	-4.00(6)	-2.79	
^{7}Be, E	37.600	-36.94(5)	extrapolated
^{7}Be, r_p	2.36(2)	2.234	
^{7}Be, μ	-1.399	-1.09(1)	converged
^{7}Be, $\mathcal{Q}$		-4.695	

- Discrepancy between expt. and calc. μ most likely due to two-body currents

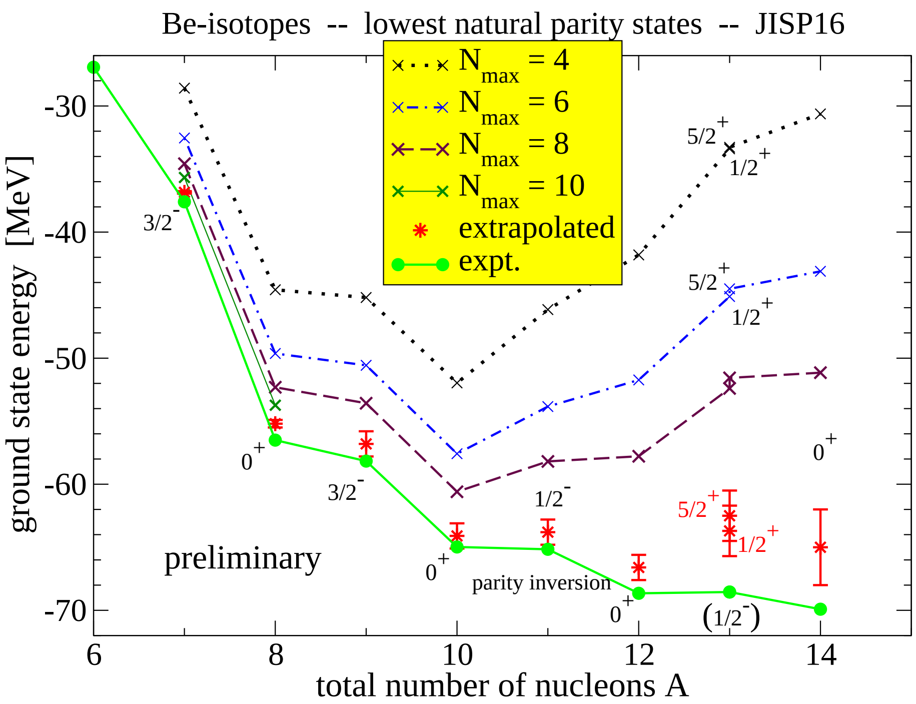


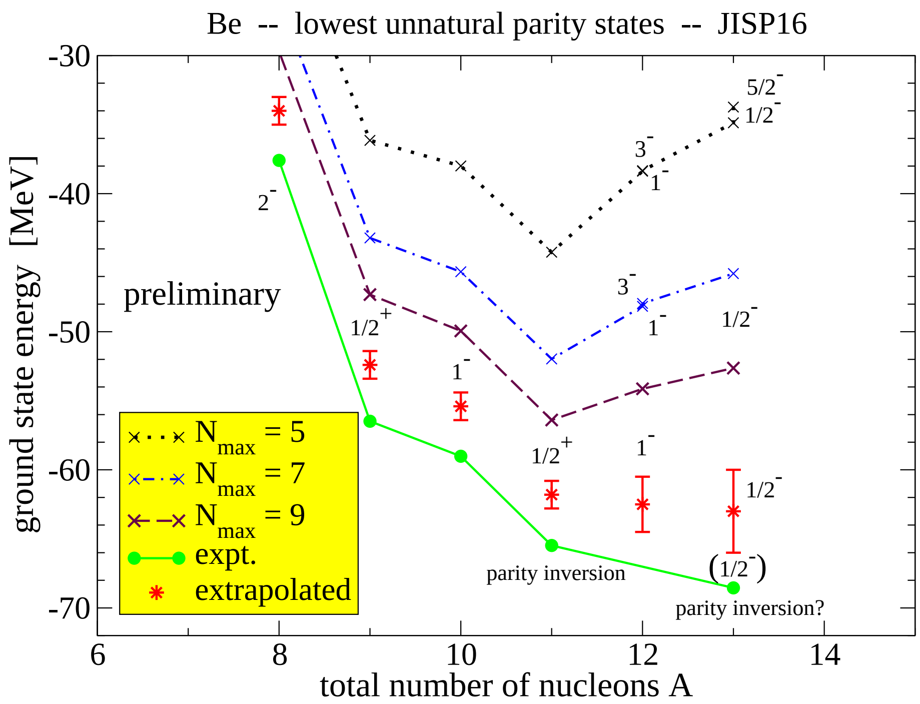


Beryllium isotopes

updated from Vary, Maris, Ng, Yang, Sosonkina, arXiv:0907.0209 [nucl-th],

J. Phys. Conf. Ser. 180, 012083 (2009)

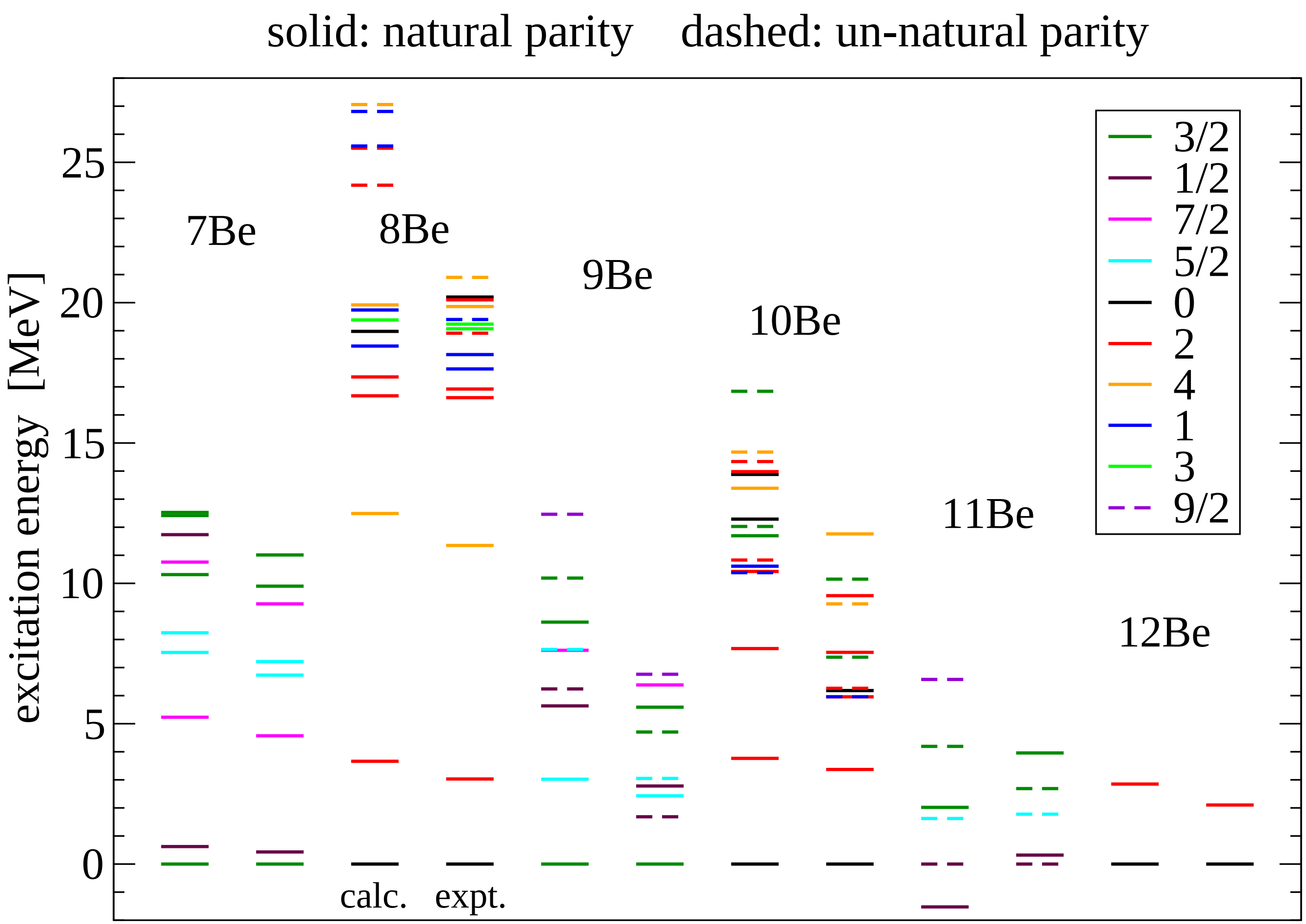




- Exploring physics near the neutron drip line – in progress
- Un-natural parity states systematically underbound with JISP16
- Similar results for He- and Li-isotopes

