Large–scale No-Core Shell Model / No-Core Full Configuration calculations

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Collaborators

Nuclear physics

ISU: James Vary, PM, students
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MSU: Scott Bogner
ANL: Harry Lee, Steve Pieper, Bob Wiringa
LANL: Joe Carlson, Stefano Gandolfi
UA: Sid Coon, Bira van Kolck, Bruce Barrett
LSU: Jerry Draayer, Tomas Dytrych, Kristina Launey
Notre Dame: Mark Caprio

International Collaborators:
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Abe, Otsuka, Shimizu, Utsuno

Computer Science/Applied Math
Ames Lab: Masha Sosonkina, Fang (Cherry) Liu, students
LBNL: Esmond Ng, Chao Yang, Hasan Metin Aktulga
ANL: Stefan Wild
OSU: Umit Catalyurek

No-Core Shell Model / No-Core Full Configuration calculations

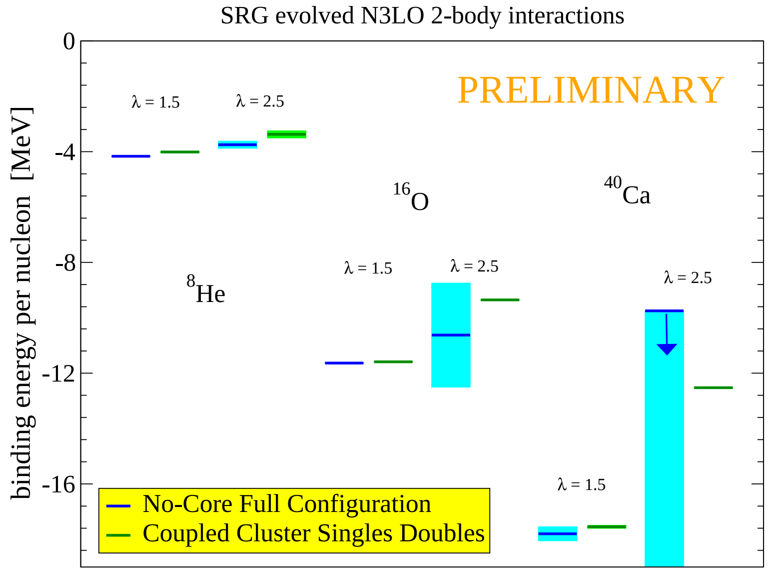
Numerical approach for bound states of nucleons
using basis-space expansion methods (CI methods)

- Given
  - a V_{NN} and V_{NNN} (and V_{NNNN}) interaction
  - number of protons and neutrons: Z, N

  calculates
  - bound state spectrum and corresponding wave functions
  - one-body density matrices
  - selected observables:
    rms radii, magnetic moments, quadrupole moments,
    transition rates between states within the same nucleus
- Ab initio calculations for nuclei throughout the p-shell
  and into the sd-shell with realistic NN and NNN potentials
- Ab initio calculations for nuclei and neutron droplets
  in external fields for comparisons with DME/DFT

Many-Fermion-Dynamics for nuclear physics

- Platform independent hybrid OpenMP/MPI Fortran code
- N_{max} truncation and HO basis:
  exact factorization CoM motion and intrinsic motion
- No-Core Shell Model:
  improved convergence in relatively small model spaces w. Lee–Suzuki–Okamoto renorm. truncated at 2- or 3-body level
- No-Core Full Configuration:
  monotonic approach to asymptotic values with increasing basis
  - Variational: upper bound for the ground state energy for any finite truncation of the basis space
- Convergence: observables independent of N_{max} and $\hbar\omega$
- Same interaction, different methods (CC, GFMC, NCFC, NCSM, ...) give same results within numerical errors



MFDn – code development progress report

- MFDn Version 13 beta02
  - interface with 'new' format from Jurgenson and Navratil for SRG-evolved chiral 2- and 3-body forces
  - minor performance improvements
  - minor bug fixes
- Integration MFDn-V13-beta02 with LCCI project

  (see LCCI session on Wednesday)

