Computational issues in ab initio nuclear structure

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UNEDF SciDAC Collaboration
Universal Nuclear Energy Density Functional

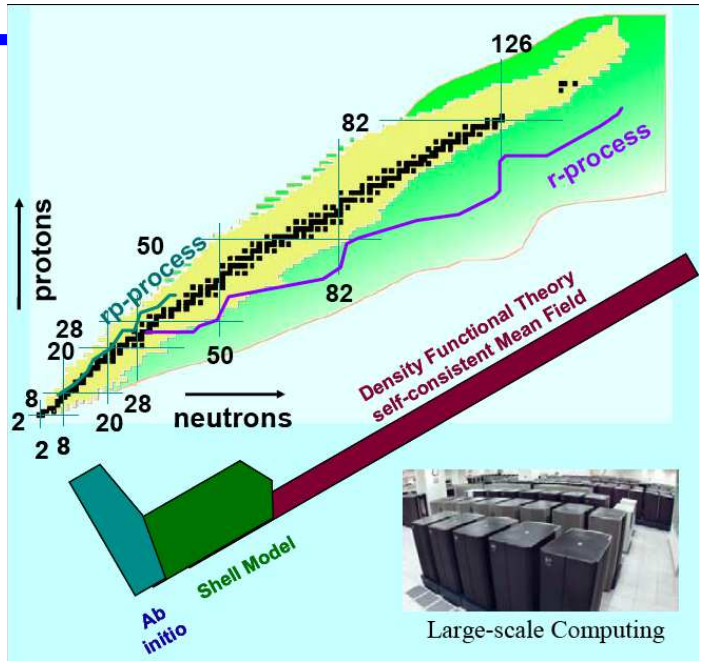
SciDAC project – UNEDF
spokespersons: Rusty Lusk (ANL), Witek Nazarewicz (ORNL/UT)
http://www.unedf.org

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

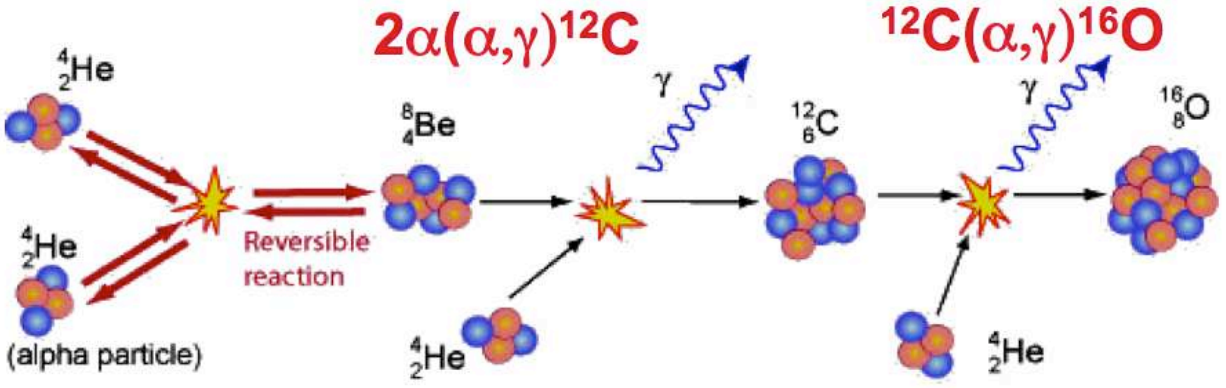
INCITE award – Computational Nuclear Structure
PI: James Vary (ISU)

NERSC CPU time

Ab initio nuclear structure – Fundamental questions



- How does the nuclear shell model emerge from the underlying theory?
- What controls nuclear saturation?
- What are the properties of nuclei with extreme neutron/proton ratios?
- Nucleo-synthesis:
  Can we understand the nuclear processes that created matter?



- Can nuclei provide precision tests of fundamental laws of nature?

Ab initio nuclear structure – Quantum many-body problem

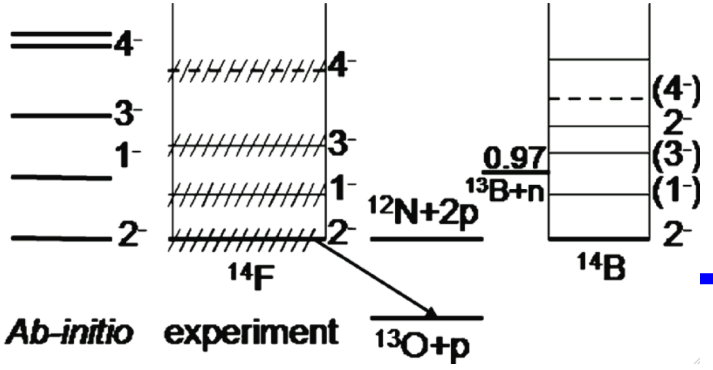
Eigenvalue problem for wave function $\Psi(r_1, \ldots, r_A)$ of A nucleons

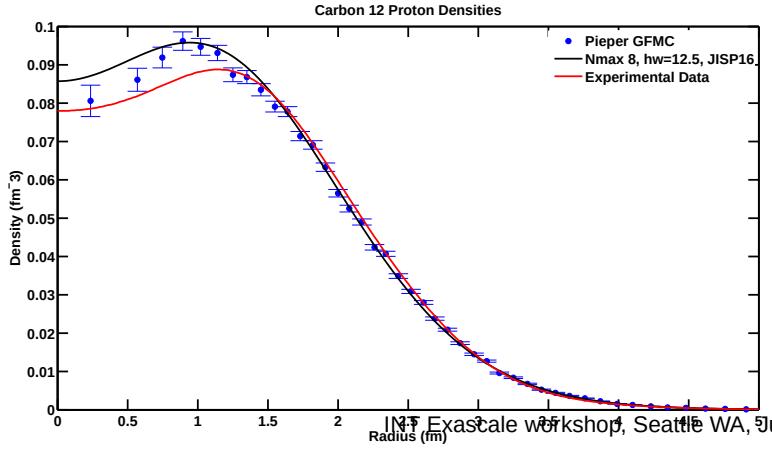
$$\hat{\mathbf{H}}\,\Psi(r_1, \ldots, r_A) \quad = \quad \lambda\,\Psi(r_1, \ldots, r_A)$$

with Hamiltonian operator

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

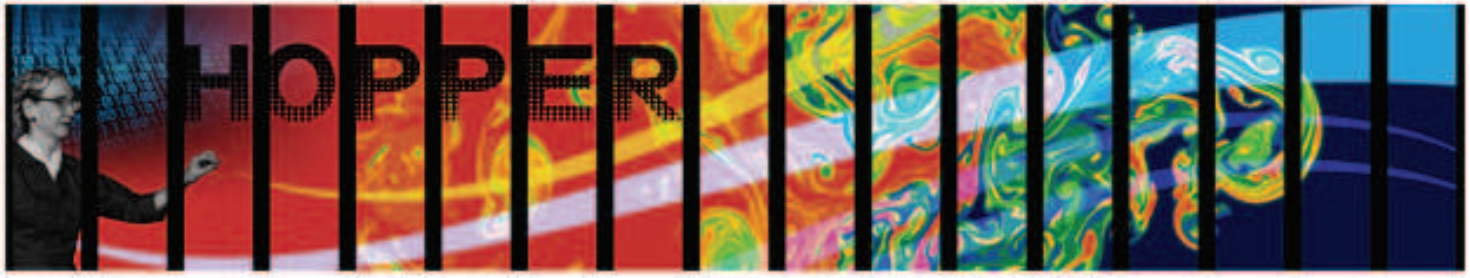
- eigenvalues λ discrete (quantized) energy levels
- eigenvectors: $|\Psi(r_1, \ldots, r_A)|^2$ probability density for finding nucleons $1, \ldots, A$ at $r_1, \ldots, r_A$



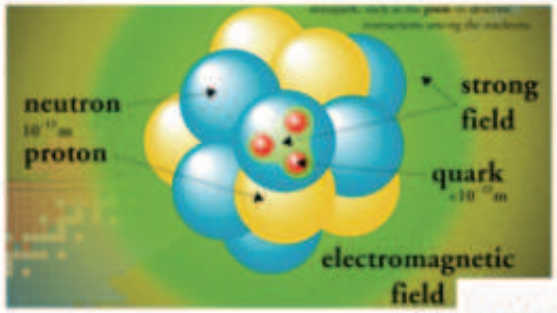


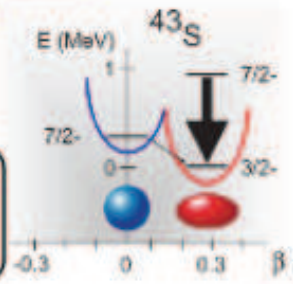
Ab initio nuclear structure – Computational challenges

- Self-bound quantum many-body problem,
  with $3A$ degrees of freedom in coordinate (or momentum) space
- Not only 2-body interactions, but also intrinsic 3-body interactions
  and possibly 4- and higher N-body interactions
- Strong interactions, with both short-range and long-range pieces
- Multiple scales, from keV's to MeV's



Ab initio nuclear structure – Extreme computing



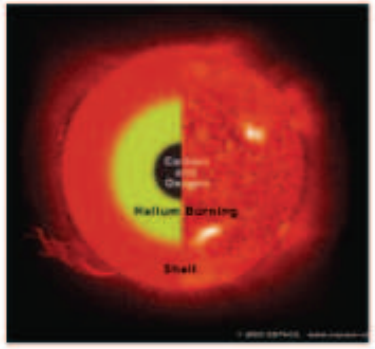


$^{12}C(\alpha,\gamma)^{16}O$
^{132}Sn structure

^{78}Ni structure

Ab initio structure in light nuclei

$^{8}Be(\alpha,\gamma)^{12}C$

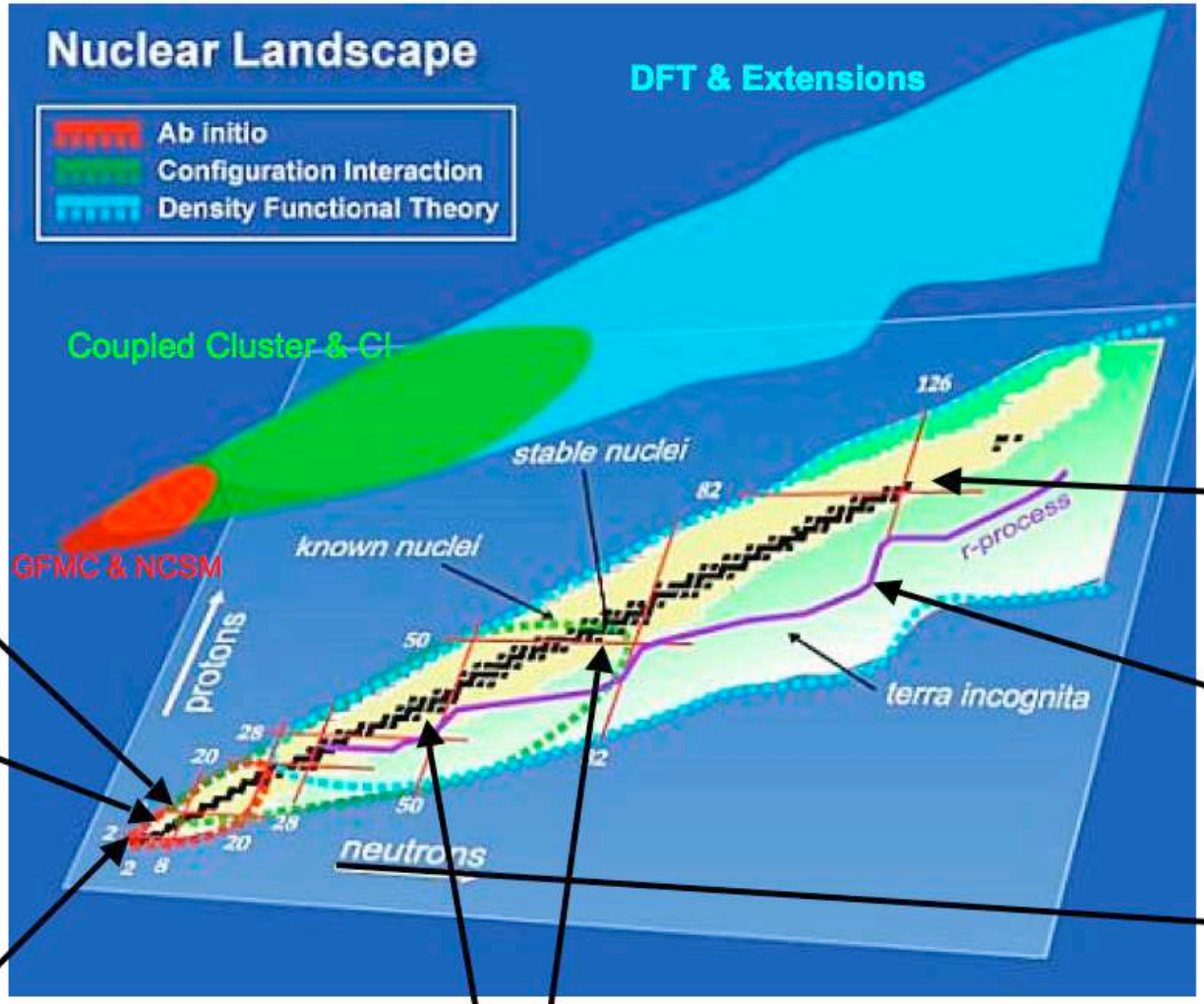


10x tera | 100x tera | peta | 10x peta | 100x peta | 1 exaflop year

~ INCITE award in 2011
~1 week of dedicated JaguarPF runs

Uniform description of nuclear structure

"Digital FRIB" and beyond



Astro

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

Hoyle

Standard Model
QCD/χEFT

Nuclear Energy

fission

Astro

r-process

neutron star crust

0ν-$\beta\beta$

Beyond Standard Model

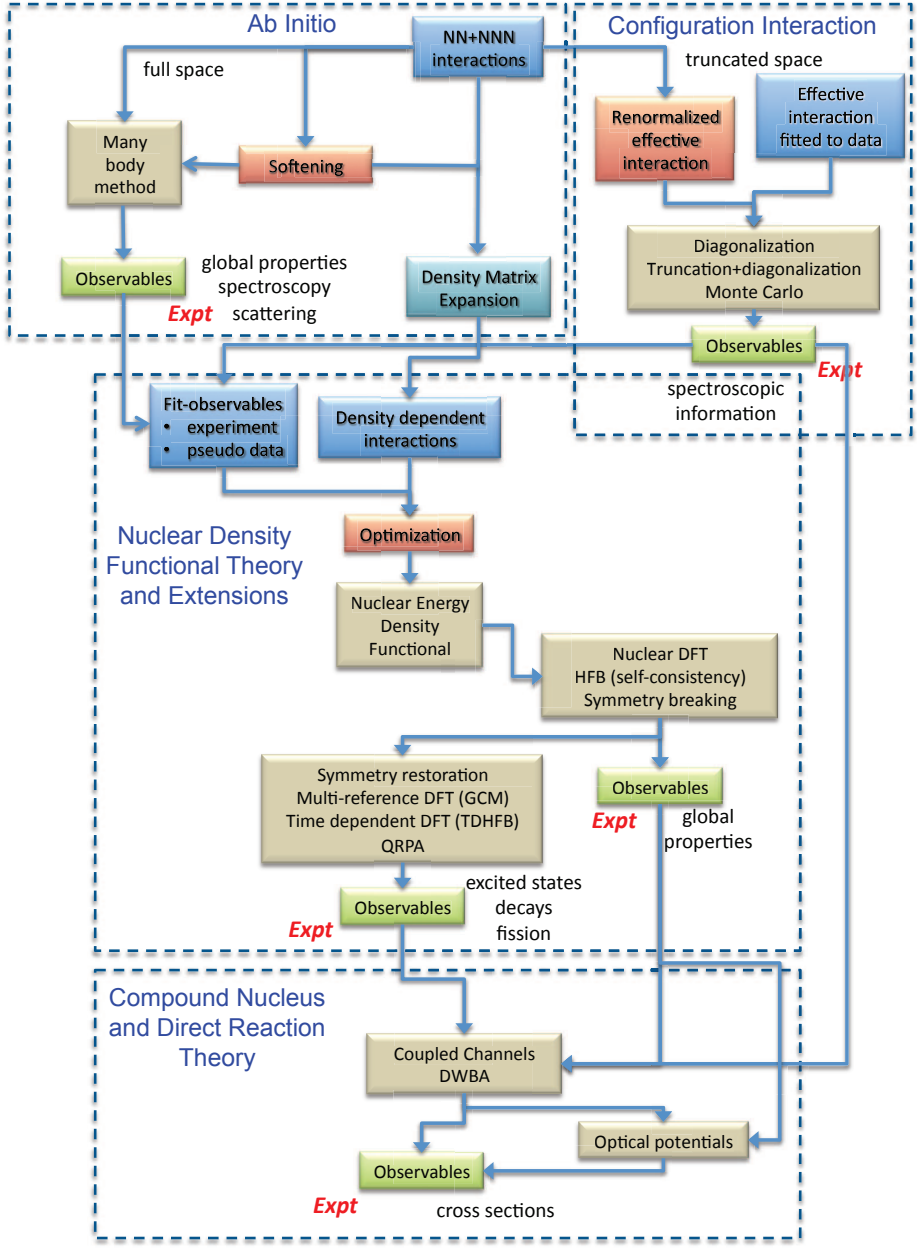
SciDAC/UNEDF – Uniform description of nuclear structure

Universal Nuclear Energy Density Functional that spans the entire mass table

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

http://www.unedf.org

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



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 – basis space expansion

- Expand wave function in basis $\Psi(r_1, \ldots, r_A) = \sum a_i \Phi_i(r_1, \ldots, r_A)$
  - Slater Determinants of single-particle states $\phi_i(r_1)$

$$\Phi_i(r_1, \ldots, r_A) = \frac{1}{\sqrt{(A!)}} \begin{vmatrix} \phi_{i1}(r_1) & \phi_{i2}(r_1) & \ldots & \phi_{iA}(r_1) \\ \phi_{i1}(r_2) & \phi_{i2}(r_2) & \ldots & \phi_{iA}(r_2) \\ \vdots & \vdots & & \vdots \\ \phi_{i1}(r_A) & \phi_{i2}(r_A) & \ldots & \phi_{iA}(r_A) \end{vmatrix}$$

  takes care of anti-symmetrization of nucleons (Fermi-statistics)
  - 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 $|n, l, s, j, m\rangle$
    - radial wavefunctions
      - Harmonic Oscillator
      - Wood–Saxon basis
      - ...