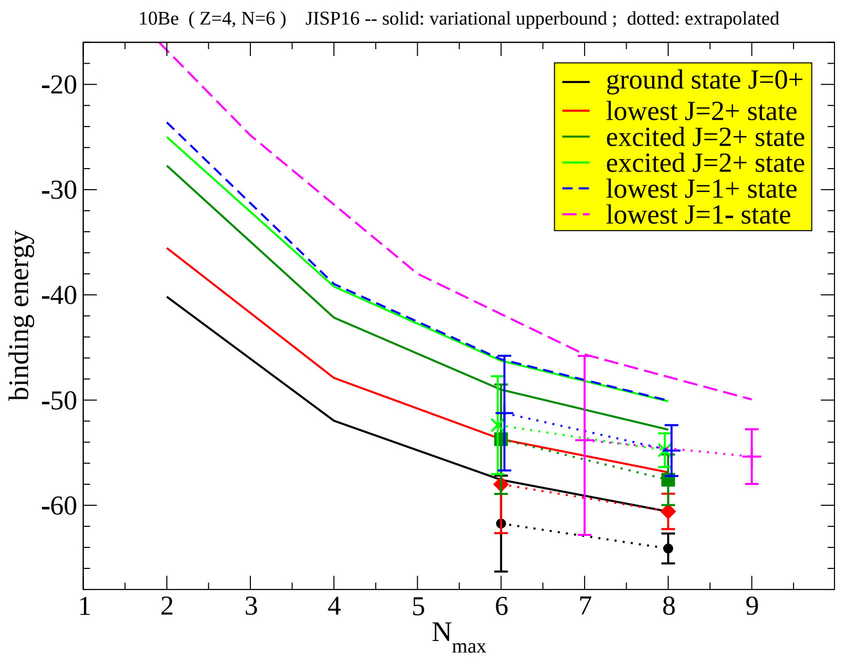
Results with JISP16 for Be spectra – work in progress

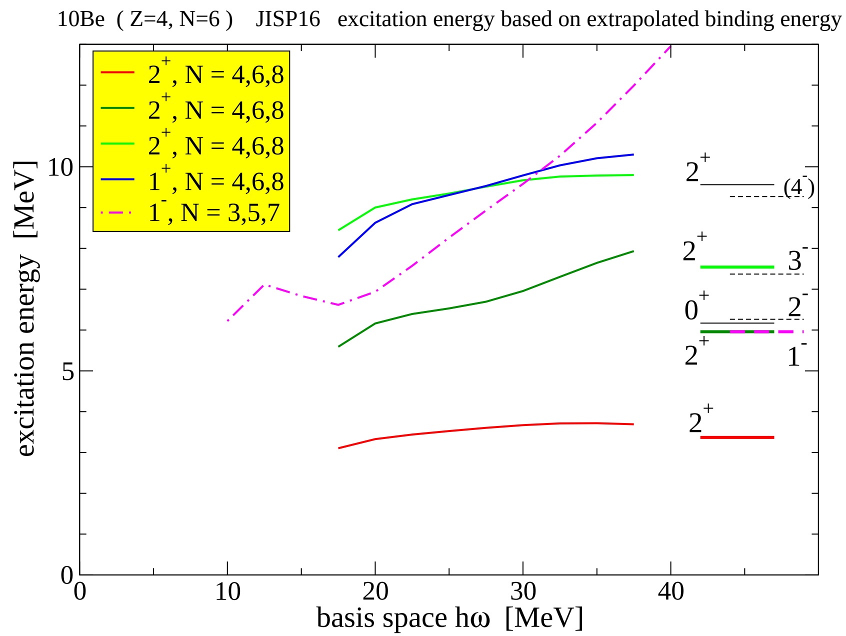
- Excitation energy at $\hbar\omega = 22.5$ MeV in largest model spaces (extrapolation to infinite model space in progress)



- Un-natural parity states systematically underbound with JISP16

Results with JISP16 for ^{10}Be – work in progress

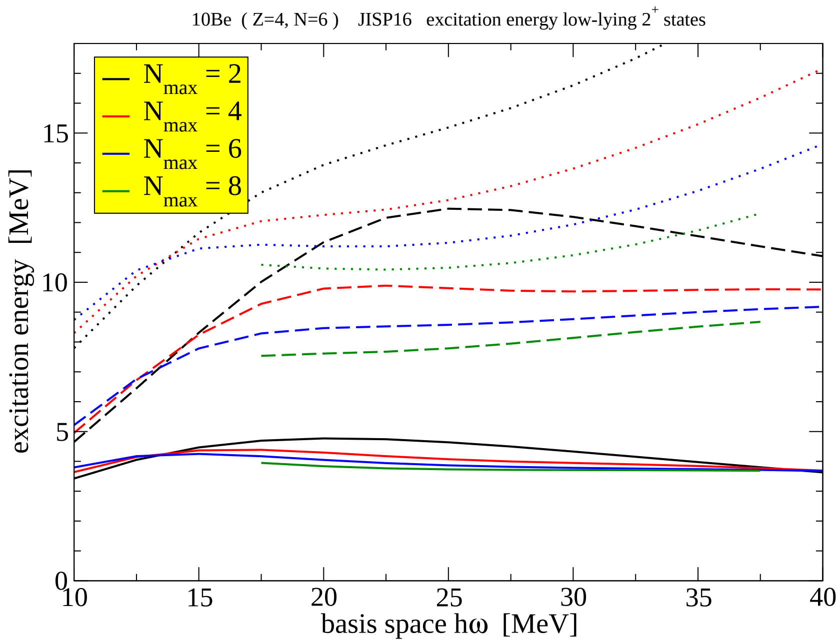


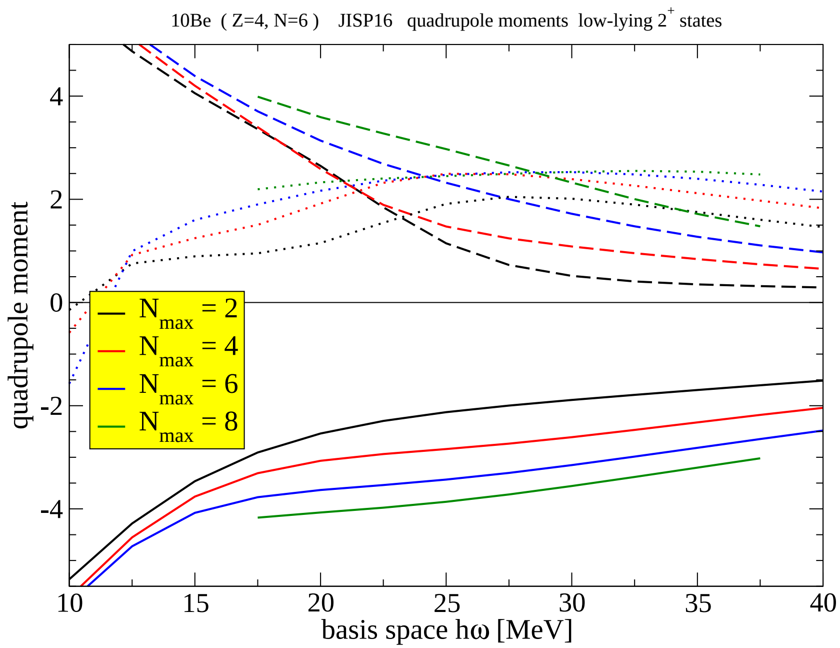


- Ground state energy in good agreement with data
  64.11 ± 1 MeV vs. 64.977 MeV
- First excited state converged and in good agreement with data
- Higher excited states and neg. parity states not converged yet
- Extrapolated spectrum in reasonable agreement with data