  `NERSC:/project/projectdirs/unedf/lcci/MFDn/`

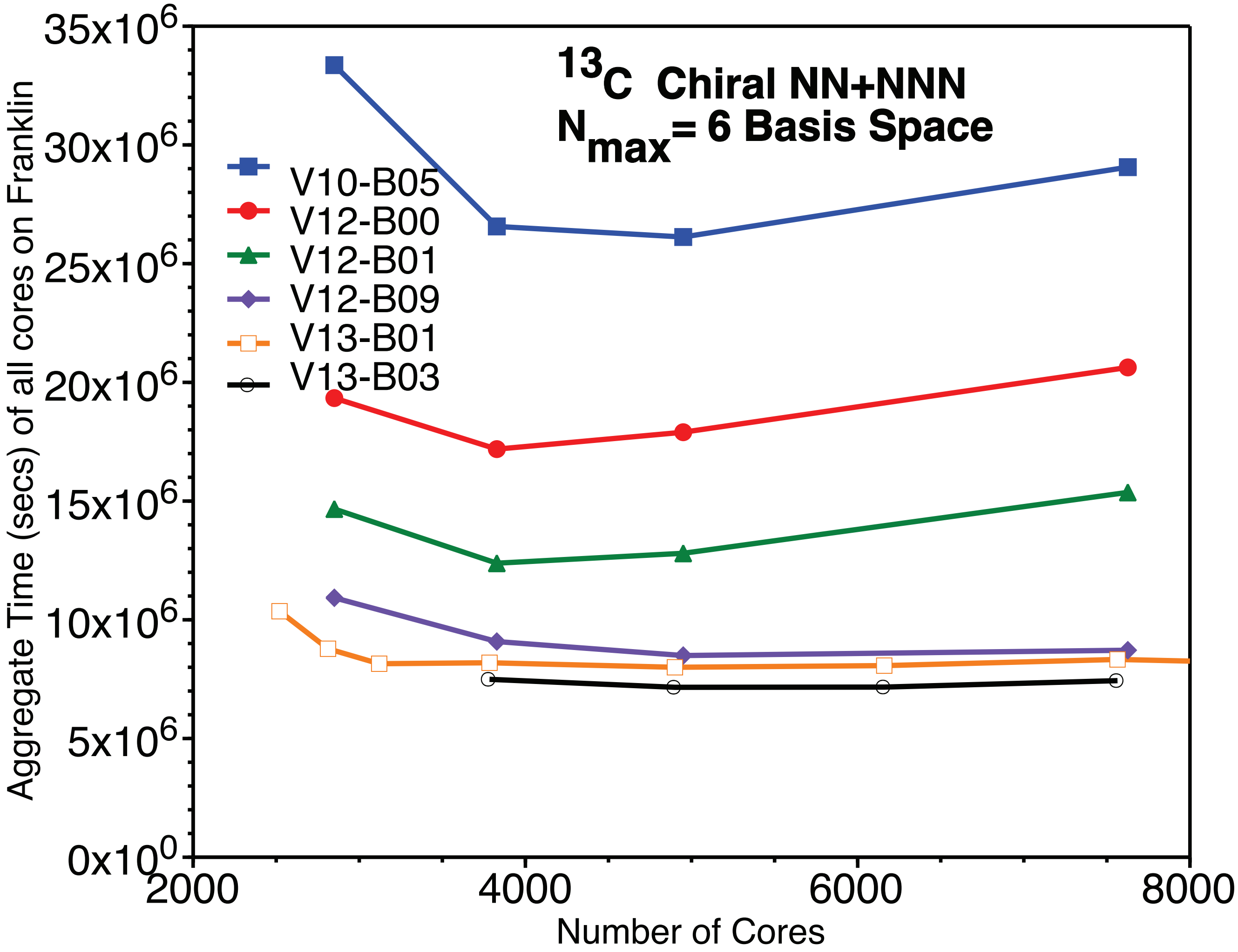
  - interactive python script for running CI codes on Leadership Class facilities
  - interface with database for archiving ab initio Shell Model / Configuration Interaction results

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

Performance improvements of MFDn over past 4 years

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

Accelerating Configuration Interaction calculations for nuclear structure, presented at SuperComputing08