Configuration Interaction Methods – basis space expansion

- Expand wave function in basis $\Psi(r_1, \ldots, r_A) = \sum a_i \Phi_i(r_1, \ldots, r_A)$
  - M-scheme: many-body basis states eigenstates of $\hat{\mathbf{J}}_\mathbf{z}$

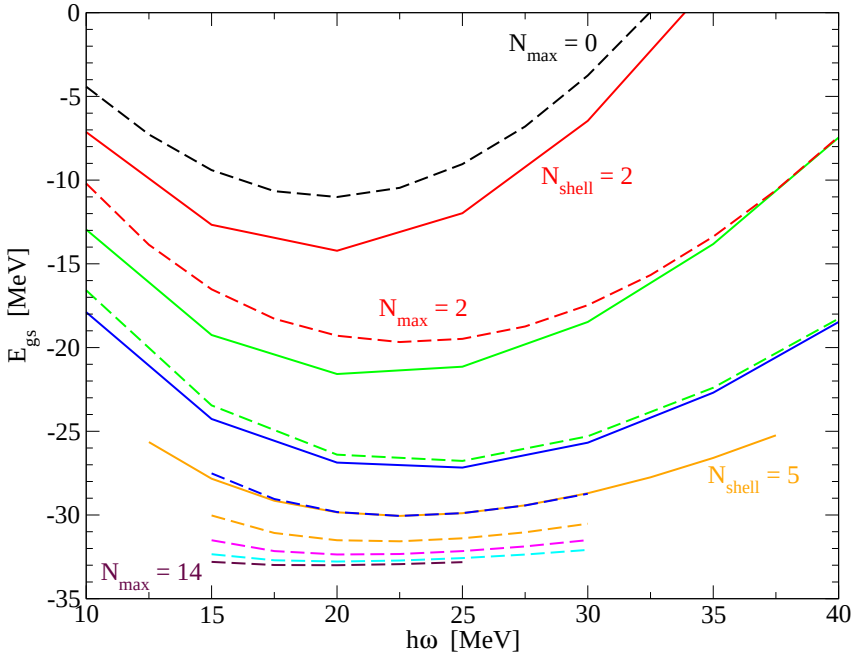
$$\hat{\mathbf{J}}_\mathbf{z}|\psi\rangle \quad = \quad M|\psi\rangle \quad = \sum_{i=1}^{A} m_i|\psi\rangle$$

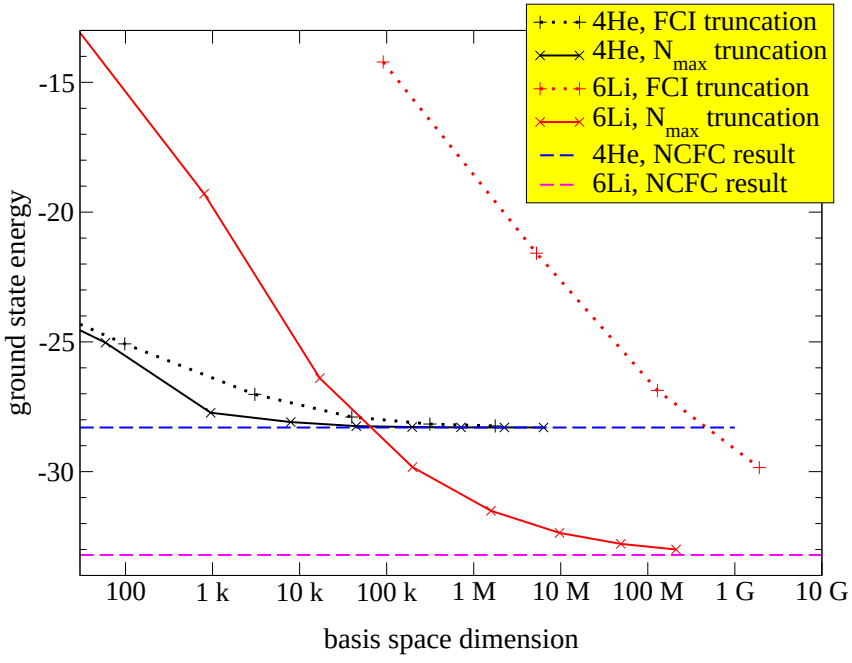
    - alternatives:
      LS scheme, Coupled-J scheme, Symplectic basis, ...
  - N_{max} truncation

$$\sum_{k=1}^{A} \left(2\, n_{ik} + l_{ik}\right) \;\leq\; N_0 + N_{\text{max}}$$

    - exact factorization of Center-of-Mass motion
    - alternatives
      Monte-Carlo No-Core Shell Model, Importance Truncation,
      FCI (truncation on single-particle basis only), ...

Intermezzo: FCI vs. Nmax truncation





$N_{\max}$ truncation

- exact factorization of Center-of-Mass motion
- converges much more rapidly than FCI truncation with basis space dimension

Configuration Interaction Methods

- Expand wave function in basis $\Psi(r_1, \ldots, r_A) = \sum a_i \Phi_i(r_1, \ldots, r_A)$
- Express Hamiltonian in basis

$$H_{ij} = \int_\Omega \left(\Phi_i^*(r'_1, \ldots, r'_A)\, \hat{\mathbf{H}}\, \Phi_j(r_1, \ldots, r_A) \right) \mathrm{d}r_1 \ldots \mathrm{d}r_A\, \mathrm{d}r'_1 \ldots \mathrm{d}r'_A$$

- Sparse matrix
  - A-body problem with 2-body (and 3-body) interactions
  - many-body basis states are single Slater Determinants

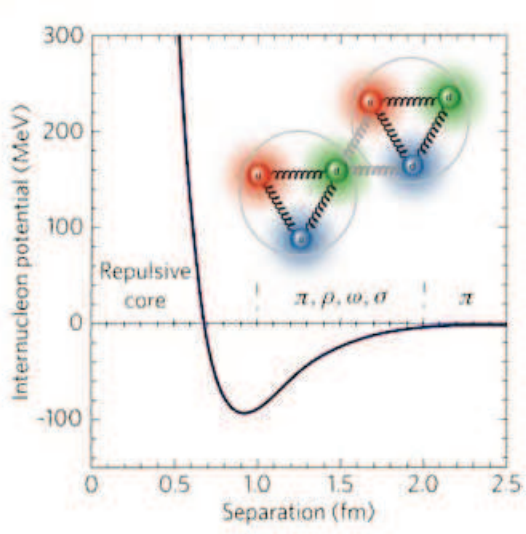
$$\begin{aligned} H_{ij}^{(A)} &= (-1)^{\text{permutations}}\, \delta_{i_1,j_1} \ldots \delta_{i_{(A-2)},j_{(A-2)}} \\ &\quad \int_\Omega \left(\Phi_i^*(r_c, r_d)\, \hat{\mathbf{H}}^{(\mathbf{2})}_{\mathbf{cd \leftarrow ab}}\, \Phi_j(r_a, r_b) \right) \mathrm{d}r_a \mathrm{d}r_b \mathrm{d}r_c \mathrm{d}r_d \\ &= (-1)^{\text{permutations}}\, \delta_{i_1,j_1} \ldots \delta_{i_{(A-2)},j_{(A-2)}}\, H^{(2)}_{cd \leftarrow ab} \end{aligned}$$

A-body problem with N-body interaction: nonzero matrix elements iff at least $A - N$ particles are in identical single-particle states

Configuration Interaction Methods

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

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

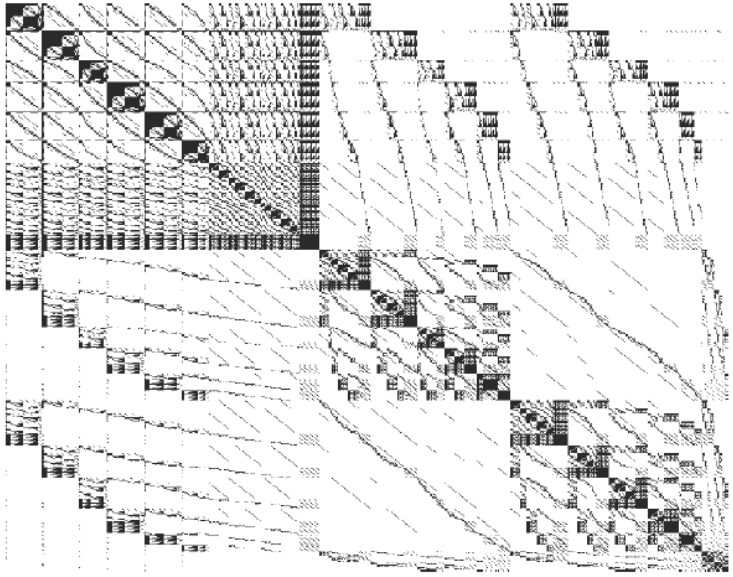


- Pick your favorite potential
  - Argonne potentials: AV8, AV18 (plus Illinois NNN interactions)
  - Bonn potentials
  - Chiral NN interactions (plus chiral NNN interactions)
  - ...
  - JISP16 (phenomenological NN potential)
  - ...

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

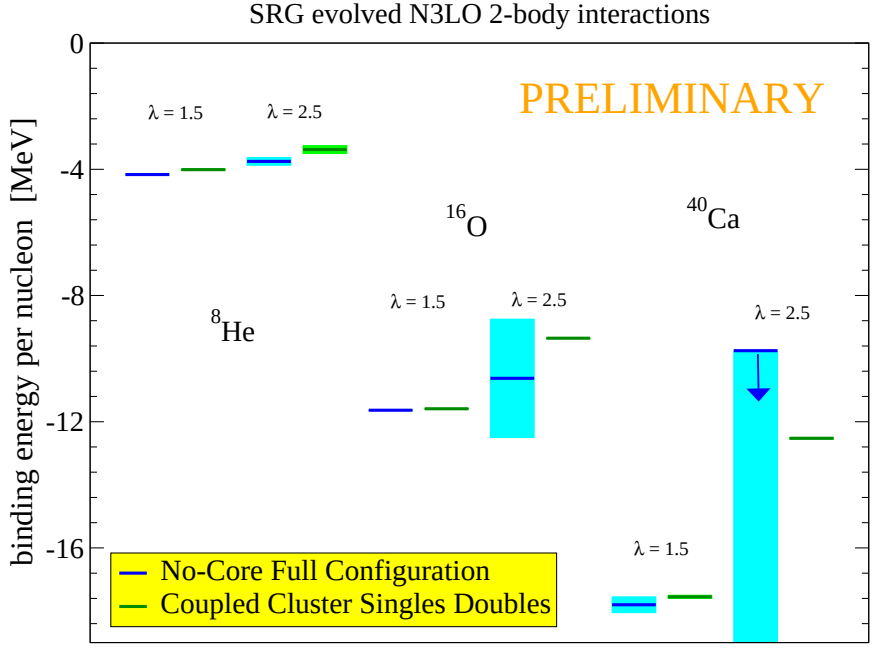


- Obtain lowest eigenvalues using Lanczos algorithm
  - Eigenvalues: bound state spectrum
  - Eigenvectors: nuclear wavefunctions

- Use wavefunctions to calculate observables
- Challenge: eliminate dependence on basis space truncation

CI calculation – convergence

- Expand wave function in basis: $\Psi(r_1, \ldots, r_A) = \sum a_i \Phi_i(r_1, \ldots, r_A)$
- Express Hamiltonian in basis: $\hat{\mathbf{H}} = H_{ij}$
- Diagonalize sparse real symmetric matrix H_{ij}
- 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



- Variational: for any finite truncation of the basis space, eigenvalue is an upper bound for the ground state energy