Quadrupole moments of ^{10}Be with JISP16 – work in progress

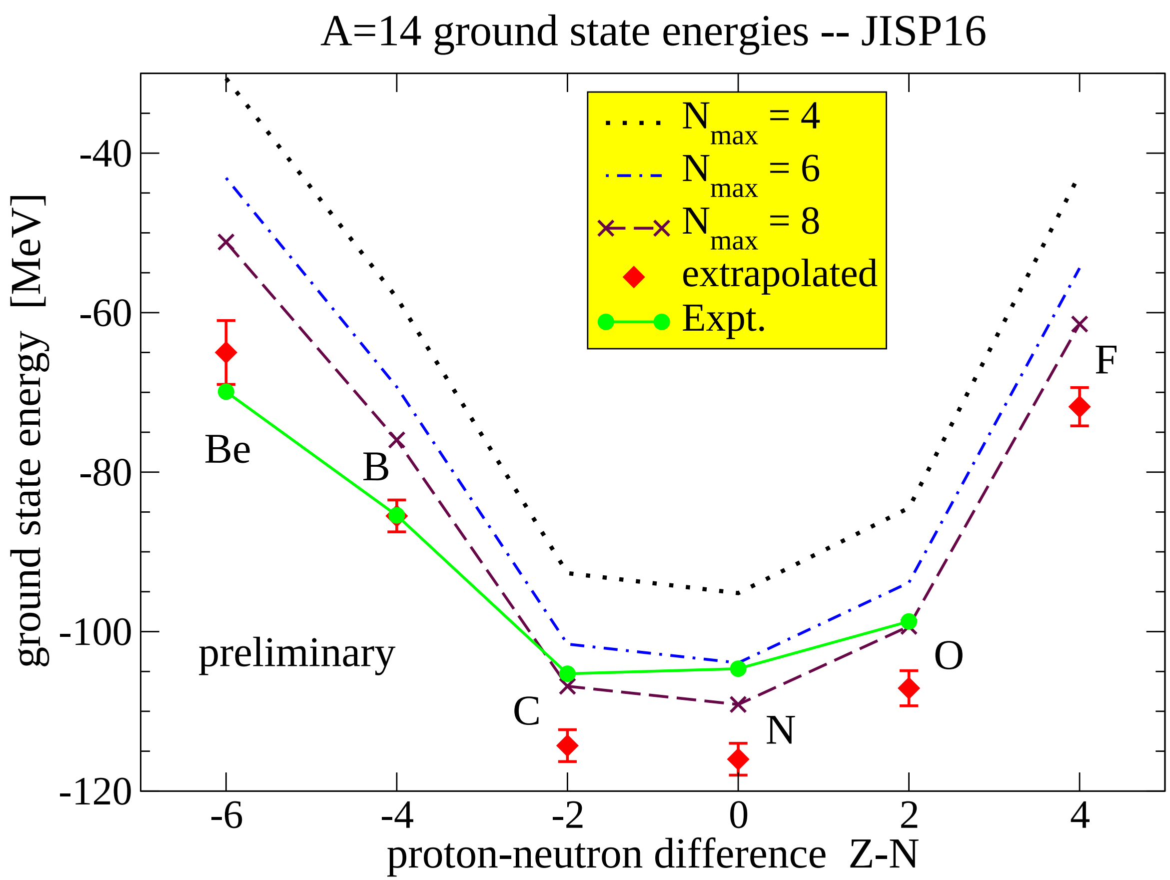
- Motivated by GFMC results
  - without 3-body forces: $\mathcal{Q}$ of lowest 2^+ state is positive
    but with 3-body forces: $\mathcal{Q}$ of lowest 2^+ state is negative
    and vice-versa for first excited 2^+ state





- JISP16 agrees qualitatively with AV18 plus 3-body forces

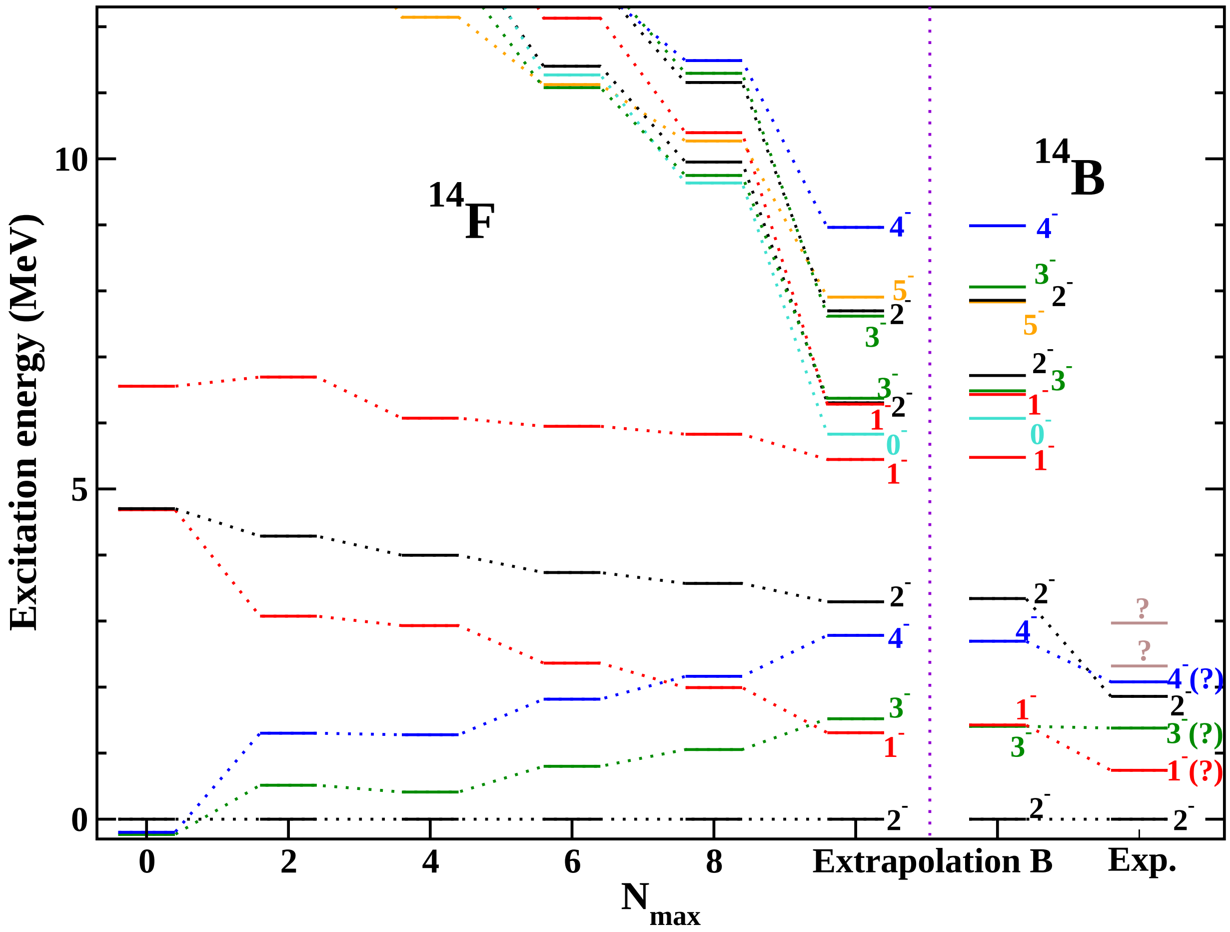
Valley of stability for $A = 14$ Nuclei



- Preliminary results
  - up to 10% overbinding for ^{14}C, ^{14}N, ^{14}O

    Maris, Vary, Shirokov, arXiv:0808.3420 [nucl-th], Phys. Rev. C79, 014308 (2009)
- Need improved (charge-dependent?) interaction