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

dimension $38 \cdot 10^6$
nonzero m.e. $56 \cdot 10^{10}$
memory for matrix: 5 TB
size input 3 GB

performance on Franklin
at NERSC

similar performance
on JaguarPF at ORNL

unpleasant surprise:
very poor performance
on Hopper at NERSC

MFDn – 2-dimensional distribution of matrix

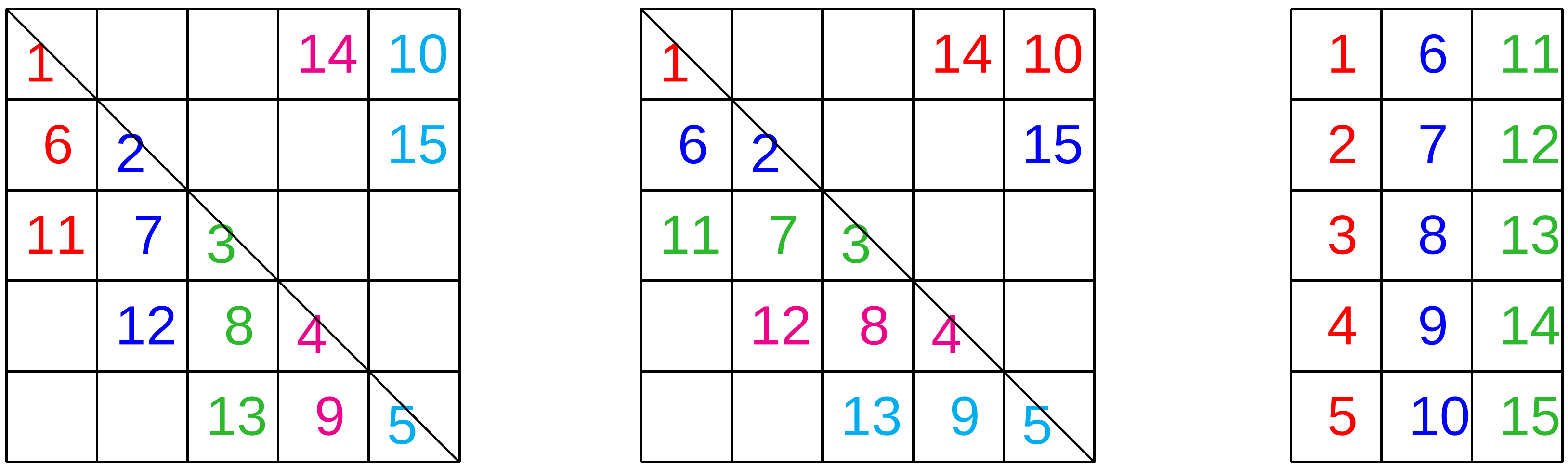
- Real symmetric matrix: store only lower (or upper) triangle
- Store Lanczos vectors distributed over all processors
- In principle, we can deal with arbitrary large vectors
  even if we cannot store an entire vector on a single processor
  - largest dimension: 8 billion, 32 GB / vector in single precision

1			14	10
6	2			15
11	7	3		
	12	8	4	
		13	9	5

1	6	11
2	7	12
3	8	13
4	9	14
5	10	15

MFDn – Communication patterns

- Matrix-vector multiplication
  - Broadcast from each of d procs to row-group of $(d+1)/2$ procs
  - B'cast from each of d procs to column-group of $(d+1)/2$ procs
  - Local (transpose) matrix vector multiplication
  - Reduce from row-group of $(d+1)/2$ off-diagonal procs
  - Reduce from column-group of $(d+1)/2$ off-diagonal procs
- Orthogonalization
  - Lanczos vectors stored over all processors
  - Local dot-product on each processor, followed by reduce