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}

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

  - 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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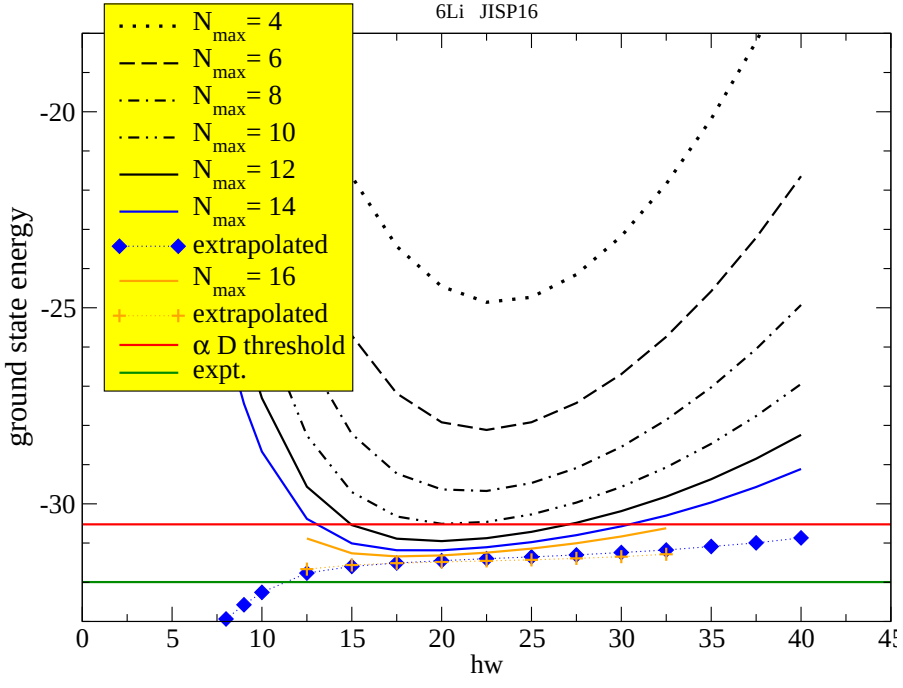
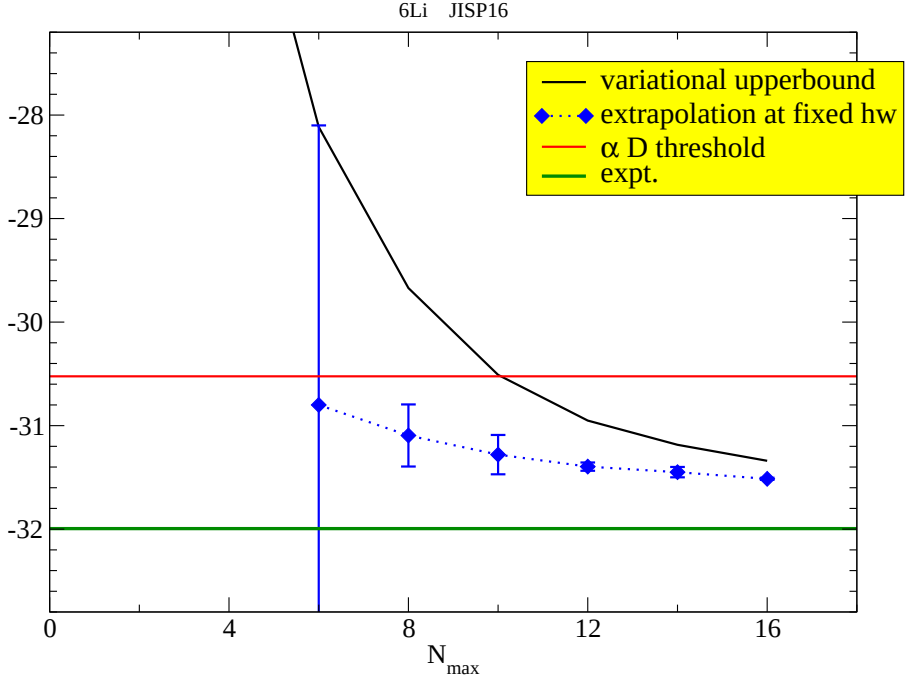
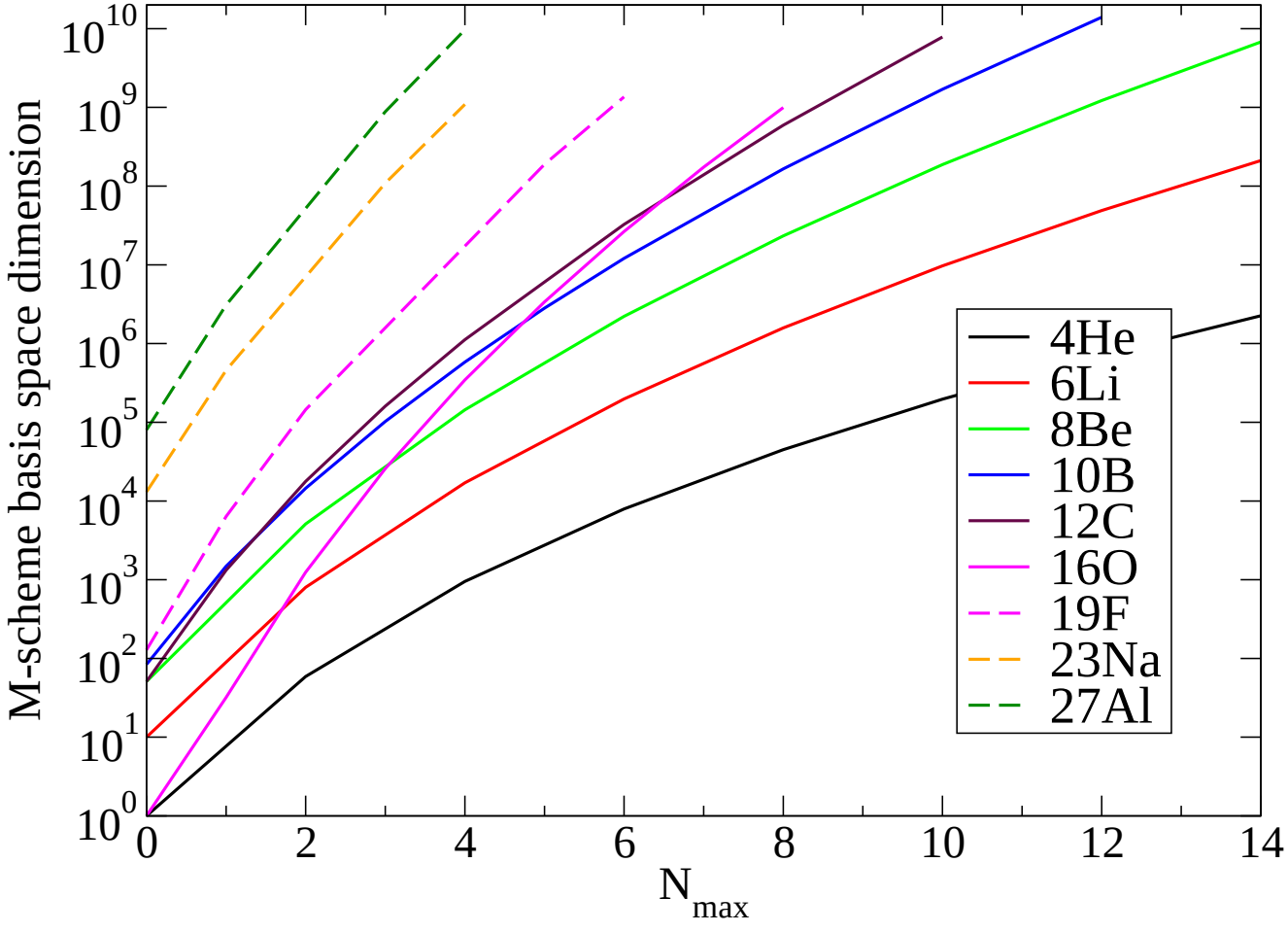
- Extrapolate to infinite model space $\longrightarrow$ exact results





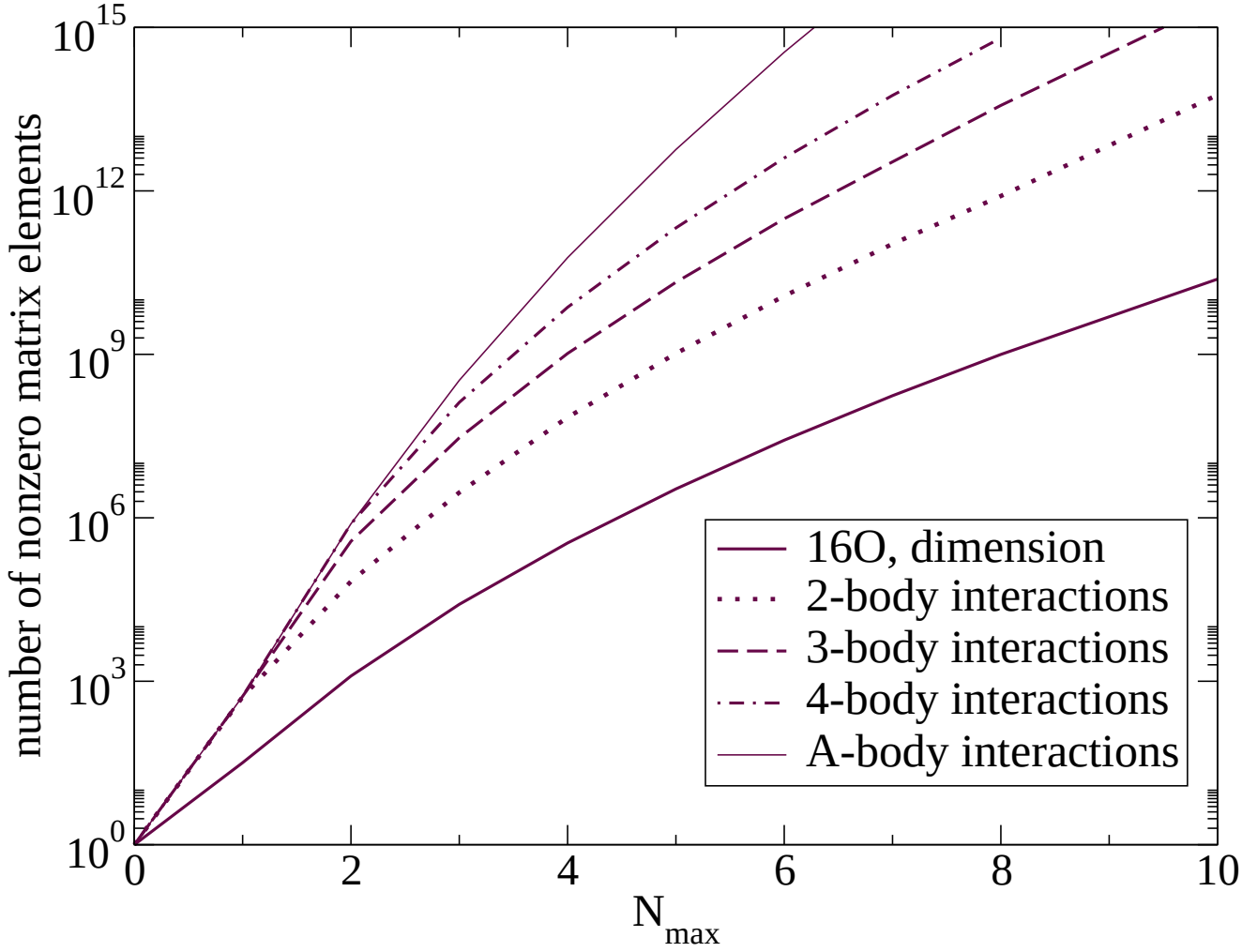
CI calculations – main challenges

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



CI calculations – main challenges

Additional computational issue:
sparseness of matrix / number of nonzero matrix elements



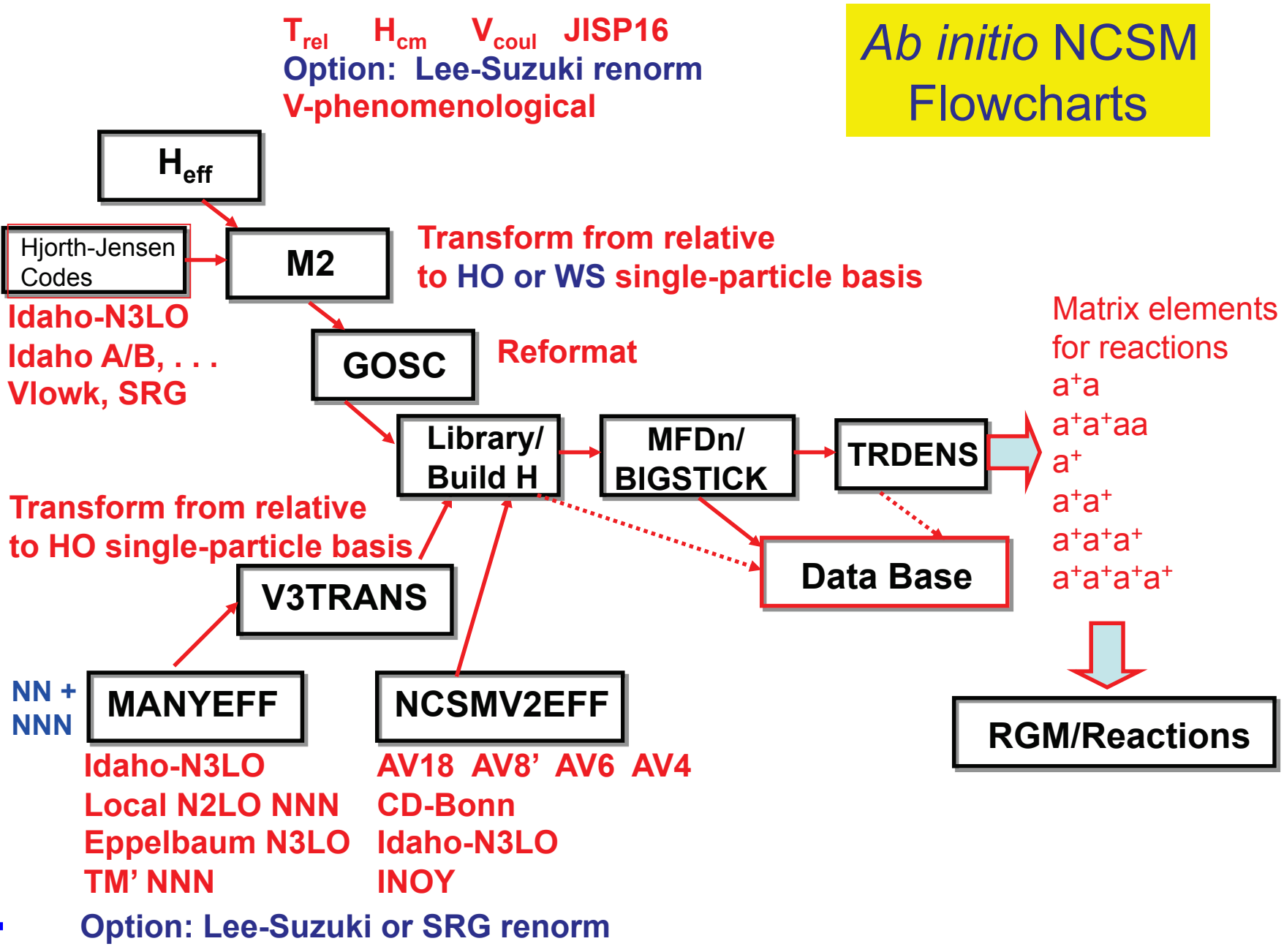
High-performance computing

- 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)
  - . . .
- 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

Many Fermion Dynamics – nuclear physics

- Platform-independent, hybrid OpenMP/MPI, Fortran 90
- Can in principle handle arbitrary N-body interactions
  however input format only specified for 2- and 3-body interactions
- Generate many-body basis space
  subject to user-defined truncation and symmetry constraints
- Construct of many-body matrix H_{ij}
  - determine which matrix elements can be nonzero
    based on quantum numbers of underlying single-particle states
  - evaluate and store nonzero matrix elements
    in compressed row/column format
- Obtain lowest eigenpairs using Lanczos algorithm
  - vectors and matrix in single precision, but accumulate
    dot-products for orthogonalization in double precision
- Calculate select one- and two-body observables
- One-body density matrices and wavefunctions available
  as input scattering and reaction calculations

Overview of pre- and post-processing codes

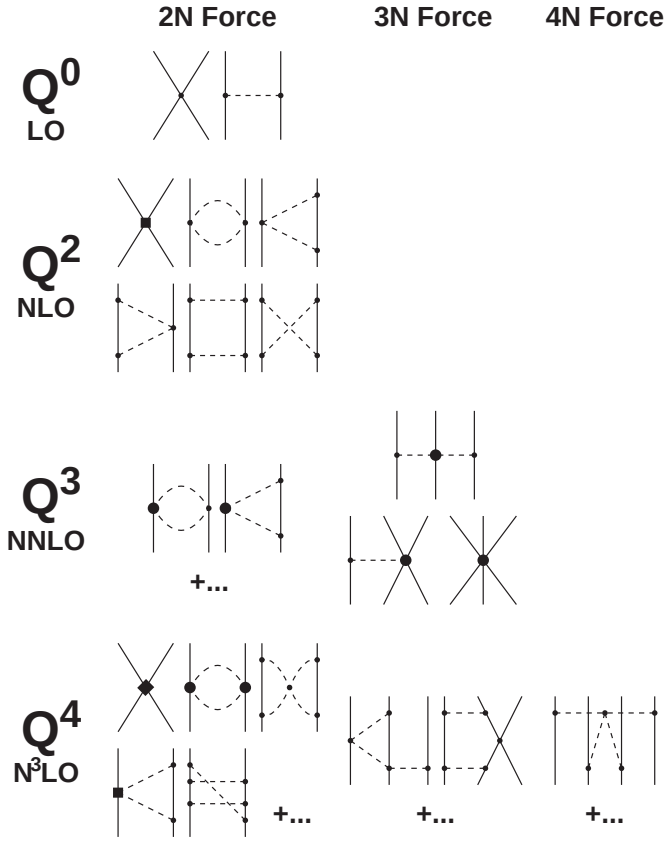


Strong force between nucleons

- 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

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

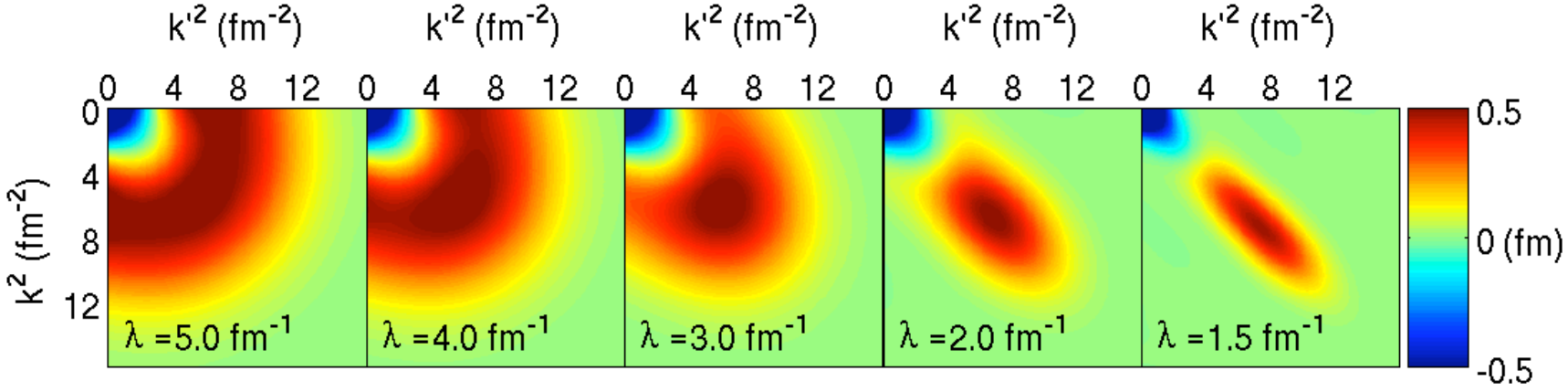
  - in principle no free parameters
    - in practice a few undetermined parameters
  - renormalization necessary
    - Lee–Suzuki–Okamoto
    - Similarity Renormalization Group