Spectrum of ^{14}F – submitted for SciDAC Highlights



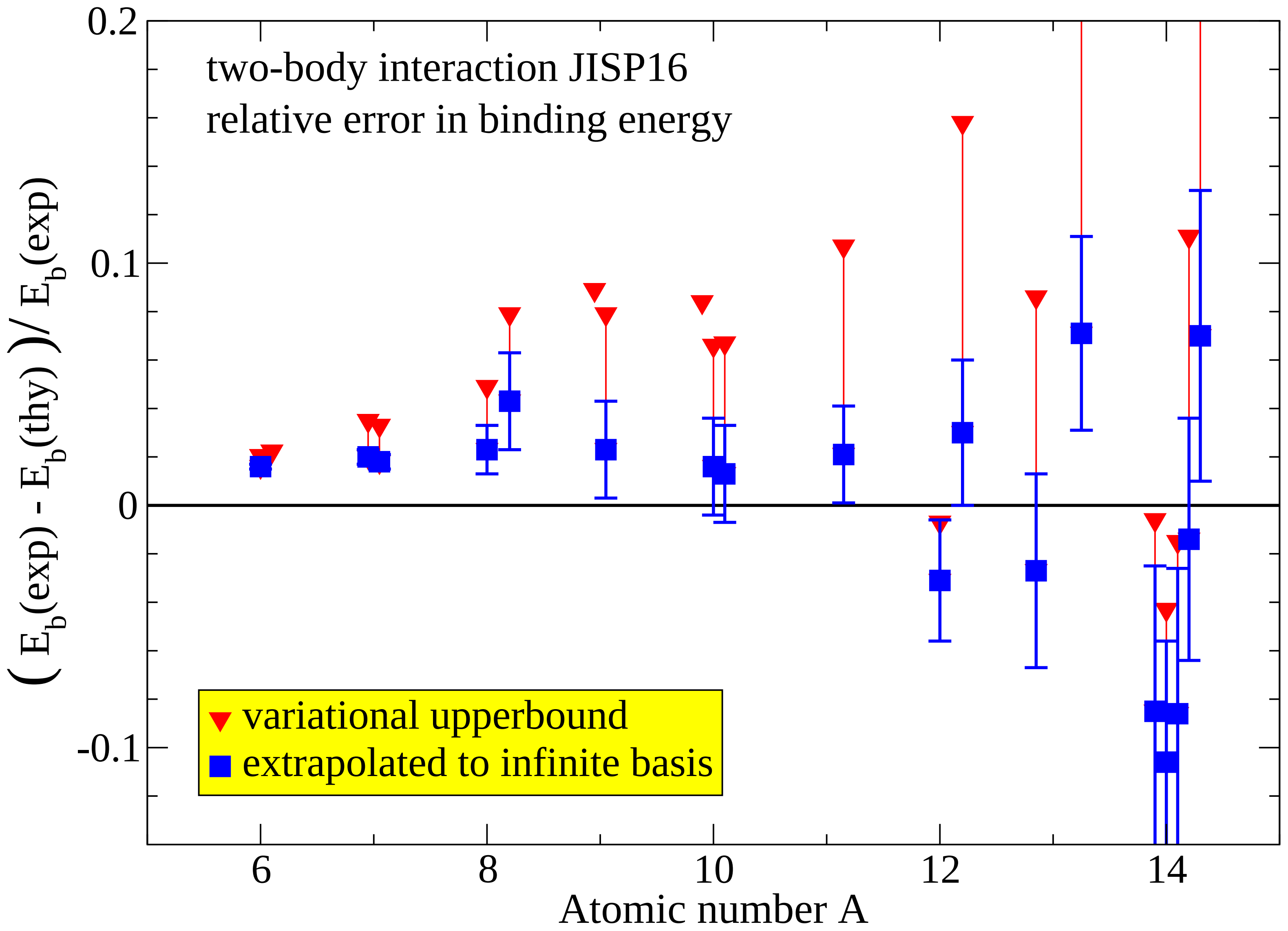
dimension $2 \cdot 10^9$
nonzero m.e. $2 \cdot 10^{12}$
runtime 2 to 3 hours on
7,626 quad-core nodes
on Jaguar (XT4)
(summer 2009)

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

- Predicted ground state energy: 72 ± 4 MeV (unstable)
- Mirror nucleus ^{14}B: 86 ± 4 MeV agrees with experiment 85.423 MeV
- Experiments in progress at Texas A&M