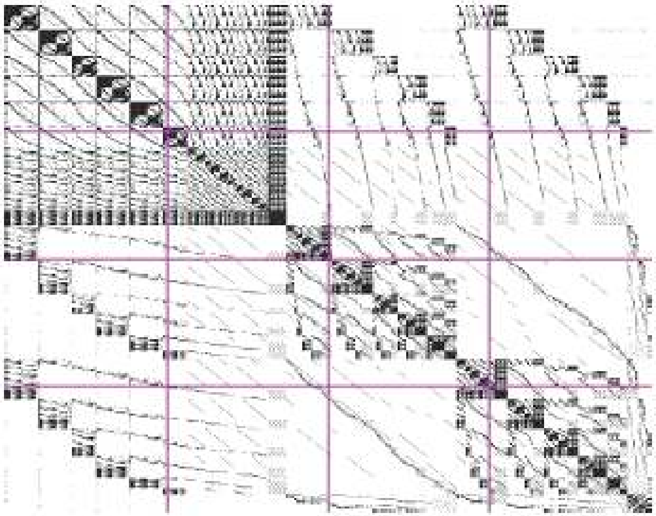


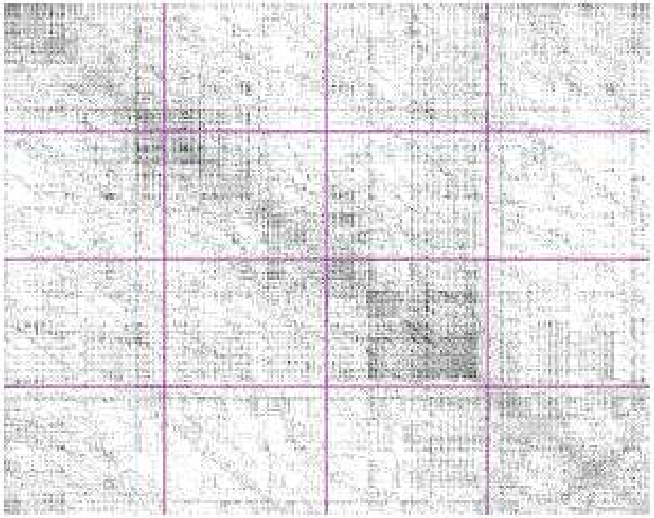
MFDn – new developments

- MFDn Version 13 beta03 (under development)
  - new interface for input of complete 2-body hamiltonian in proton-neutron format
  - allows for general basis functions and external fields
- MFDn – Total-J code
  see next talk (Hasan Metin Aktulga)
- MFDn Version 14
  - different distribution of basis states:
    retain part of the natural block-sparsity pattern
    of many-body matrix
    - significant improvement in efficiency of constructing many-body matrix
    - not as well load-balanced as Version 13
  - checkpoint / restart capability
  - enabling larger model-space calc. using partial “on-the-fly”