Similarity Renormalization Group – NN interaction

- SRG evolution

Bogner, Furnstahl, Perry, PRC 75 (2007) 061001



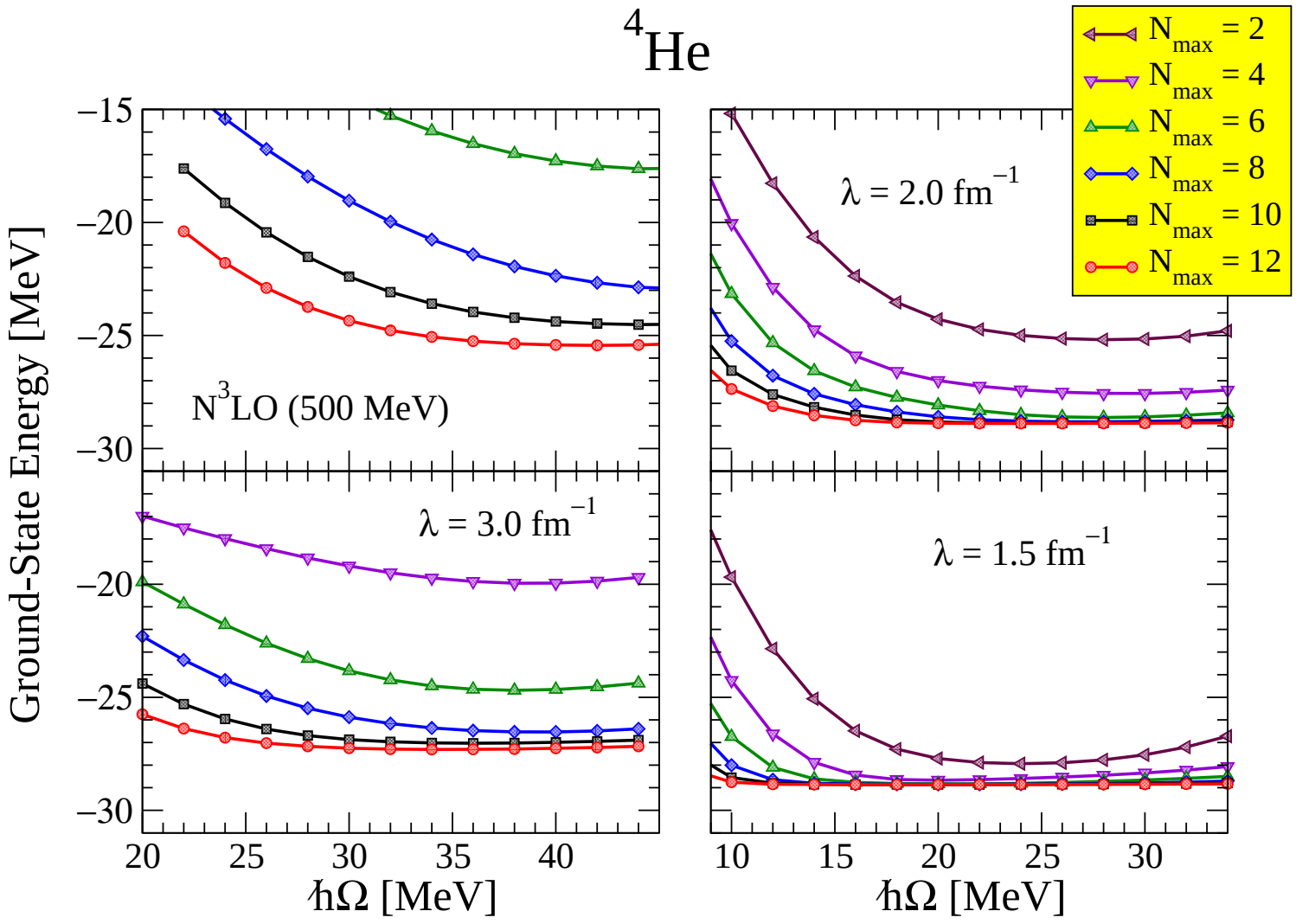
  - drives interaction towards band-diagonal structure
  - SRG shifts strength between 2-body and many-body forces

- Initial chiral EFT Hamiltonian
  power-counting hierarchy A-body forces

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

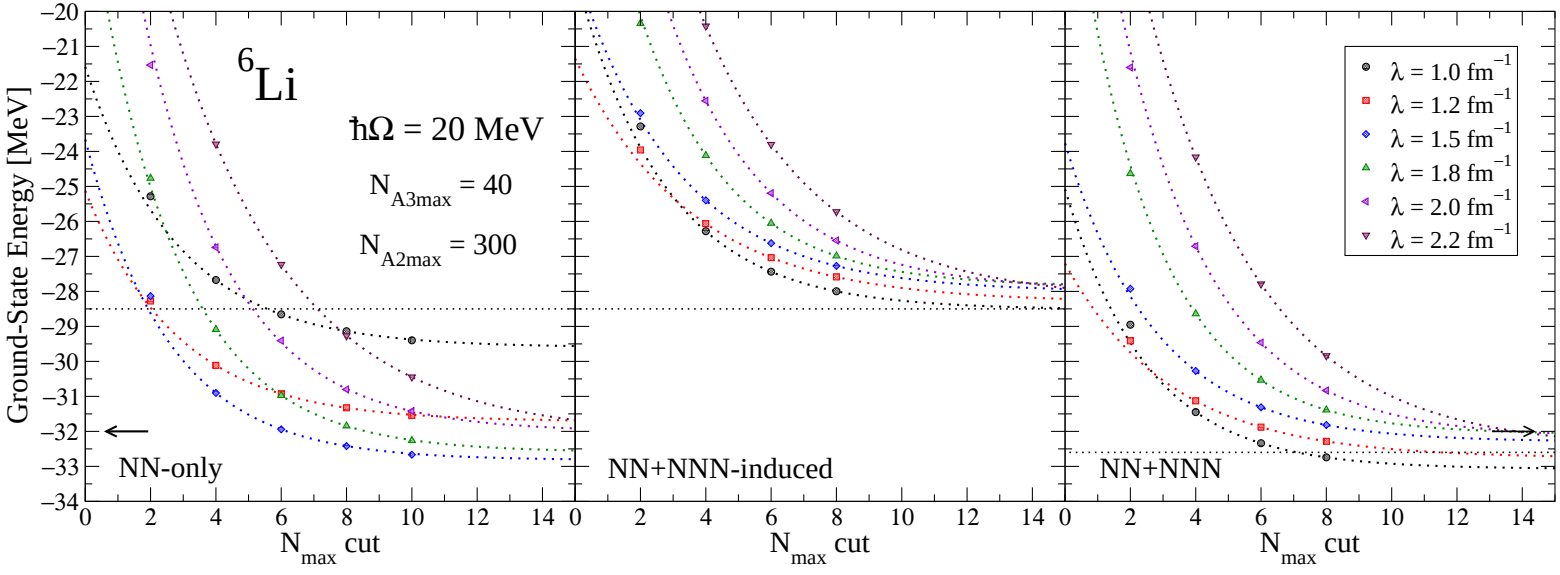
  - key issue: preserve hierarchy of many-body forces

Improve convergence rate by applying SRG to N3LO



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

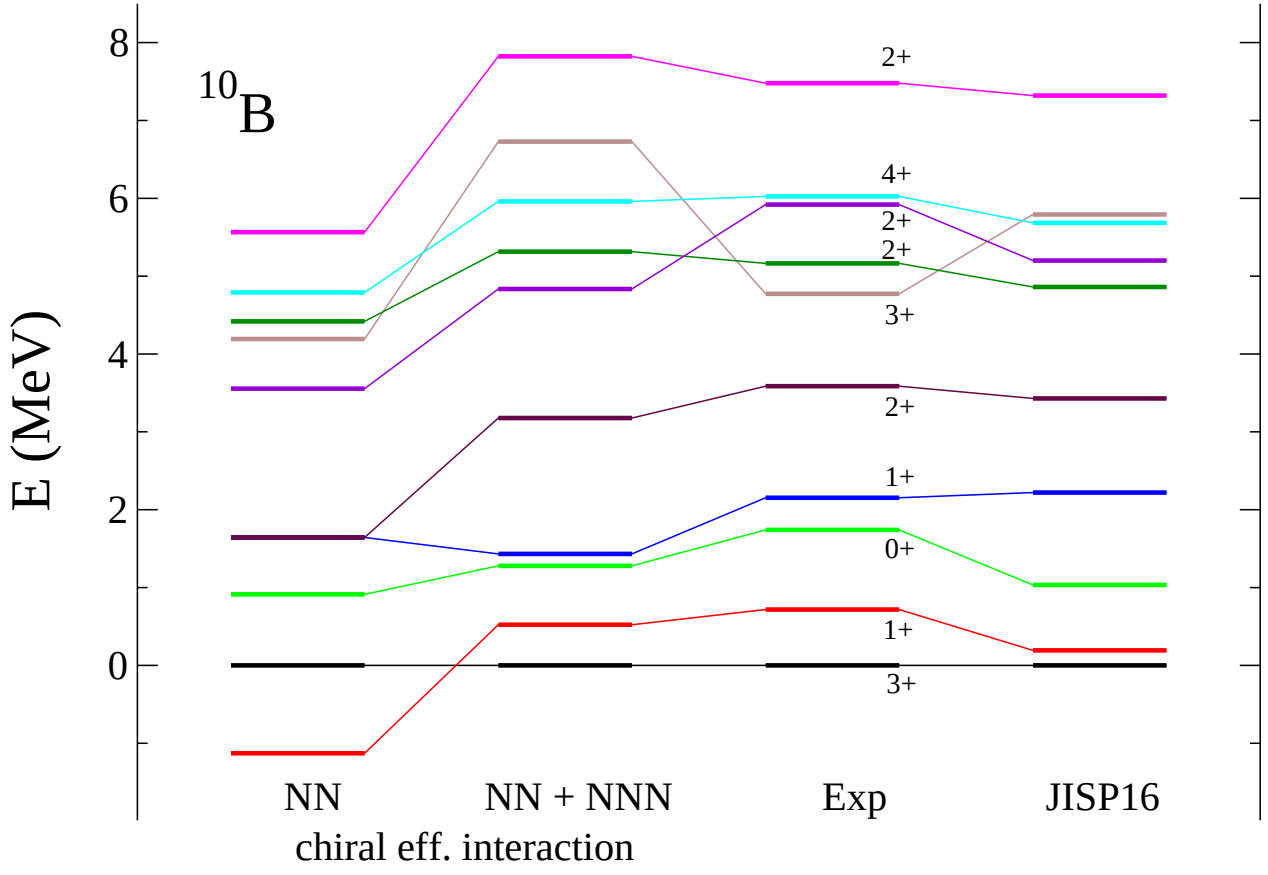
Effect of three-body forces



(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?



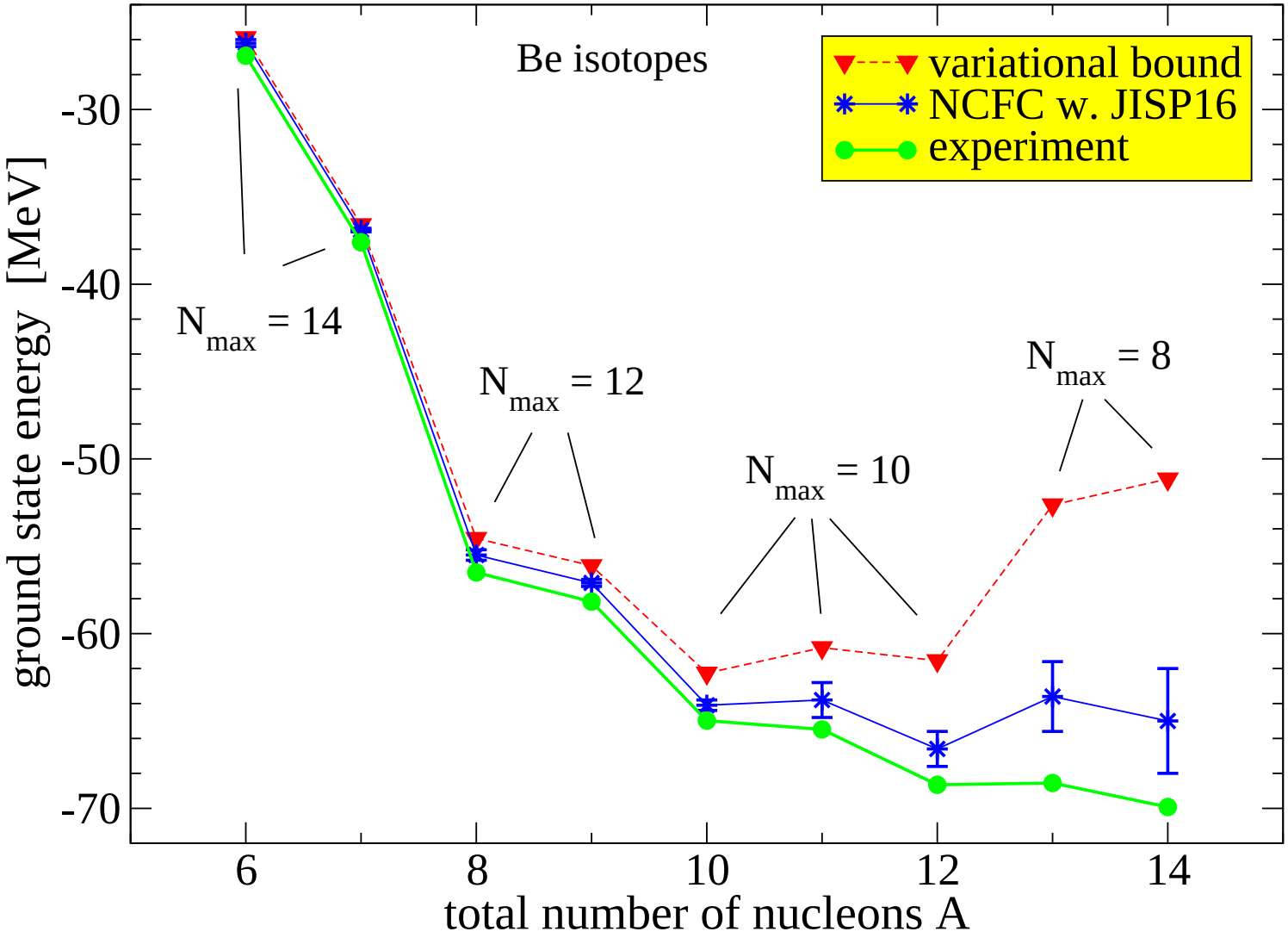
Spectrum of ^{10}B

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

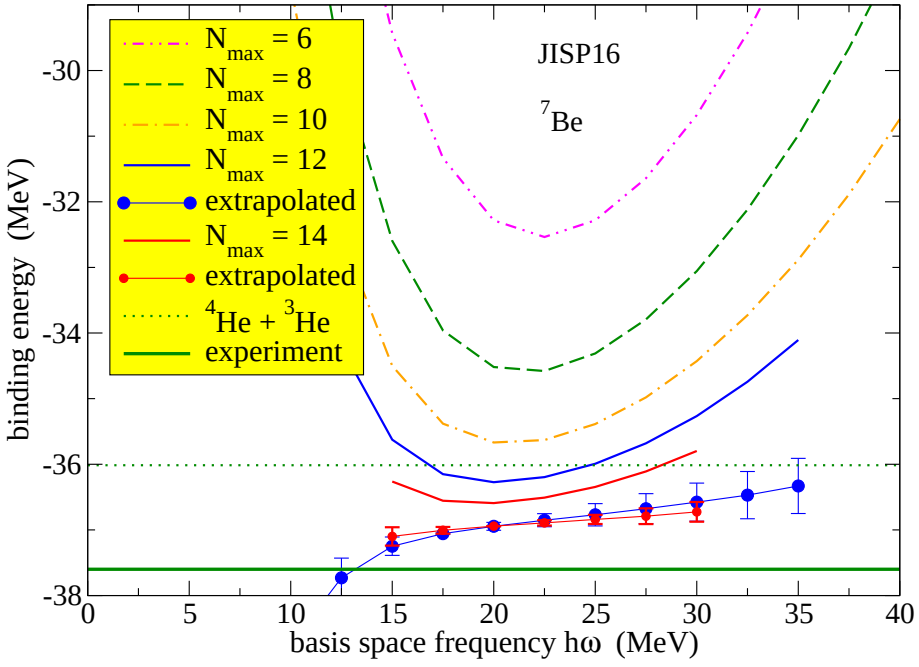
nonlocal 2-body interaction JISP16 at $N_{\max} = 8$