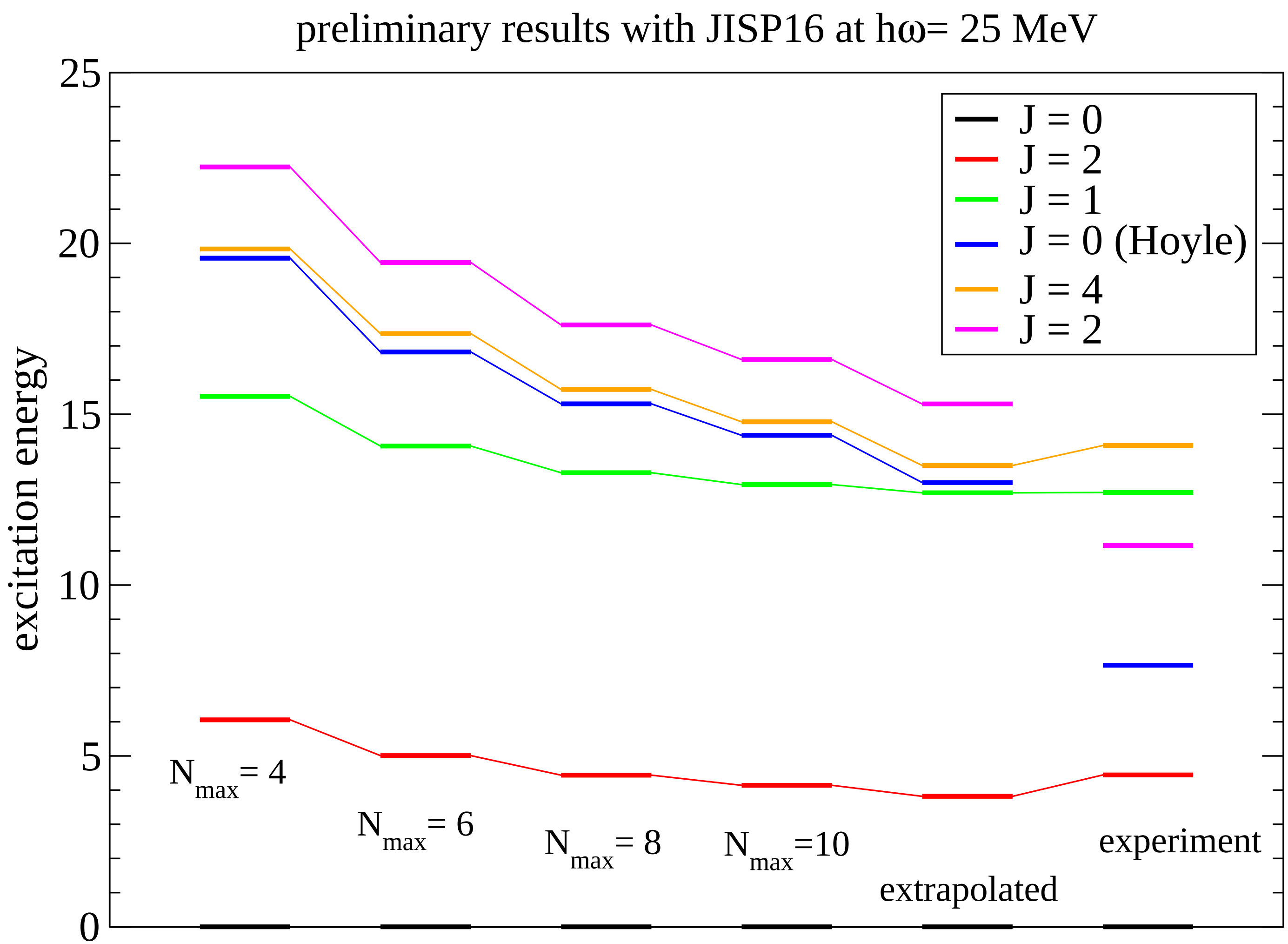
Summary of NCFC results with JISP16

Comparison of data and theory for natural parity ground state energies



12C spectrum with JISP16 – work in progress

- Excitation energy at $\hbar\omega = 25$ MeV up through $N = 10$

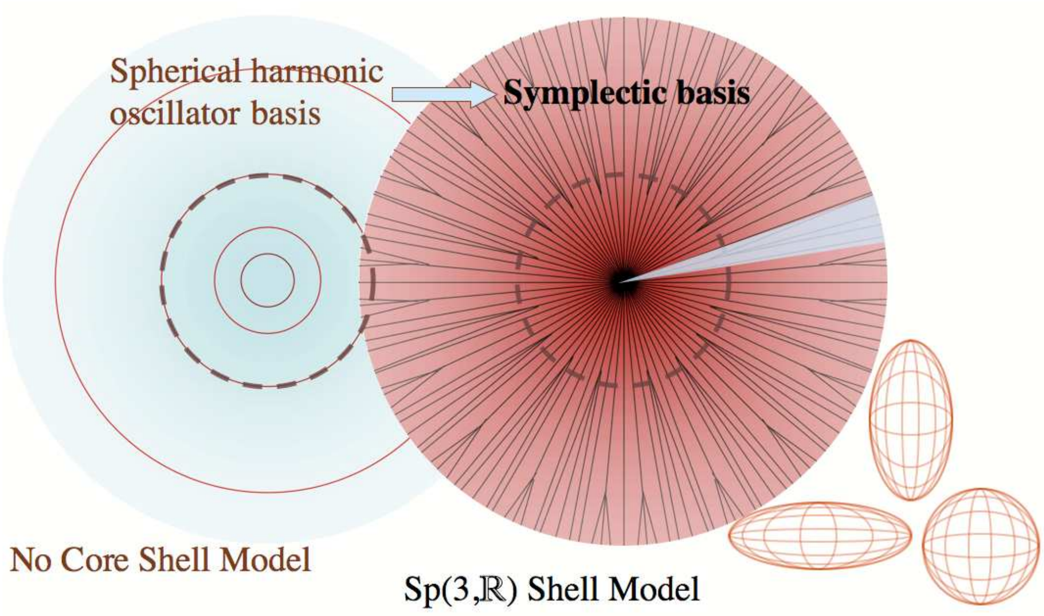


- Hoyle state not converged and/or far from experiment w. JISP16

Taming the scale explosion in nuclear structure calculations

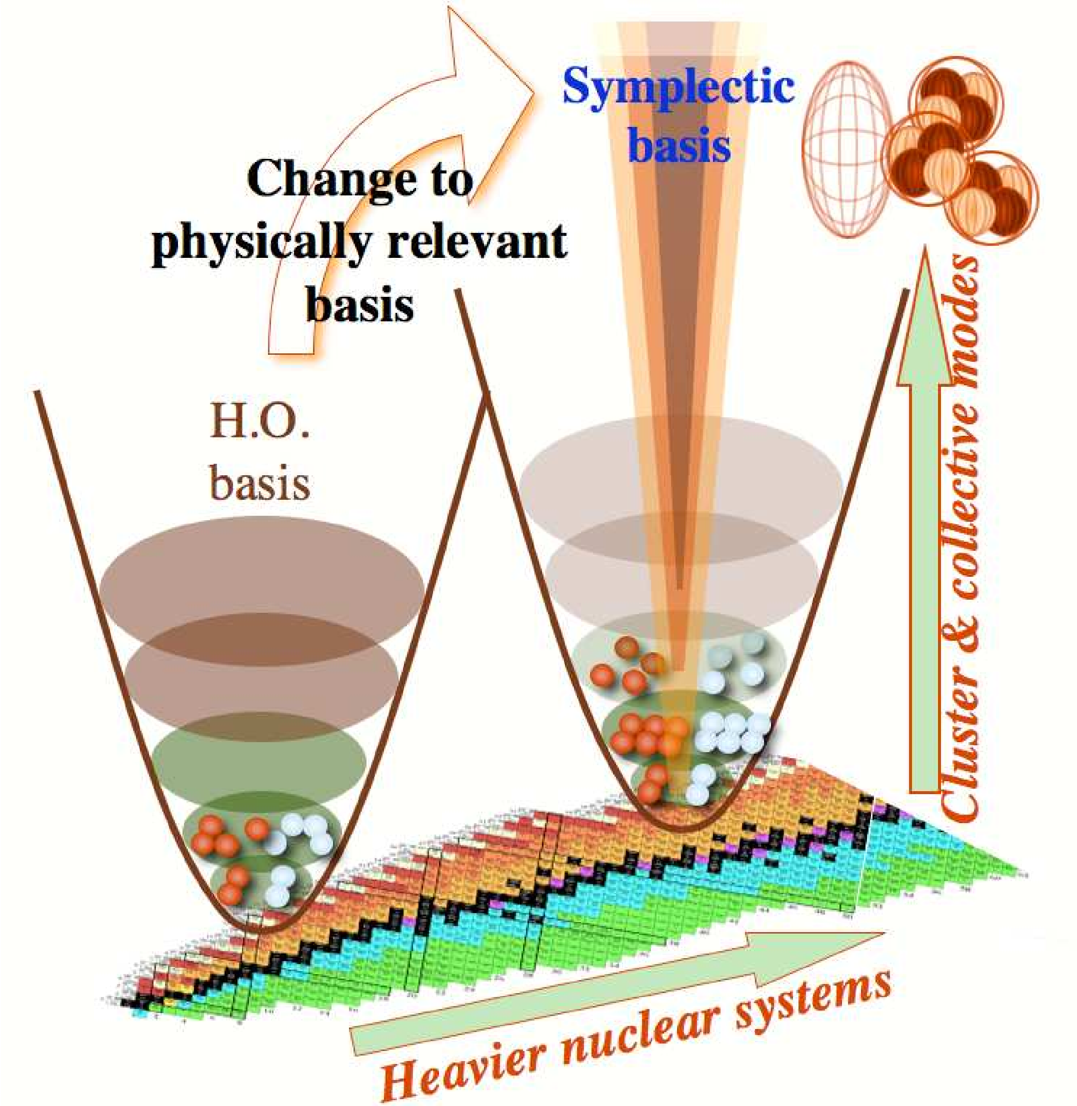
PetaApps award (2009)
PIs: Jerry Draayer (LSU), Umit Catalyurek (OSU),
Masha Sosonkina, James Vary (ISU)

- Harmonic Oscillator basis: spherically symmetric
- Symplectic Sp$(3, \mathbb{R})$ basis: exploit symmetries of nuclear physics
  - highly deformed states (oblong, oblate)
  - α-cluster states
- Unitary transformation from H.O. to Sp$(3, \mathbb{R})$ basis: reducing the exponential increase of the basis space dimension with $N_{\max}$ while incorporating important physics associated with clustering and deformations



Taming the scale explosion in nuclear structure calculations

PetaApps award (2009)



- Allows for ab initio calculations of
  - cluster states
  - deformed nuclei
  - nuclei in sd-shell (beyond ^{16}O)
- Requires innovative loadbalancing techniques
- Astrophysical applications: Hoyle state in ^{12}C (3 α-cluster state) crucial for nucleosynthesis

Conclusions

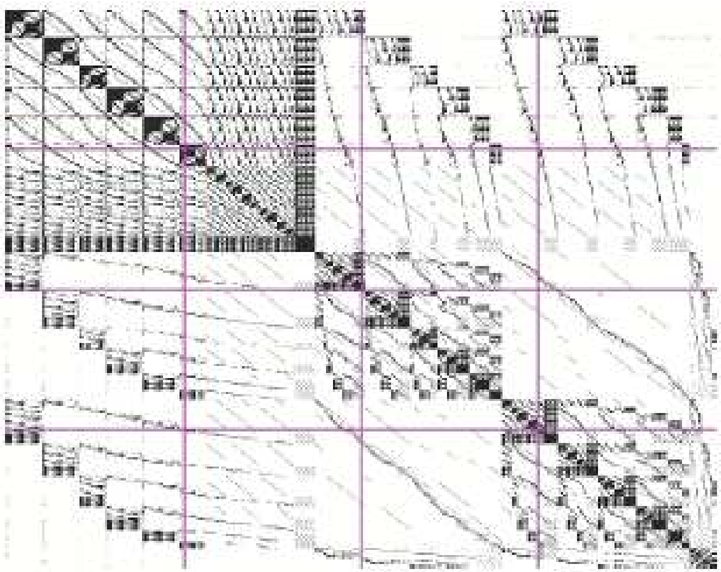
- No-core Full Configuration nuclear structure calculations
  - Binding energy, spectrum
  - $\langle r^2 \rangle$, μ, $\mathcal{Q}$, transitions, wfns, one-body densities
- Numerical convergence
  - Extrapolation to infinite basis space for (absolute) energies
  - Other observables:
    convergence rate depends on observable
- JISP16
  - Nonlocal phenomenological 2-body interaction
  - Good description of a range of light nuclei
  - Rapid convergence
- Chiral effective interactions
  - True ab-initio – nuclear interaction obtained from QCD
  - 3-body forces necessary for description of light nuclei
  - Renormalization techniques necessary

and Outlook

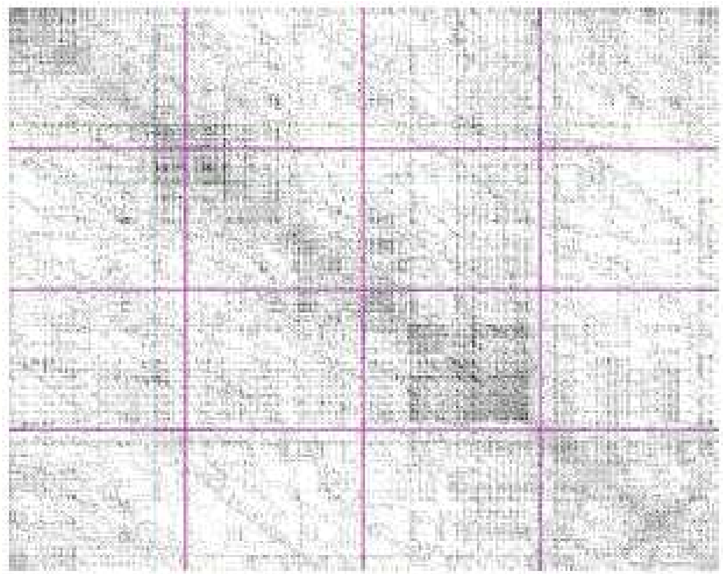
- Need realistic basis function
  to improve convergence $\langle r^2 \rangle$, $\mathcal{Q}$ — Negoita, PhD work in progress
- Need improved (charge-dependent) nonlocal NN-interaction
  Shirokov, Mazur, work in progress
  - tuned to selected light nuclei and Nuclear Matter?
- Need SRG evolution of — (OSU/LLNL), work in progress
  - chiral 3-body forces
  - operators
- Symplectic basis — Draayer *et al.*, PetaApps award
  - significantly larger model spaces
- Quantum field theory — Honkanen *et al.*
  - QED and QCD in lightfront dynamics