MFDn – load-balancing

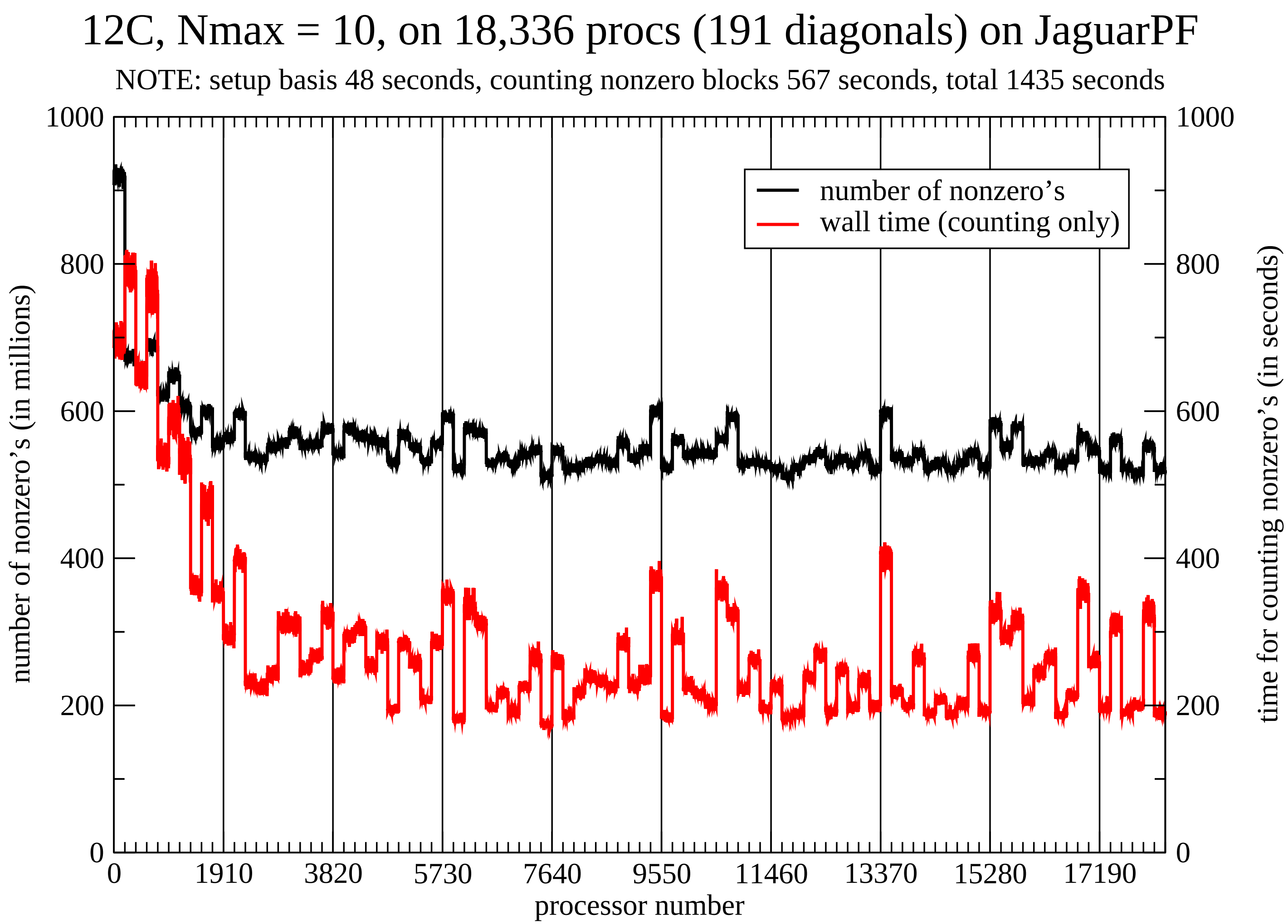
- Version 13
  - Lexico-graphical enumeration of basis states on d procs
  - Round-robin distribution of basis states over d procs





  - Almost perfect load balancing
  - However, no (apparent) structure in sparse matrix
    - multi-level blocking scheme to locate nonzero's (Sternberg 2008)
- Version 14: distribute groups of basis states over d procs
  in order to retain part of the natural structure of the matrix

MFDn – load-balancing, Version 14



Checkpointing

- Version 13: no checkpoint/restart capability
- Version 14:
  - No IO of many-body matrix
    - construction of many-body matrix much faster than in Version 13
    - IO time of many-body matrix larger than re-construction in case of a restart
  - IO of Lanczos vectors by 'diagonal processors'
    - one binary file per diagonal processor
    - each Lanczos vector written to file at each iteration
  - Tri-diagonal matrix elements written by single processor at each iteration
  - Restart option (on same number of processors!): read in previously calculated Lanczos vectors and tri-diagonal matrix

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

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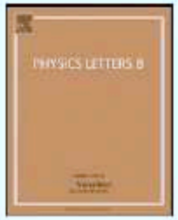


First observation of ^{14}F

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

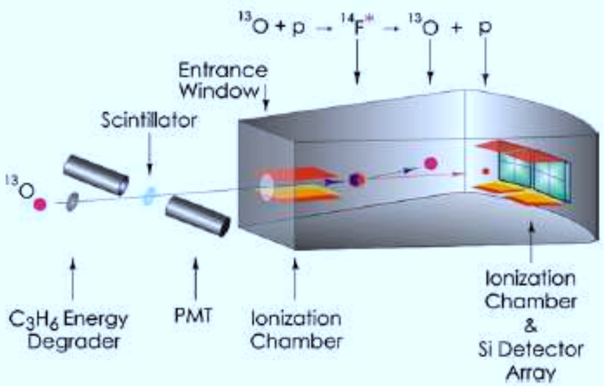


Fig. 1. (Color online.) The setup for the ^{14}F experiment. The "gray box" is the scattering chamber. See explanation in the text.