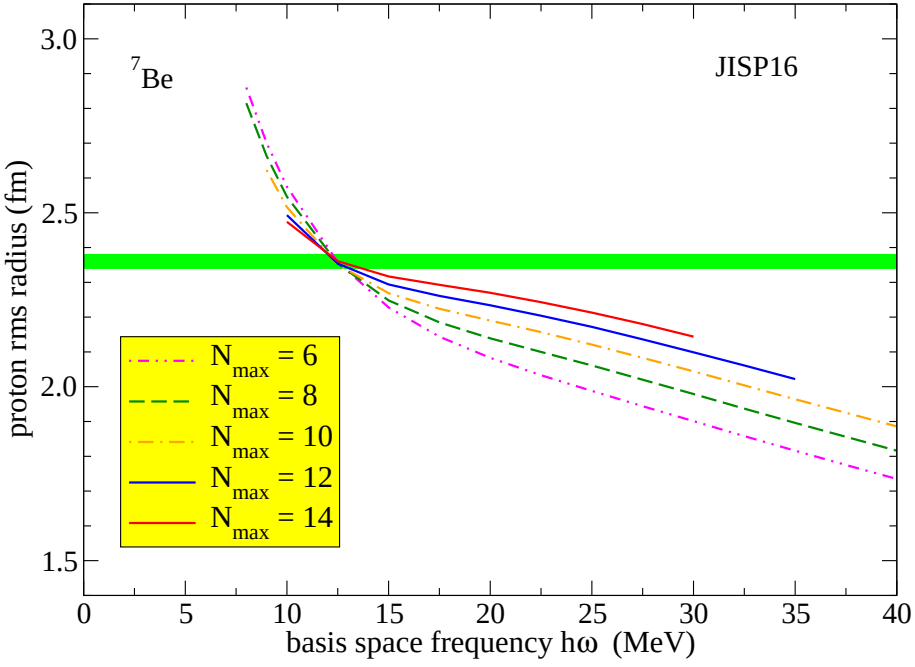
Vary, Maris, Negoita, Navratil, Gueorguiev, Ormand, Nogga, Shirokov, and Stoica, in “Exotic Nuclei and Nuclear/Particle Astrophysic (II)”, AIP Conf. Proc. 972, 49 (2008); N3LO+3NF from Navratil, Gueorguiev, Vary, Ormand, and Nogga, PRL 99, 042501 (2007); for JISP16 see Shirokov, Vary, Mazur, Weber, PLB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

Ground state energy Be-isotopes with JISP16



7Be – Ground state properties



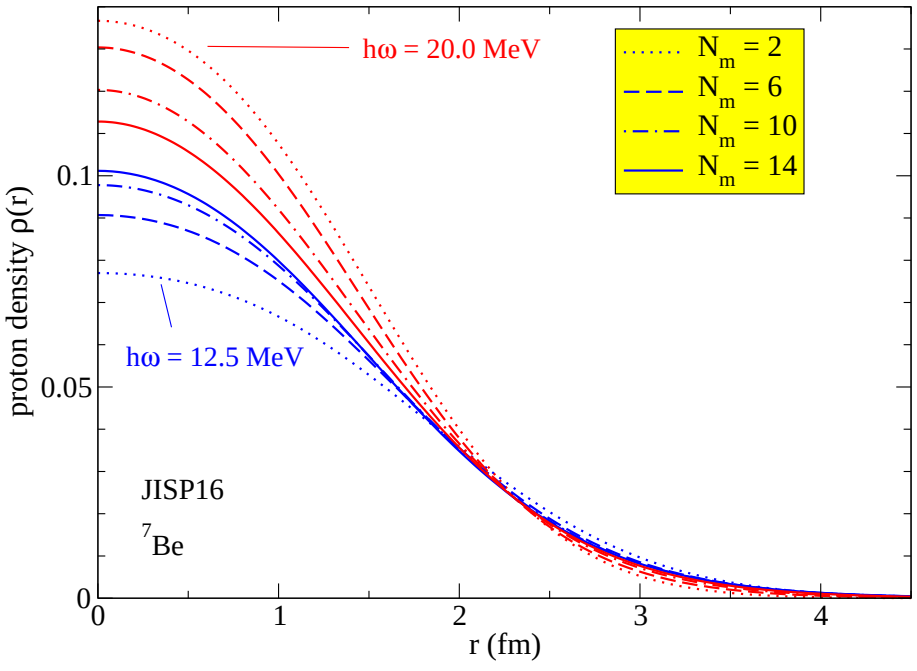


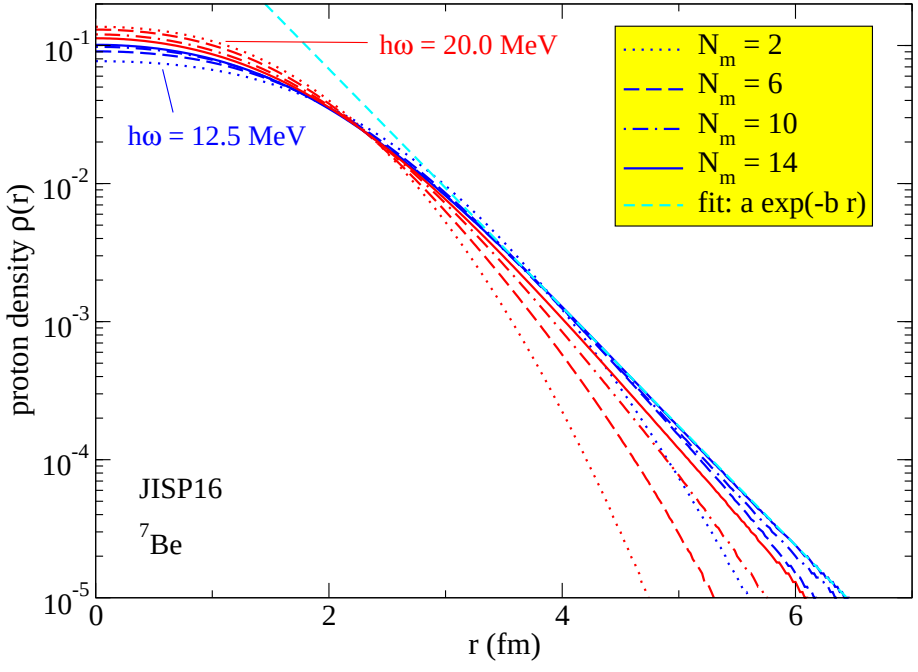
- Binding energy converges monotonically,
  with optimal H.O. freuqency around $\hbar\omega = 20$ MeV to 25 MeV
- Ground state about 0.7 MeV underbound with JISP16
- Proton point radius does not converge monotonically

7Be – Proton density

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

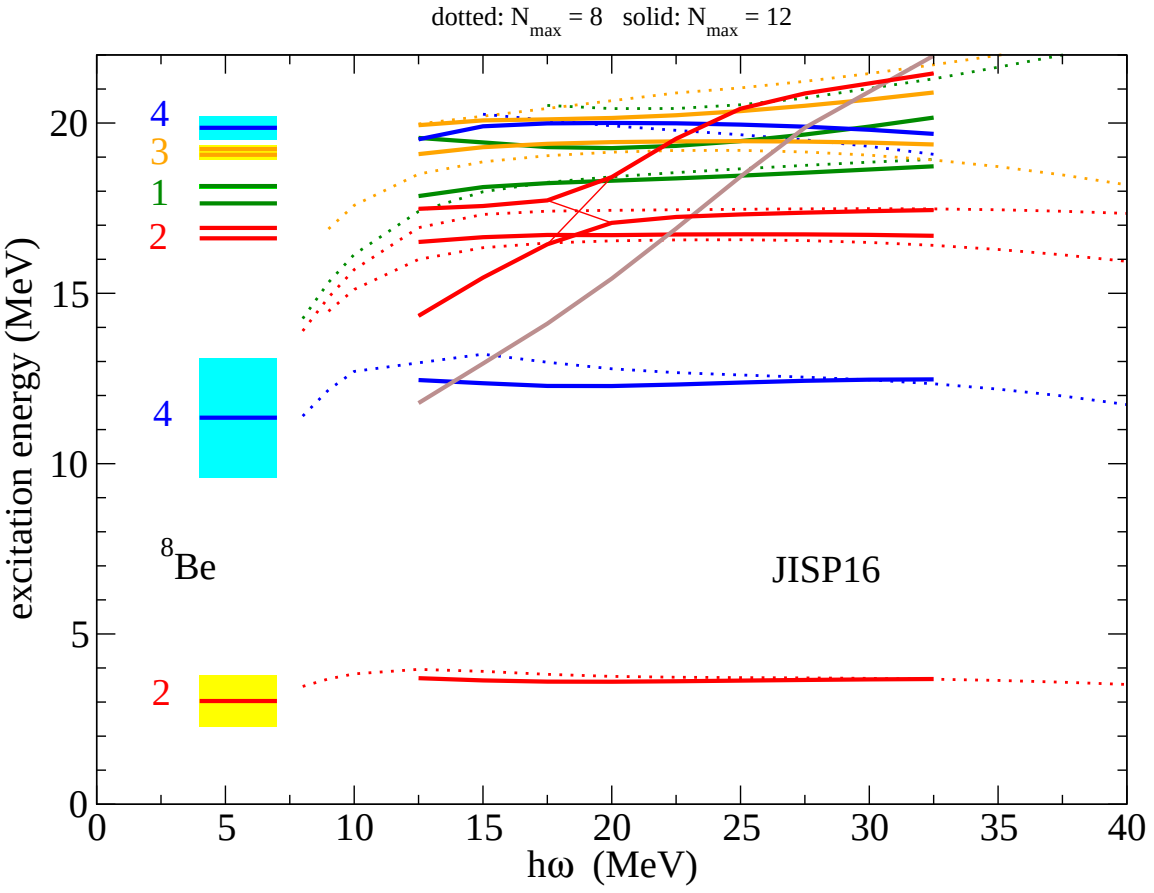
w. Cockrell, PhD student ISU





- 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

8Be – Spectrum positive parity

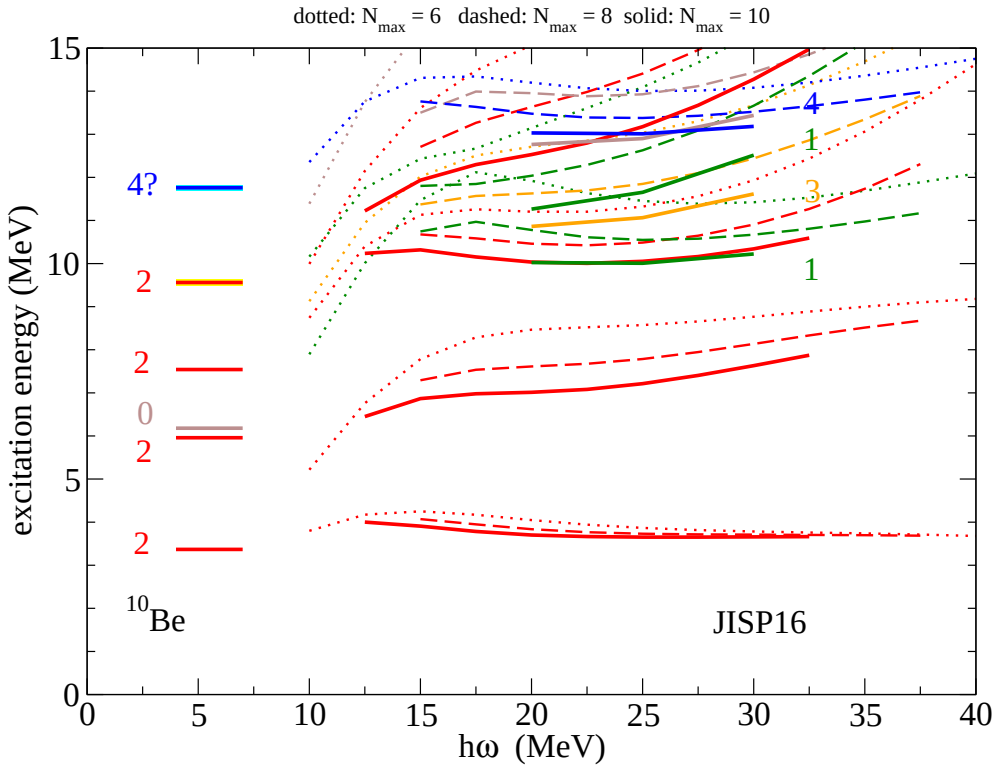


- Pairs of isospin 0 and 1 states with J = 2, 1, and 3
- Evidence of continuum states (J = 0 and 2) at $N_{\max} = 12$
- Rotational band

	expt.	calc	rotor
E_4/E_2	3.75	3.40	3.33

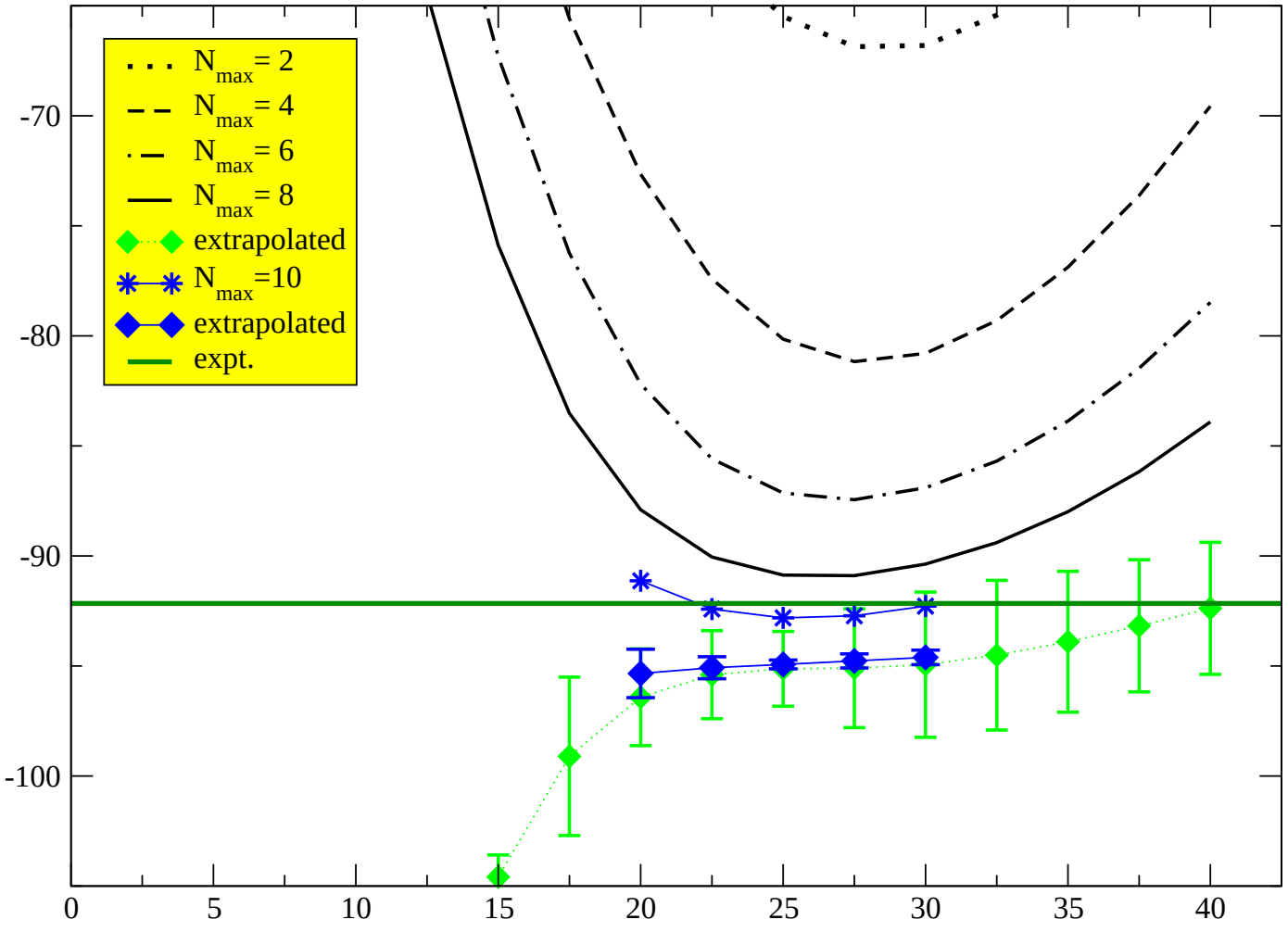
- Ground state above 2α threshold: radius not converged
- Quadrupole moments 2^+ and 4^+ not converged, nor B(E2)'s, but in qualitative agreement with rotational structure