Many Fermion Dynamics – nuclear physics

- Platform-independent F90 code with both MPI and OpenMP
- Scalable (has run successfully on 45k+ cores on JaguarPF)
- Load-balanced



on single processor



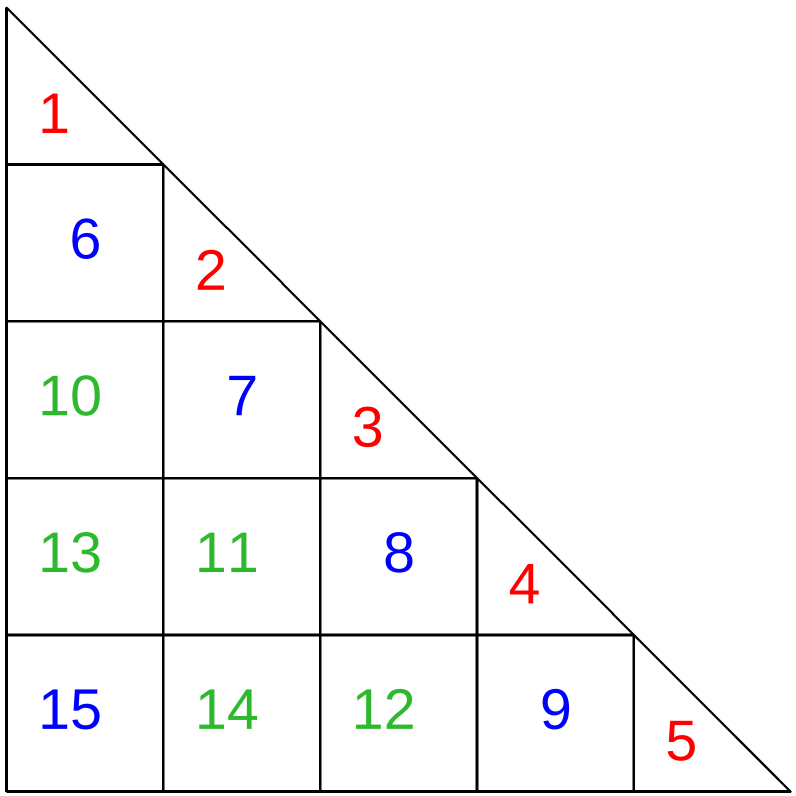
on 10 processors

- round-robin distribution of many-body states over d procs
- however, no (apparent) structure in sparse matrix

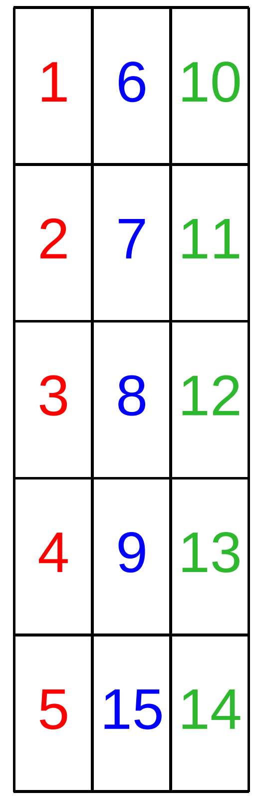
Distribution of matrix and vectors

- Store lower half of symmetric matrix, distributed over $n = d \cdot (d+1)/2$ processors with d “diagonal” proc’s
- Store Lanczos vectors on one of $(d+1)/2$ groups of d proc’s