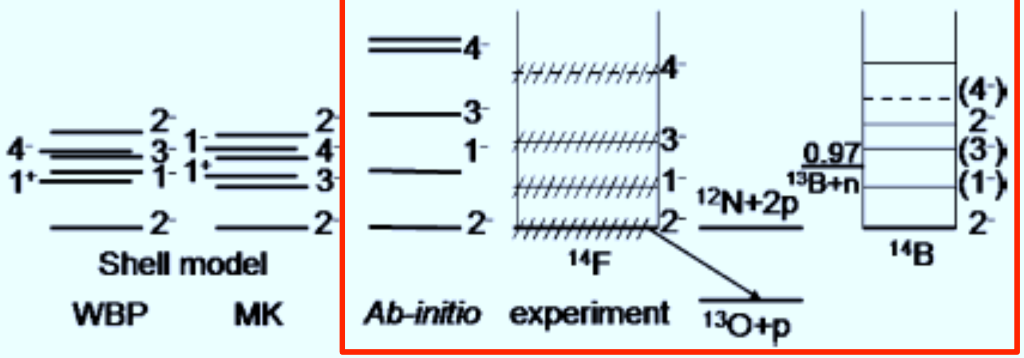
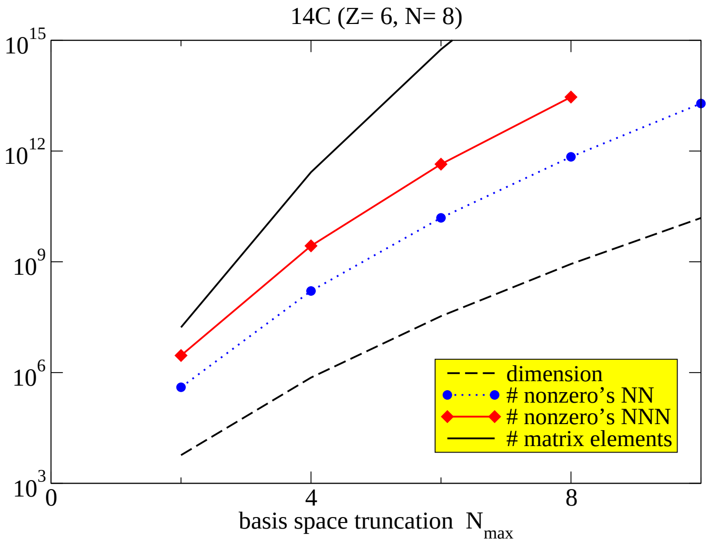
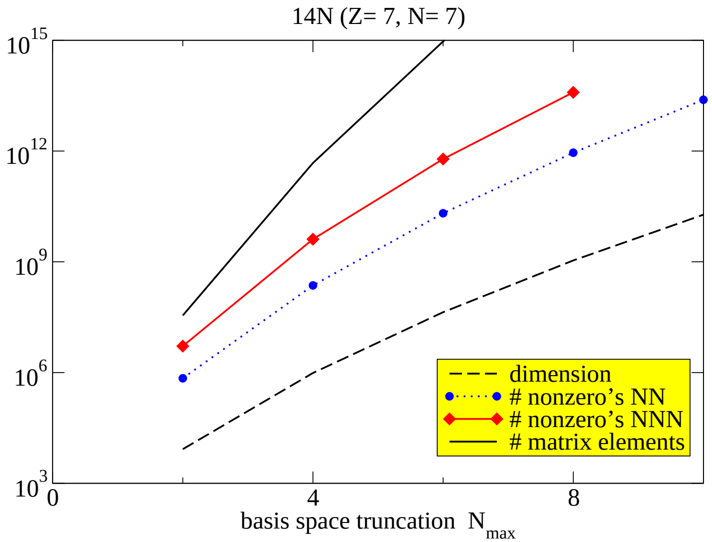


Fig. 6. ^{14}F level scheme from this work compared with shell-model calculations, *ab-initio* calculations [3] and the ^{14}B level scheme [16]. The shell model calculations were performed with the WBP [21] and MK [22] residual interactions using the code COSMO [23].