10Be – positive parity states



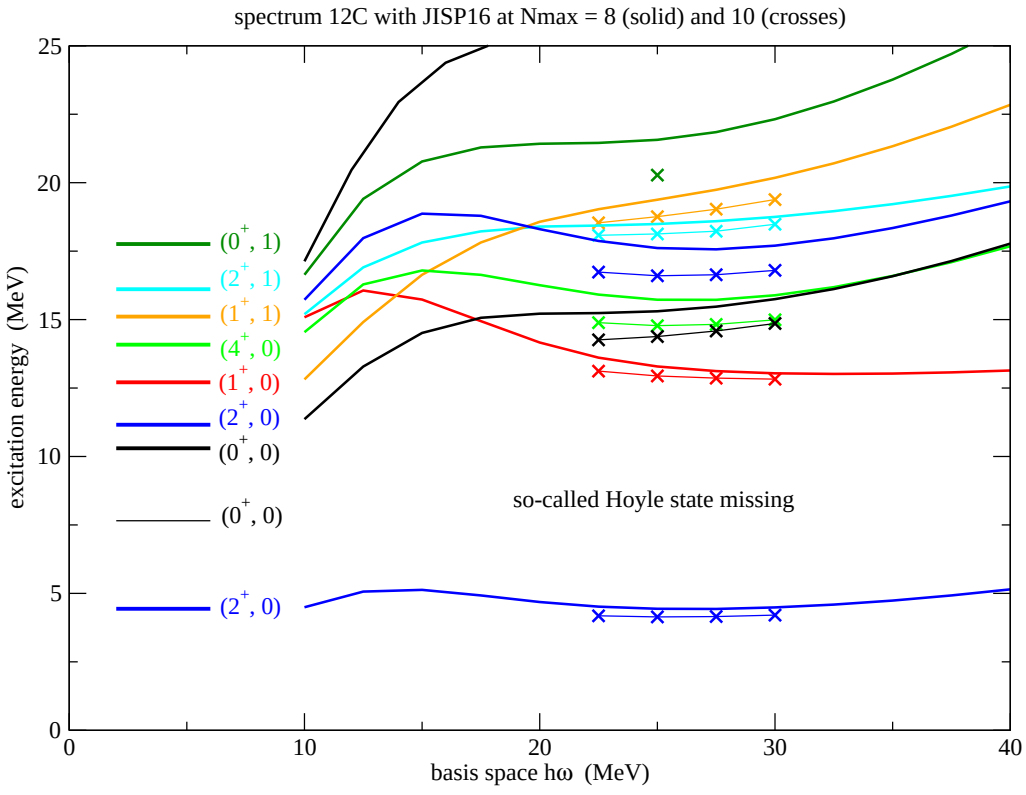
- Several 2^+ state in reasonable agreement with data
- Note: 0^+ state at 6 MeV missing from calculations?
  or coming down in spectrum with increasing basis space?
- Additional 1^+ and 3^+ states predicted

Results with JISP16 for ^{12}C



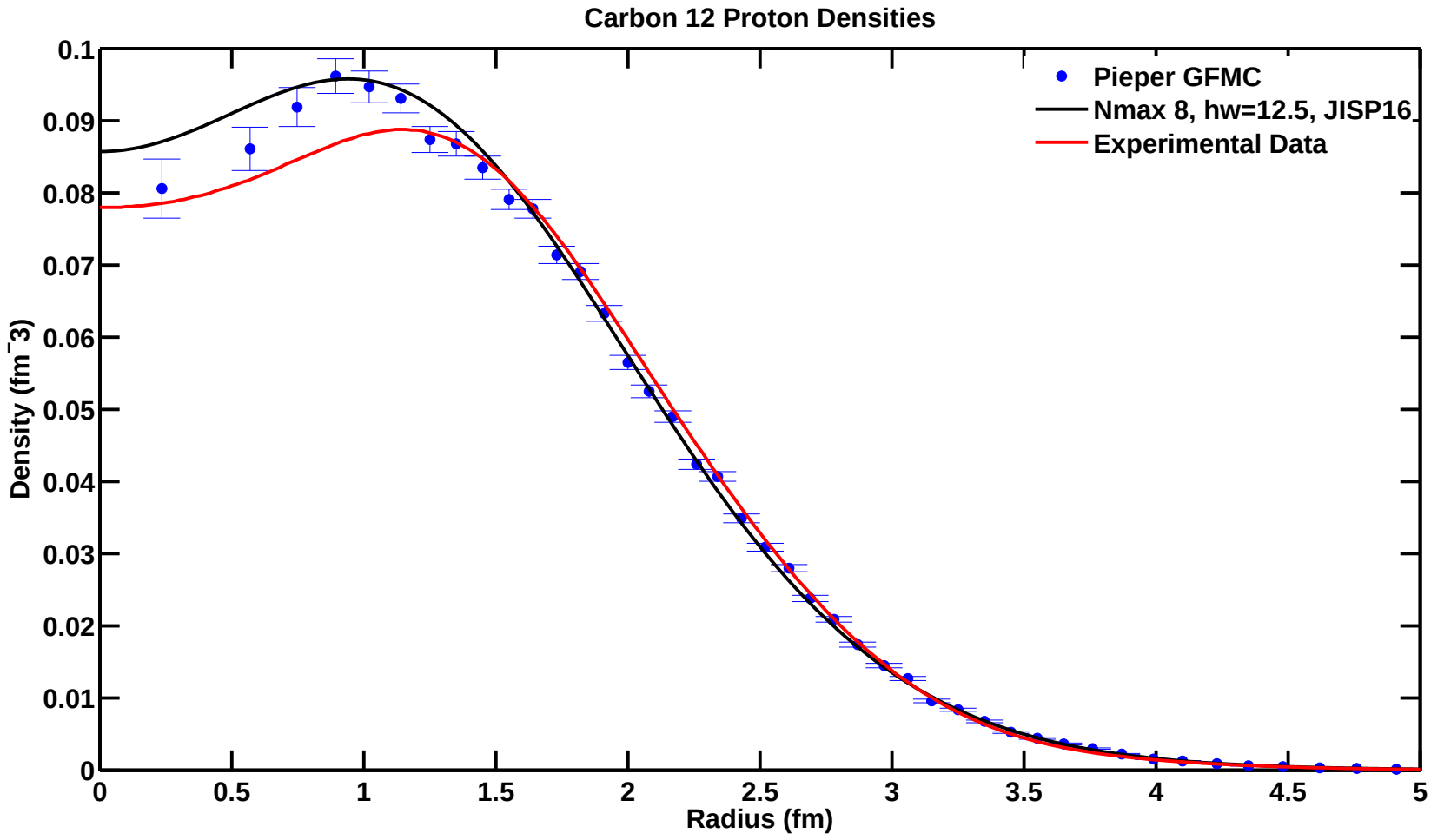
- calculations for $N_{\max} = 10$ underway (D = 8 billion)
  using 100,000 cores on JaguarPF (ORNL) under INCITE award

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



- pos. parity states in agreement with data, except for Hoyle state
- neutrino and pion scattering calculations in progress
- electromagnetic transitions in progress
  - rotational 2^+ and 4^+ states:
    significantly enhanced B(E2) (though not converged)

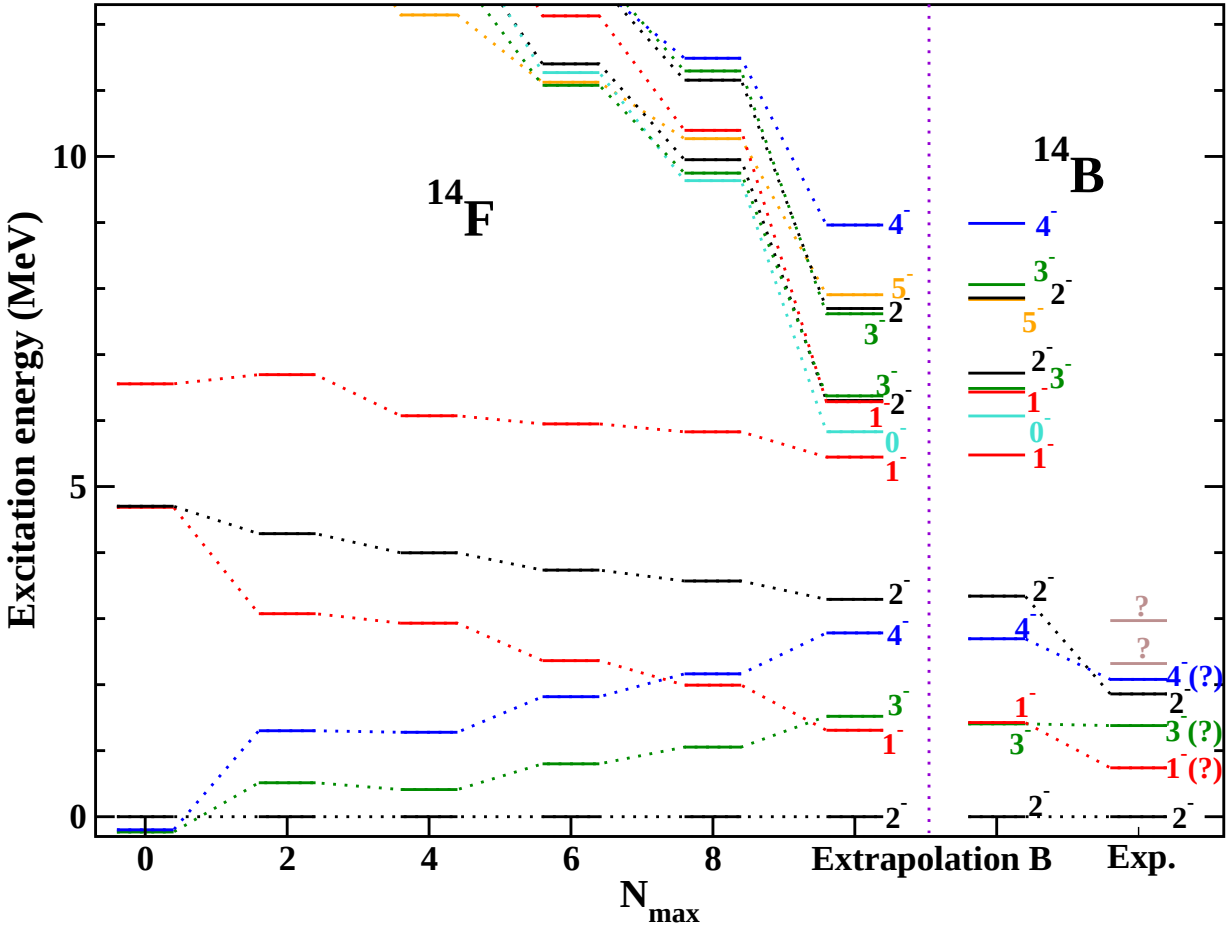
Density of ^{12}C with JISP16



- 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 $N_{\max} = 8$, $\hbar\omega = 12.5$ MeV (not converged)

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

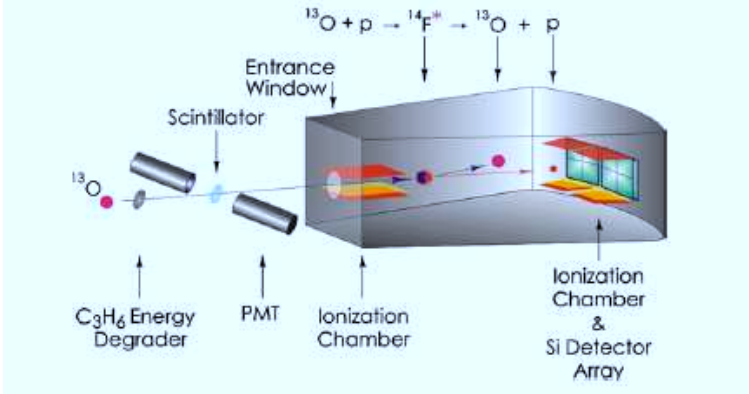


Fig. 1. (Color online.) The setup for the ^{14}F experiment. The "gray box" is the scattering chamber. See explanation in the text.

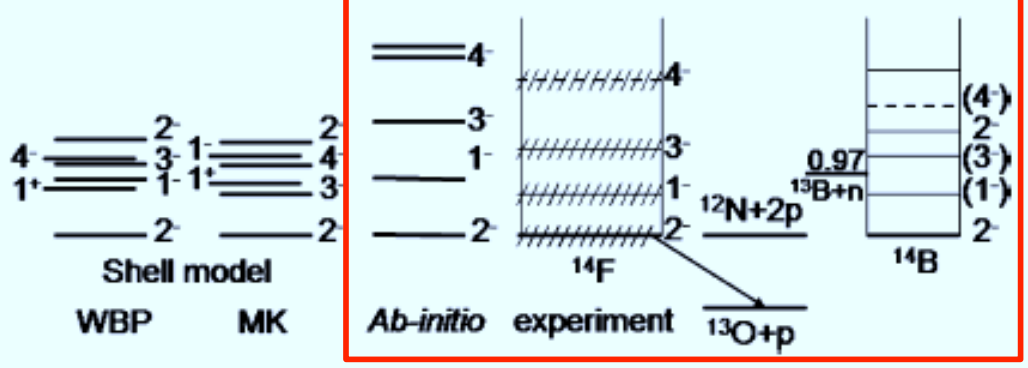


Fig. 6. ^{14}F level scheme from this work compared with shell-model calculations, *ab-initio* calculations [3] and the ^{14}B level scheme [16]. The shell model calculations were performed with the WBP [21] and MK [22] residual interactions using the code COSMO [23].

Lifetime of ^{14}C: A puzzle for nuclear theory

Puzzling to scientists …

What is the nuclear structure of ^{14}C that leads to its anomalously long half-life?

$\tau_{1/2}$ = 5730 years

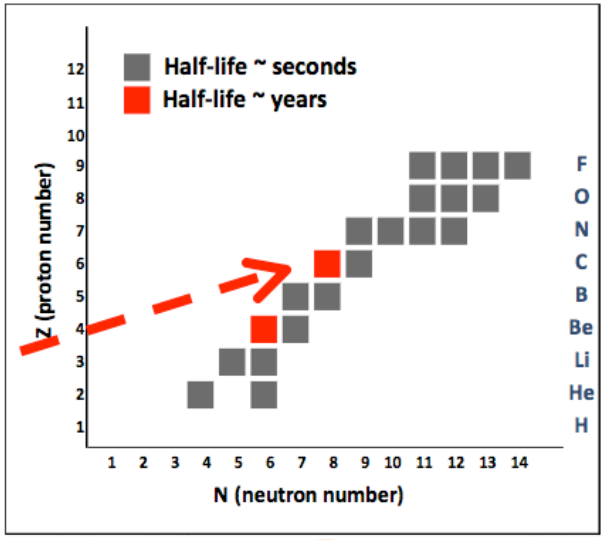


Chart of light nuclei that decay via beta emissions

$n \rightarrow p + e^- + n_e$

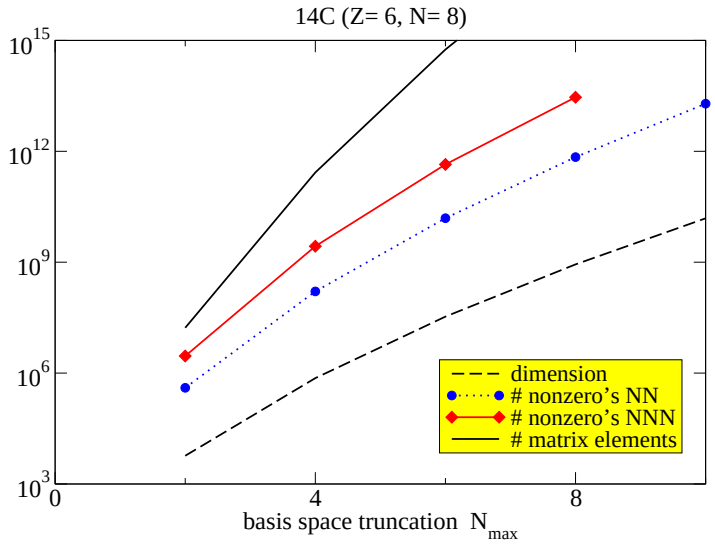
^{10}Be and ^{14}C have extremely long half-lives compared to other light nuclei (1.6 x 10^6 years / 5,730 years) . Their long half-lives make both isotopes useful for radioactive dating.