lower triangle matrix

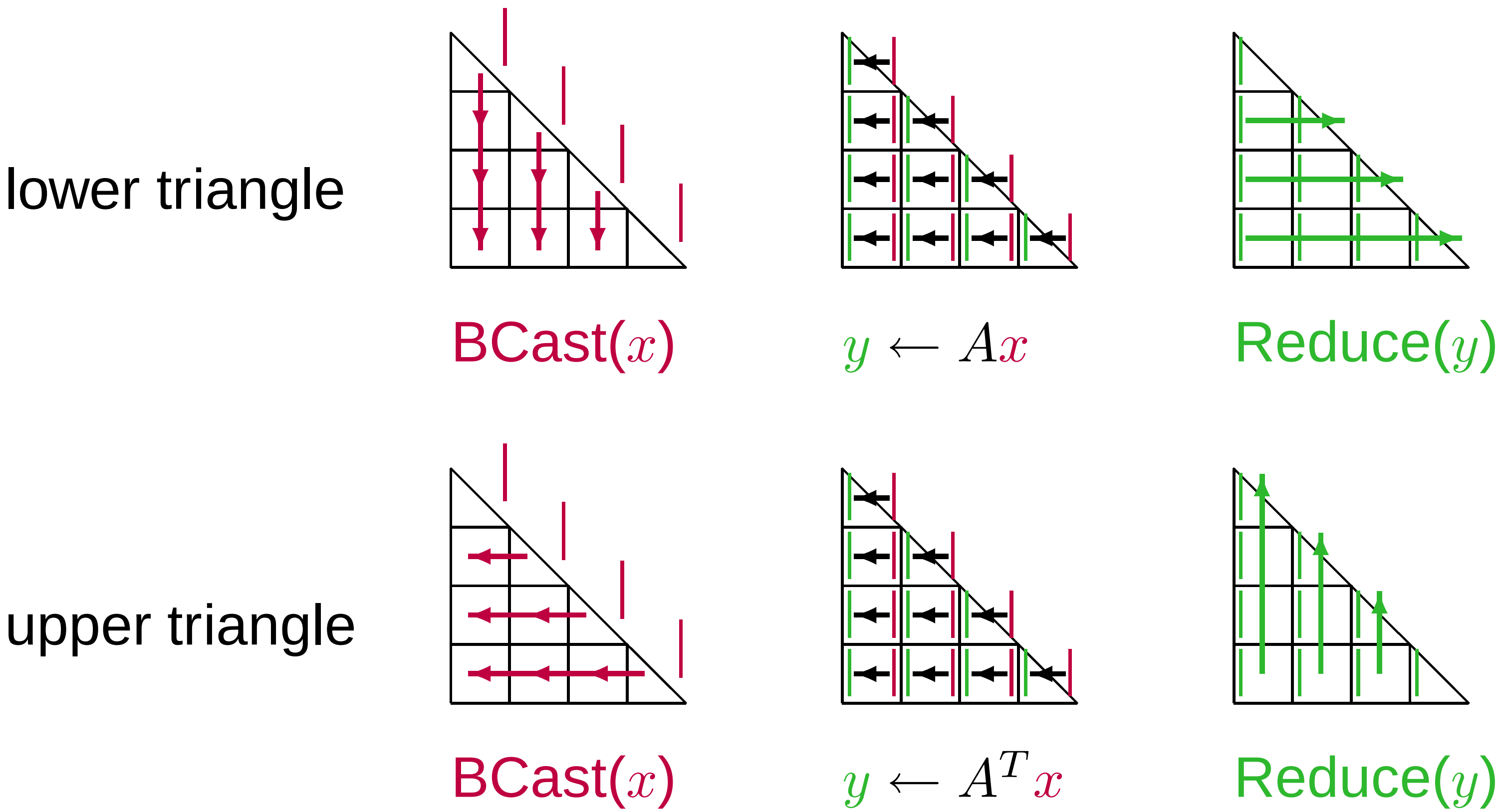


storage Lanczos vectors



Distribution of matrix and vectors

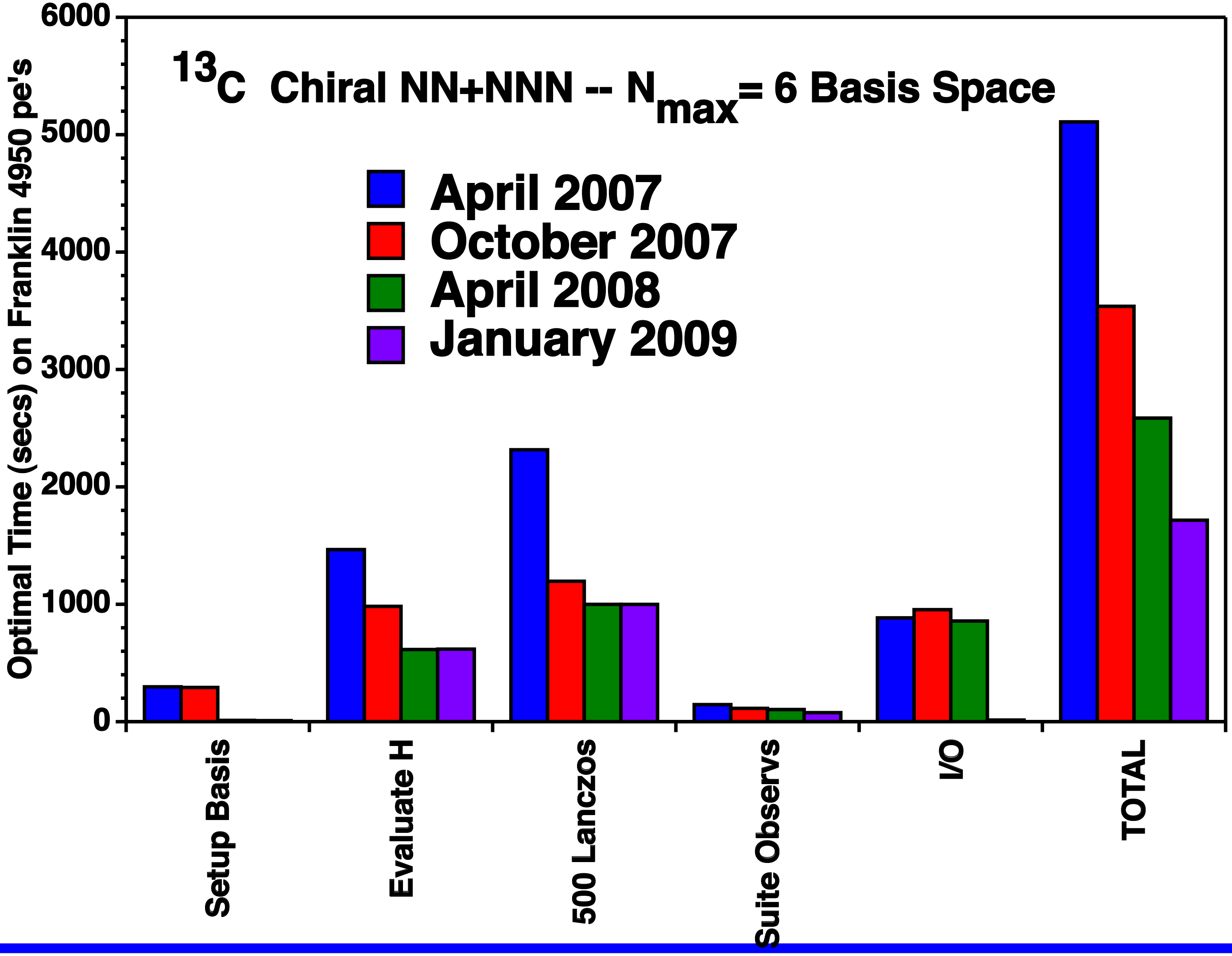
- Store lower half of symmetric matrix, distributed over $n = d \cdot (d+1)/2$ processors with d "diagonal" proc's
- Store Lanczos vectors on one of $(d+1)/2$ groups of d proc's
- Communication pattern matrix-vector multiplication



Recent performance improvements

updated from Sternberg, Ng, Yang, Maris, Vary, Sosonkina, Le,

Accelerating Configuration Interaction calculations for nuclear structure, presented at SuperComputing08

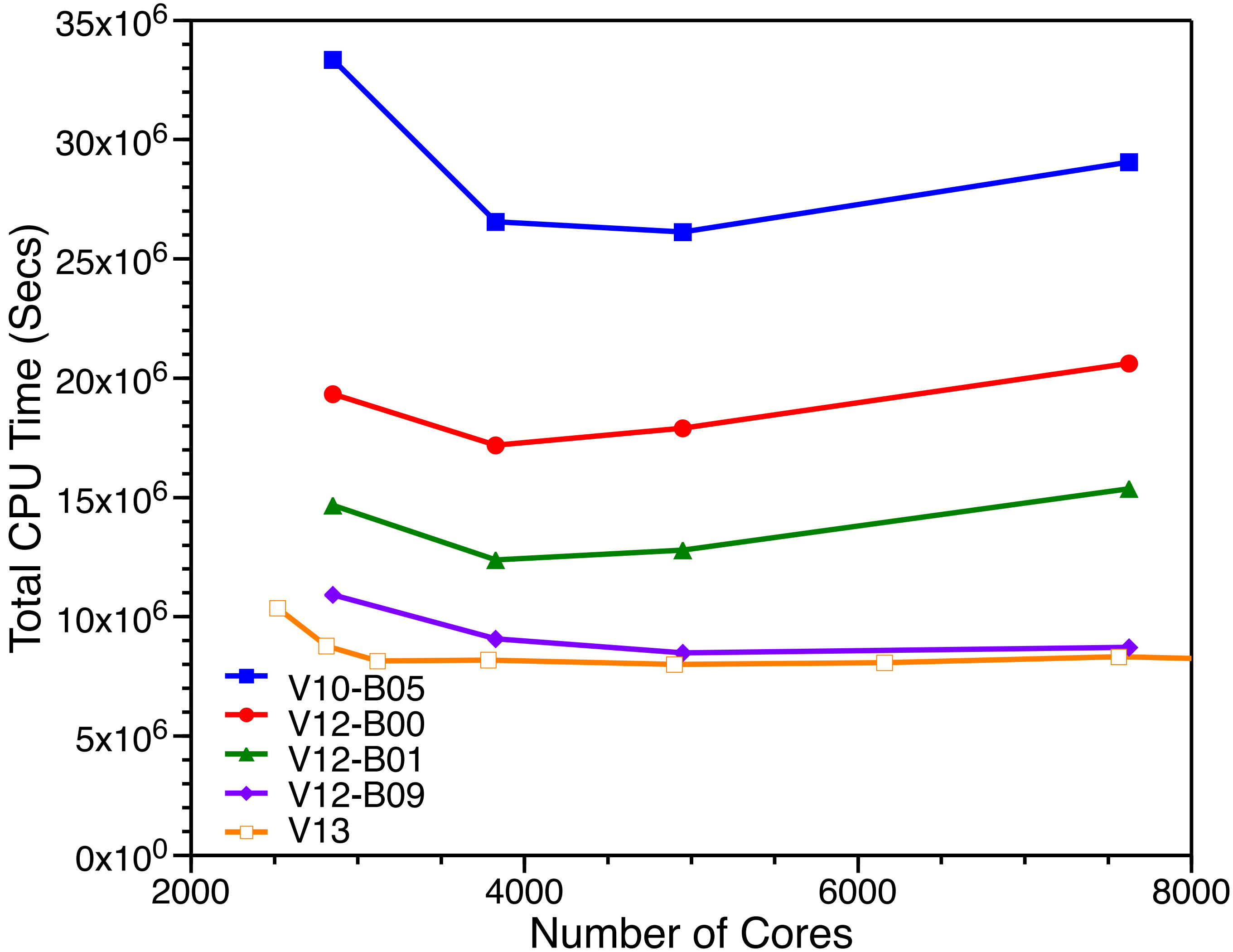


dimension $38 \cdot 10^6$

nonzero m.e. $56 \cdot 10^{10}$

size input 3 GB

Strong Scaling on Cray XT4



^{13}C chiral N3LO
2- and 3-body
interactions

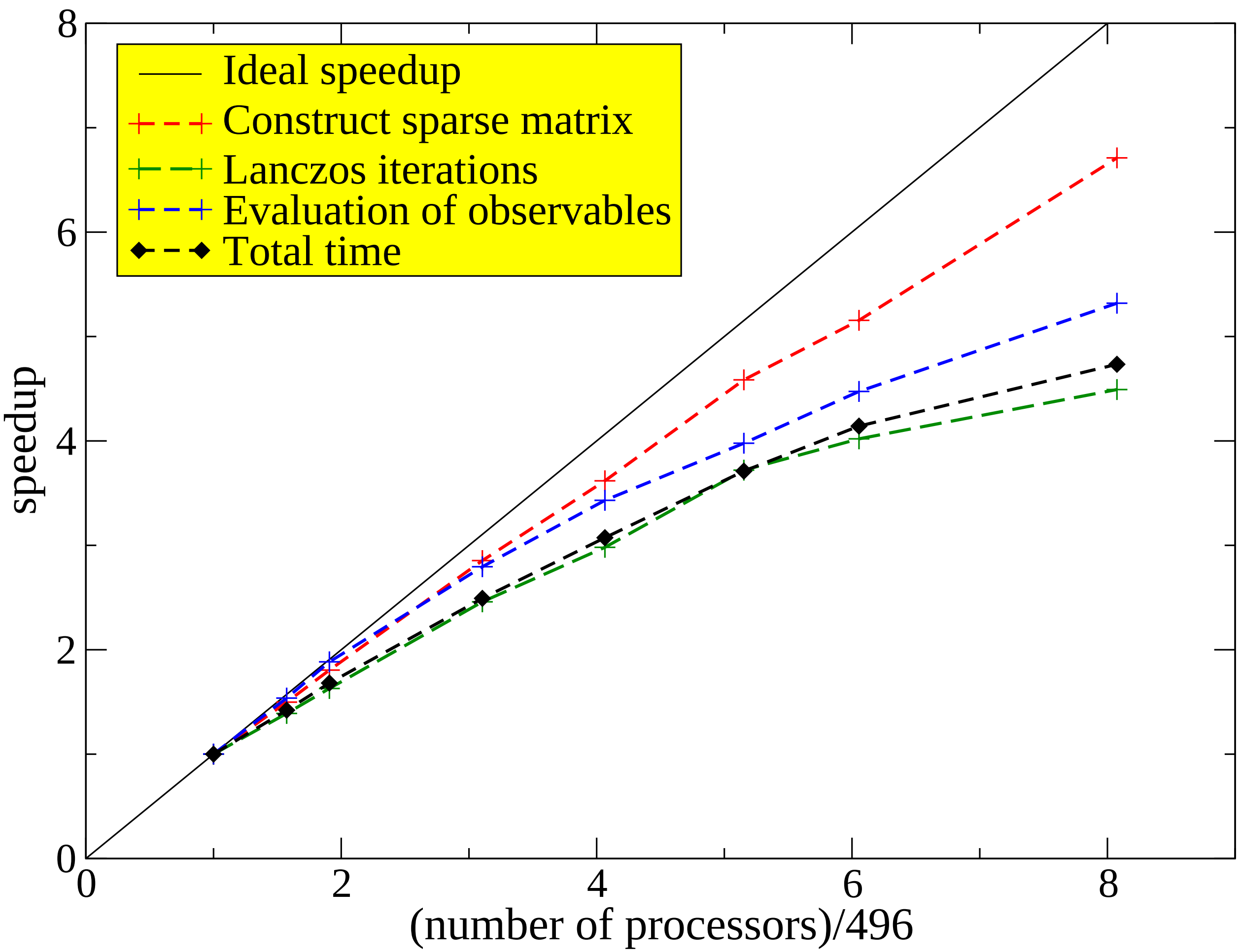
dimension $38 \cdot 10^6$
nonzero m.e. $56 \cdot 10^{10}$
size input 3 GB

Version 13:
hybrid MPI
and OpenMP
(Aug. 2009)

Strong Scaling of MFDn on Cray XT4

adapted from Maris, Sosonkina, Vary, Ng, Yang, submitted to ICCS 2010

Scaling of ab-initio nuclear physics calculations on multicore computer architectures



^{6}Li, $N_{\max} = 12$,
2-body interactions
strong scaling
from 496 PE's
to over 4,000 PE's

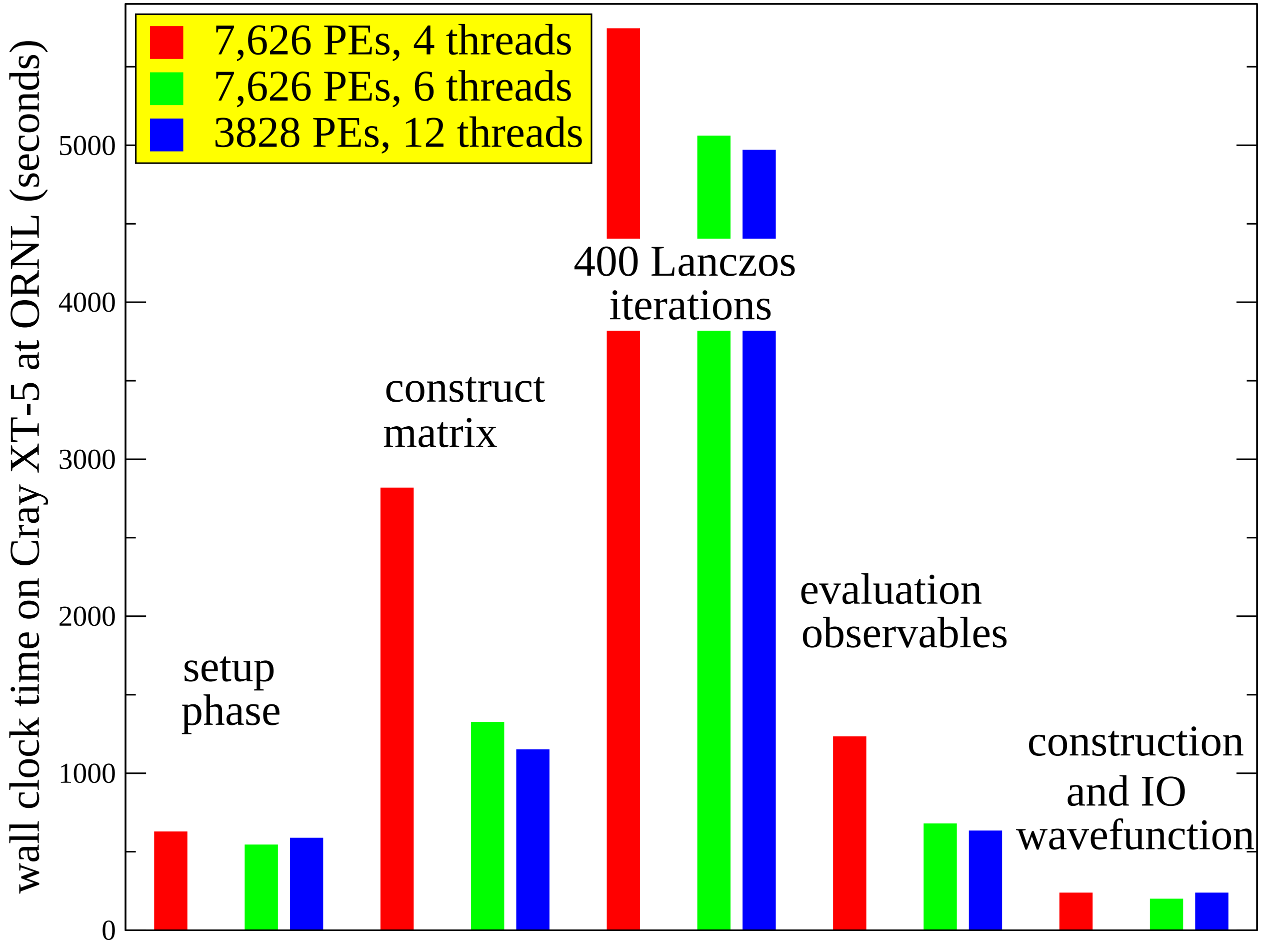
$$\text{speedup} = \frac{T_{\text{496 PE's}}}{T_{\text{\# PE's}}}$$

dimension $49 \cdot 10^6$

nonzero m.e. $74 \cdot 10^9$

memory for storing matrix: 600 GB

Quad core vs. Hex core performance on Cray XT5



^{14}Be

2-body interaction

dimension $2.8 \cdot 10^9$

nonzero m.e. $2.8 \cdot 10^{12}$