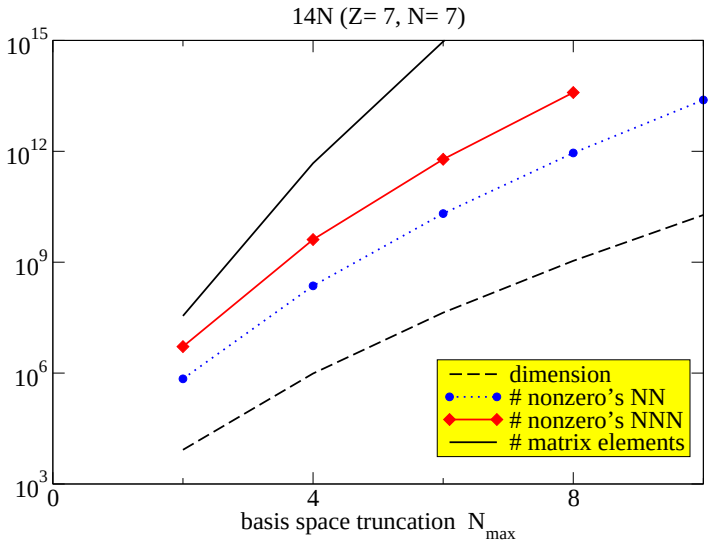
compare e.g. β decay $^6\mathrm{He}(0^+) \rightarrow {}^6\mathrm{Li}(1^+)$

- half-life $\tau_{1/2}$ = 806.7 ± 1.5 msec
- Gamov–Teller transition B(GT) = 4.71
- good agreement between ab-initio calculations and experiment

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

Petascale Early Science – Ab initio structure of Carbon-14



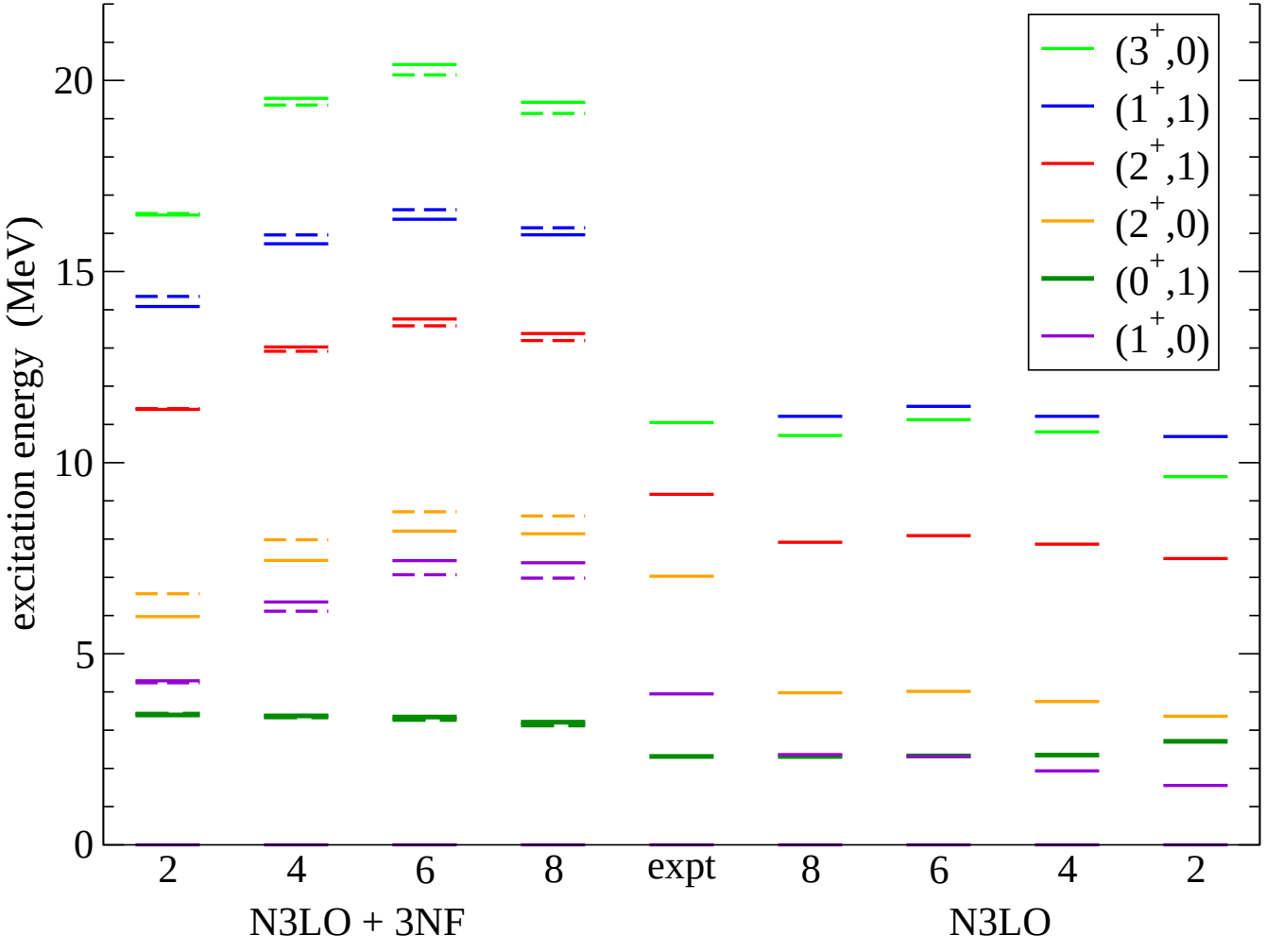


- Chiral effective 2-body plus 3-body interactions at $N_{\max} = 8$
- Basis space dimension 1.1 billion
- Number of nonzero m.e. 39 trillion
- Memory to store matrix (CRF) 320 TB
- Total memory on JaguarPF 300 TB

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

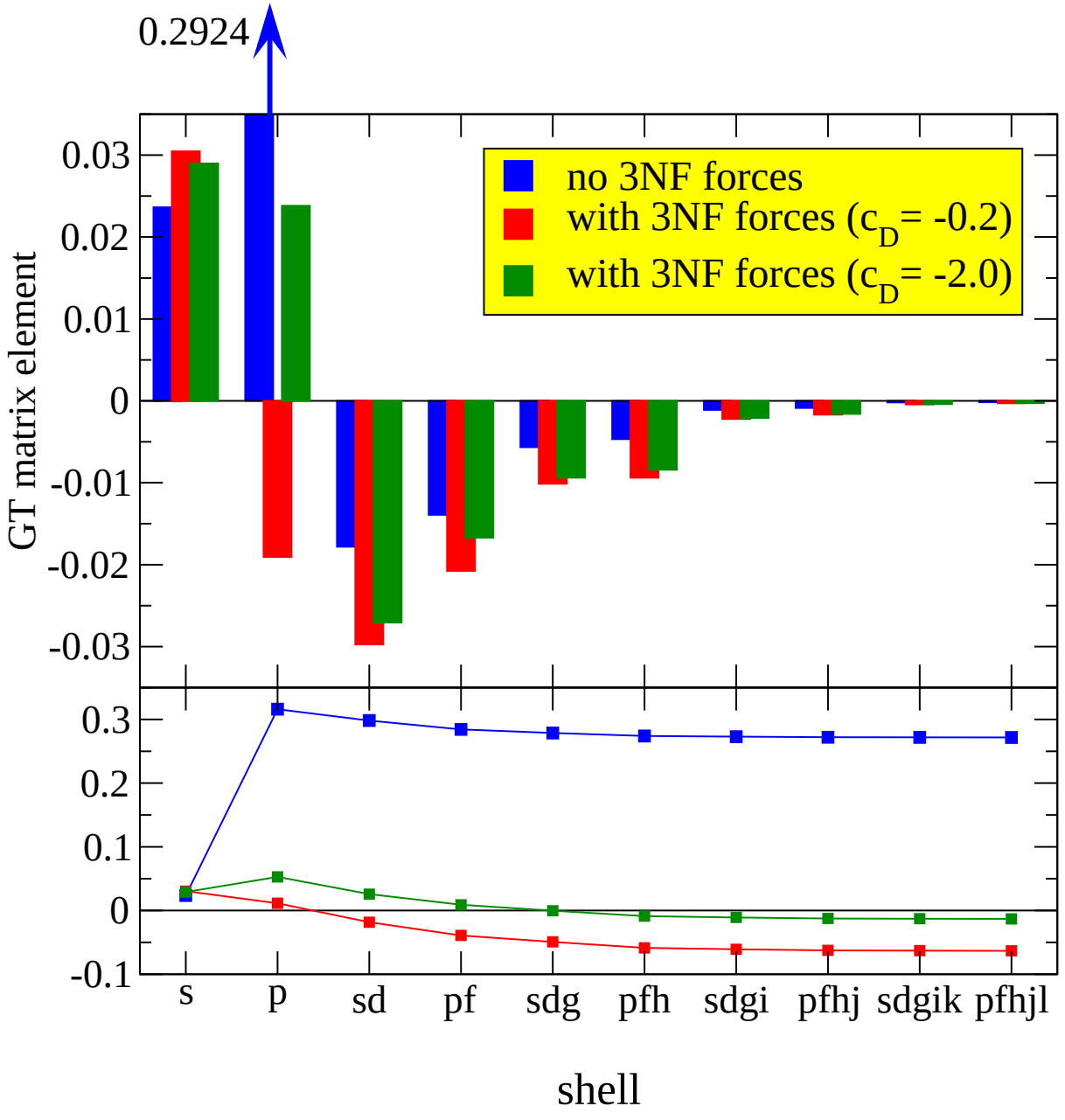
Ab initio structure of Carbon-14 and Nitrogen-14

Maris, Vary, Navratil, Ormand, Nam, Dean, PRL106, 202502 (2011)



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

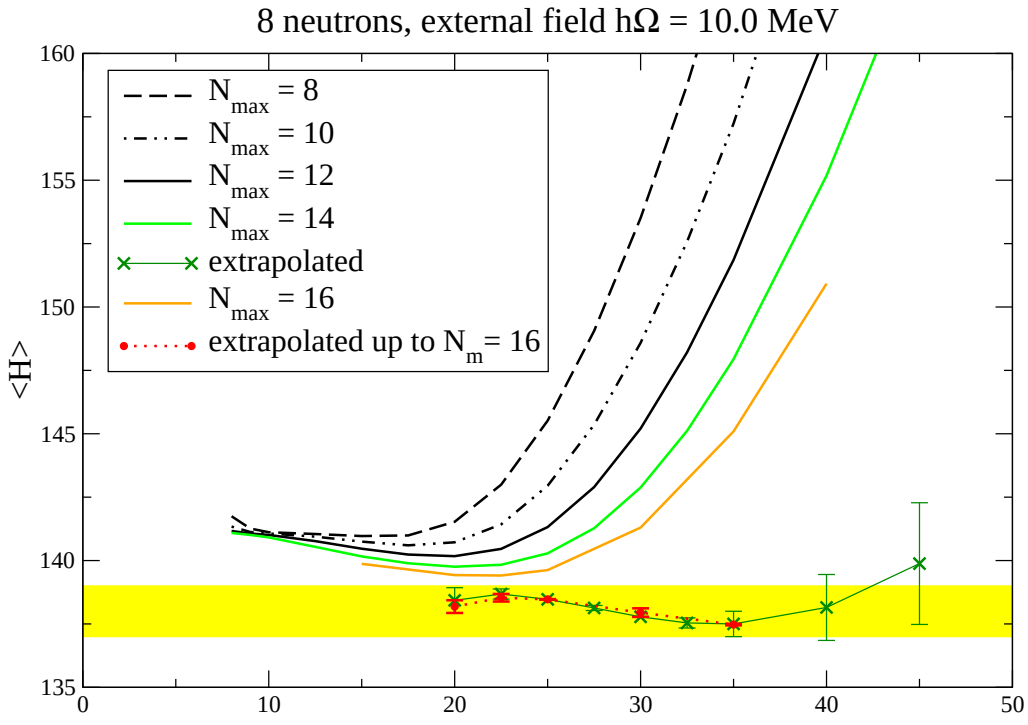
Maris, Vary, Navratil, Ormand, Nam, Dean, PRL106, 202502 (2011)

Validating ab-initio DME/DFT calculations

Bogner, Furnstahl, Kortelainen, Maris, Stoistov, Vary, arXiv:1106.3557

- 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
  - DME supplemented by fitted Skyrme-like contact terms
- DFT fit to NCFC results
- Comparison for 8 and 20 neutrons
  - total and internal energy per neutron, rms radius
  - densities, form factors

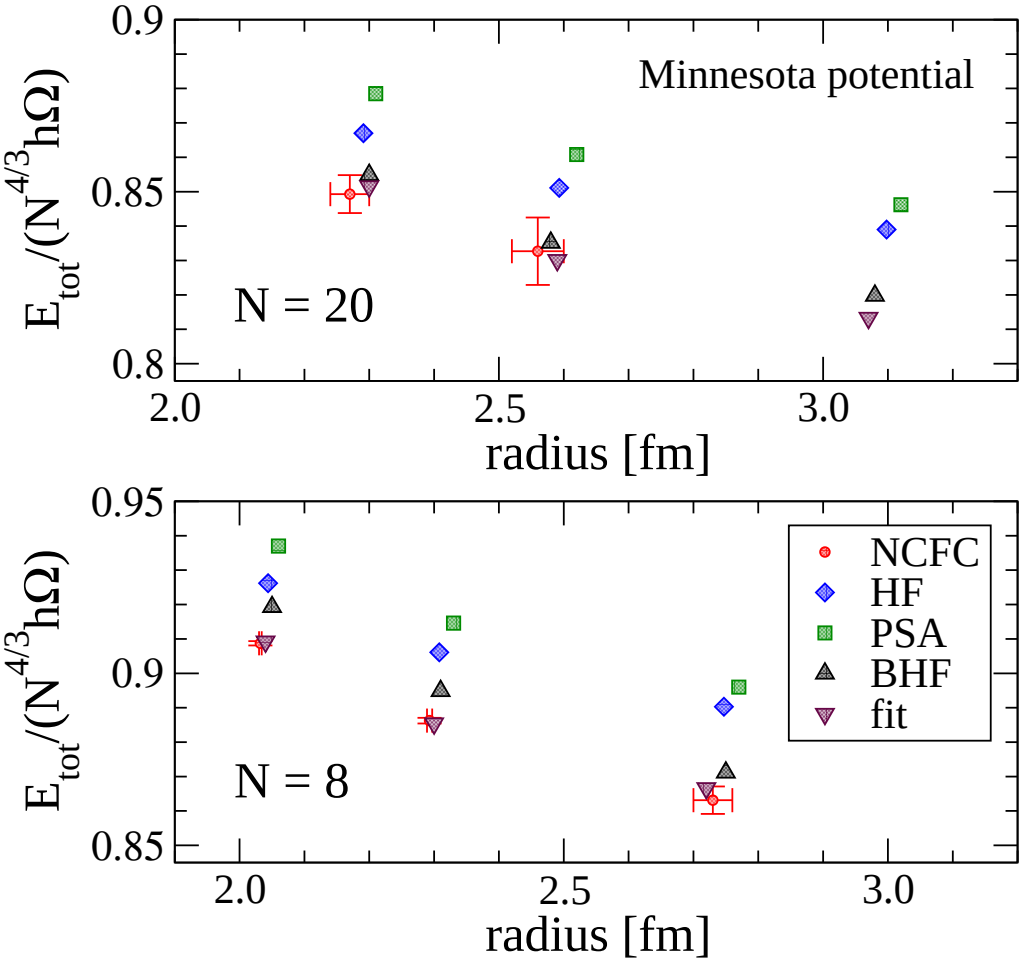
Minnesota potential – total energy



- Location variation minimum shifts to higher basis space $\hbar\omega$ with increasing N_m
- Optimal basis $\hbar\omega$ for Minnesota around 30 to 40 MeV
- Slow convergence in external field of 10 MeV

Minnesota potential – Total energy vs. radius

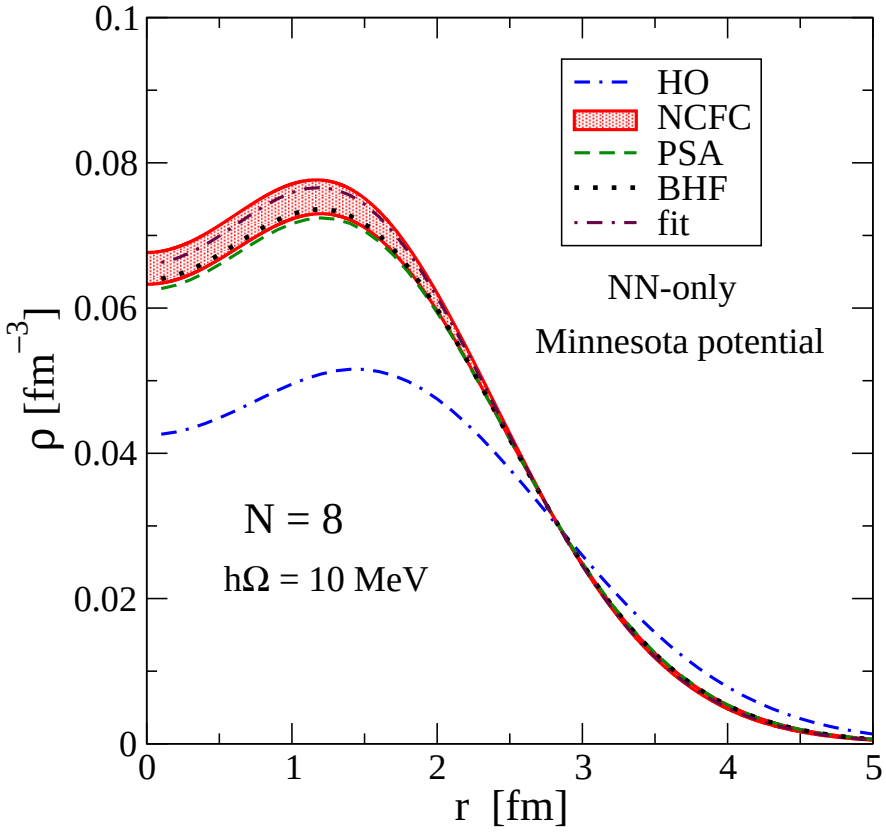
Bogner, Furnstahl, Kortelainen, Maris, Stoistov, Vary, arXiv:1106.3557

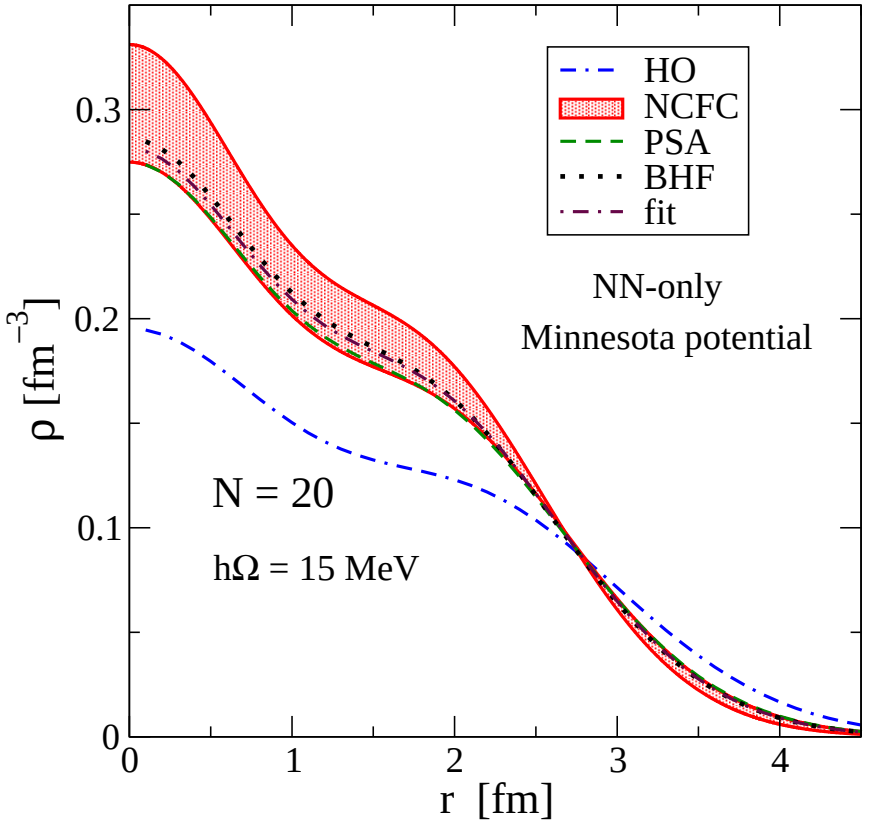


- Hartree–Fock does not agree with NCFC
- Brueckner–Hartree–Fock close to NCFC
- Fit with volume term and surface term can reproduce NCFC data

Minnesota potential – density

Bogner, Furnstahl, Kortelainen, Maris, Stoistov, Vary, arXiv:1106.3557

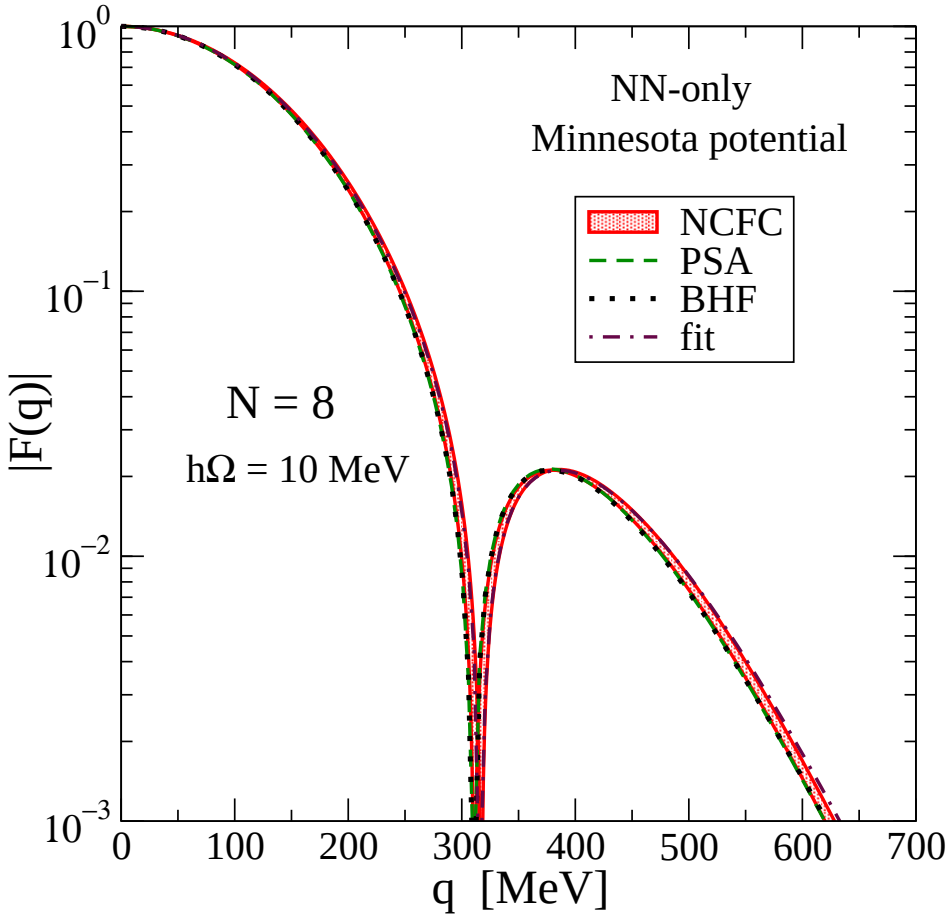




- Agreement between DME/DFT calculations and NCFC
- Density profile dominated by H.O. external field modefied by NN interaction

Minnesota potential – form factor

Bogner, Furnstahl, Kortelainen, Maris, Stoistov, Vary, arXiv:1106.3557



- Agreement between DME/DFT calculations and NCFC

Taming the scale explosion

- Reaching the limit of M-scheme $N_{\max}$ truncation
  - extremely large, extremely sparse matrices
- Reduce basis dim. by keeping only most important basis states
  errors due to reduced basis dimension can be estimated
  and hopefully kept under control
  - Importance Truncation Roth, Phys. Rev. C79, 064324 (2009)
    - reduce basis dimension by factor of order of ten
    - many-body states single Slater Determinants in M-scheme
  - Monte-Carlo No-Core Shell Model

    Abe, Maris, Otsuka, Shimizu, Utsuno, Vary, AIP Conf Proc 1355, 173 (2011)
    - reduce basis to (few) hundred highly optimized states
    - many-body states linear combination of Slater Deteminants
    - projected to good Total-J
    - hotspot:
      construction of optimized basis and of many-body matrix

Taming the scale explosion

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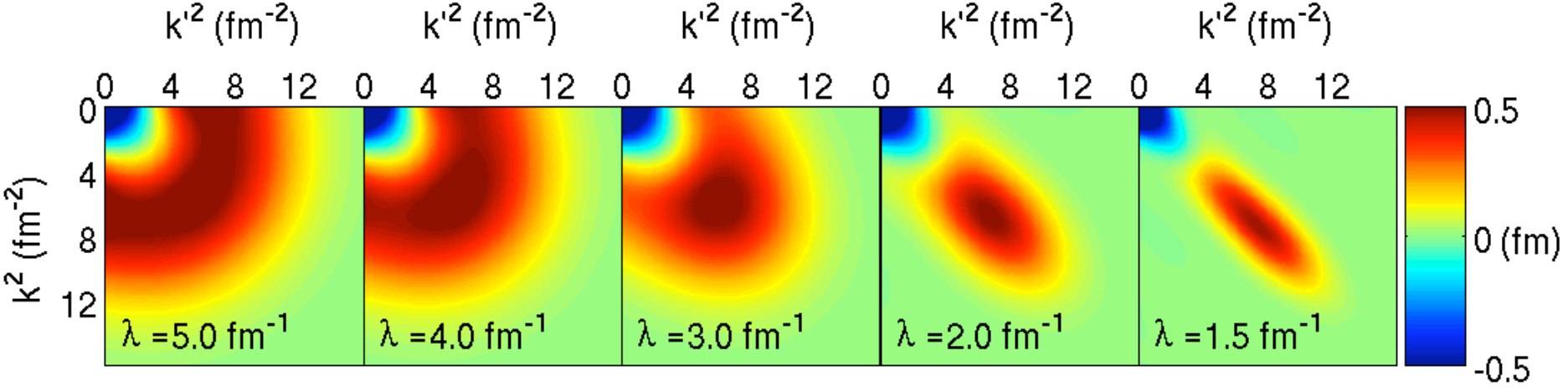
  - extremely large, extremely sparse matrices
- Reduce basis dim. by keeping only most important basis states
  errors due to reduced basis dimension can be estimated
  and hopefully kept under control
- Renormalization techniques to accelerate convergence w. $N_{\max}$
  Lee–Suzuki–Okamoto, Similarity Renormalization Group, . . .
  - bottlenecks
    - construction of renormalized input Hamiltonian
    - including induced many-body interactions



Taming the scale explosion

- Reaching the limit of M-scheme $N_{\max}$ truncation
  - extremely large, extremely sparse matrices
- Reduce basis dim. by keeping only most important basis states
  errors due to reduced basis dimension can be estimated
  and hopefully kept under control
- Renormalization techniques to accelerate convergence w. $N_{\max}$
- More flexible / realistic (radial) basis functions

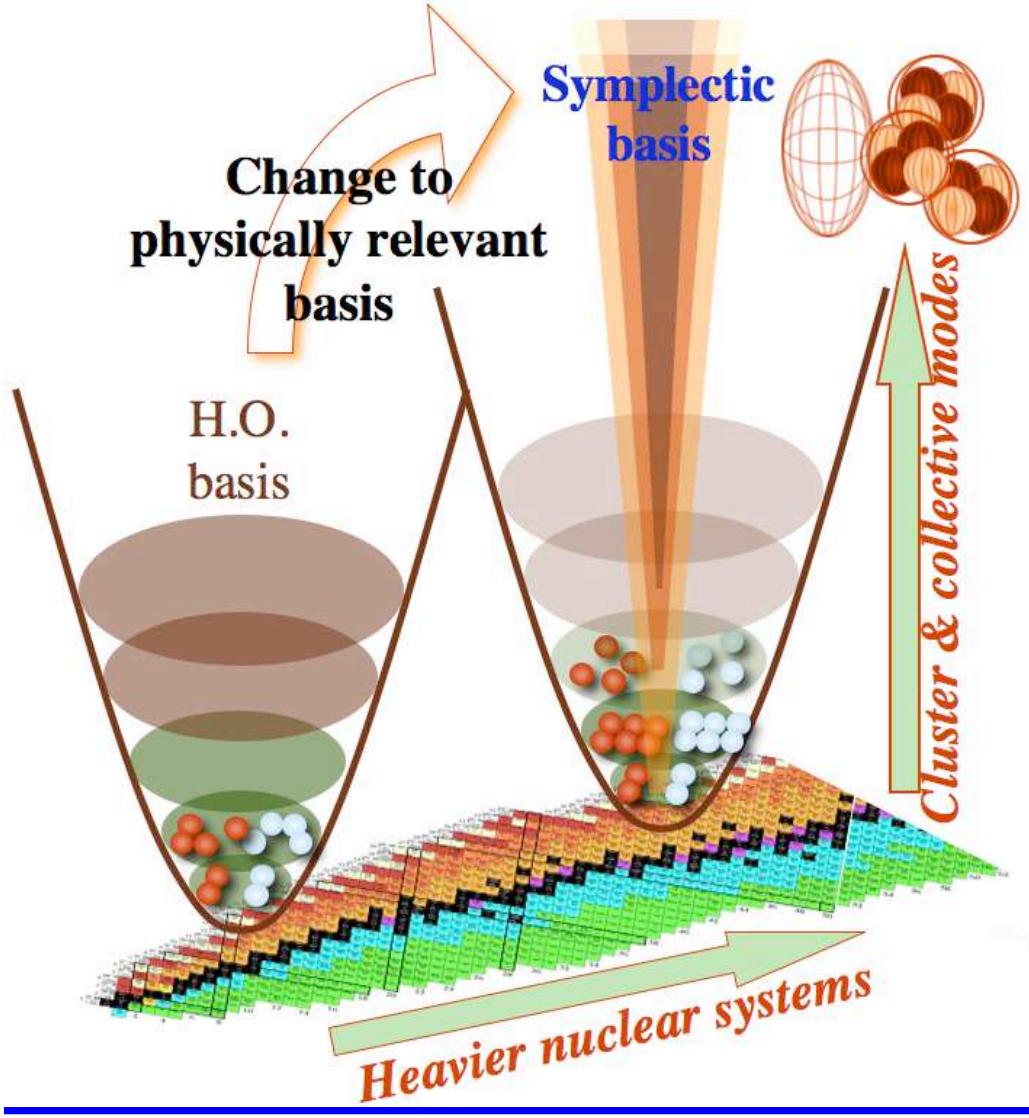
  Negoita, PhD thesis 2010; Caprio, Maris, Vary, in progress
- Reduce basis dim. by exploiting additional symmetries

  Coupled-J basis — Aktulga, Yang, Ng, Maris, Vary, in preparation

  SU(3) / Sp(3,R) basis — Draayer et al, PetaApps Award 2009 - 2014
  - smaller, but less sparse matrices
  - construction of matrix more costly, but diagonalization cheaper
  - number of nonzero matrix elements often actually
    (significantly) larger than in M-scheme

Symmetry-Adapted CI truncation

PetaApps award (2009) PI: Draayer(LSU)



- Allows for ab initio calculations of
  - cluster states
  - deformed nuclei
  - nuclei in sd-shell (beyond ^{16}O)
- Astrophysical applications: Hoyle state in ^{12}C (3 α-cluster state) crucial for nucleosynthesis
- Status
  - SU(3) based CI code up and running (T. Dytrych
  - requires innovative loadbalancing techniques

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
- Main challenge: construction and diagonalization of extremely large (D > 1 billion) sparse matrices
- Significant benefits from collaboration between nuclear physicists, applied mathematicians, and computer scientists
- Has led to
  - prediction of new isotope, ^{14}F
  - understanding of the anomalously large lifetime of ^{14}C
  - validation of DFT/DME calculations (in progress)
- Future developments: Taming the scale explosion
  - reduce basis space dimension
  - matrix generally becomes less sparse, but more expensive to construct