Petascale Early Science – Ab initio structure of Carbon-14



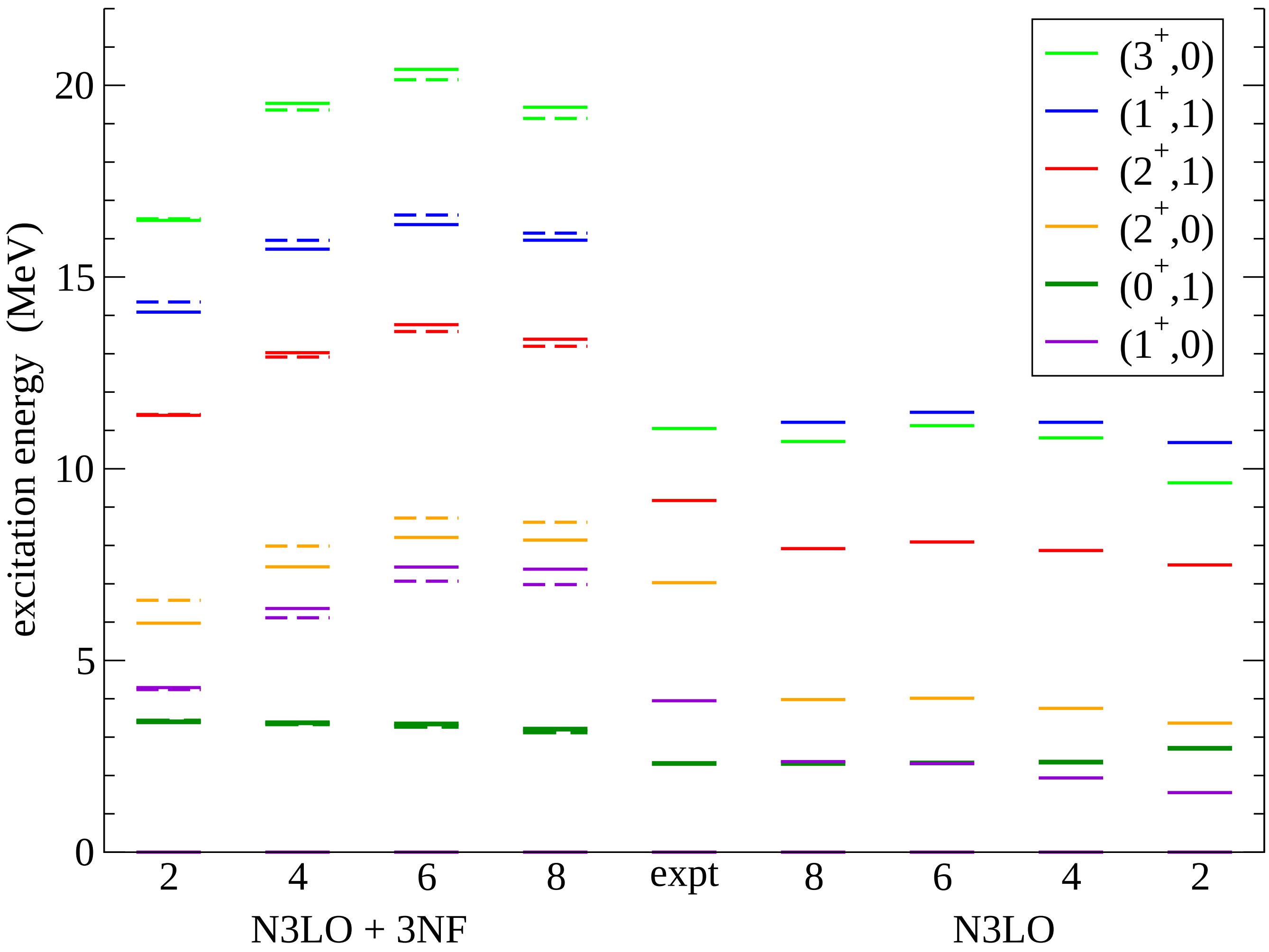


- Chiral effective 2-body plus 3-body interactions at $N_{\text{max}} = 8$
- Basis space dimension 1.1 billion
- Number of nonzero m.e. 39 trillion
- Memory to store matrix (CRF) 320 TB
- Total memory on JaguarPF 300 TB

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

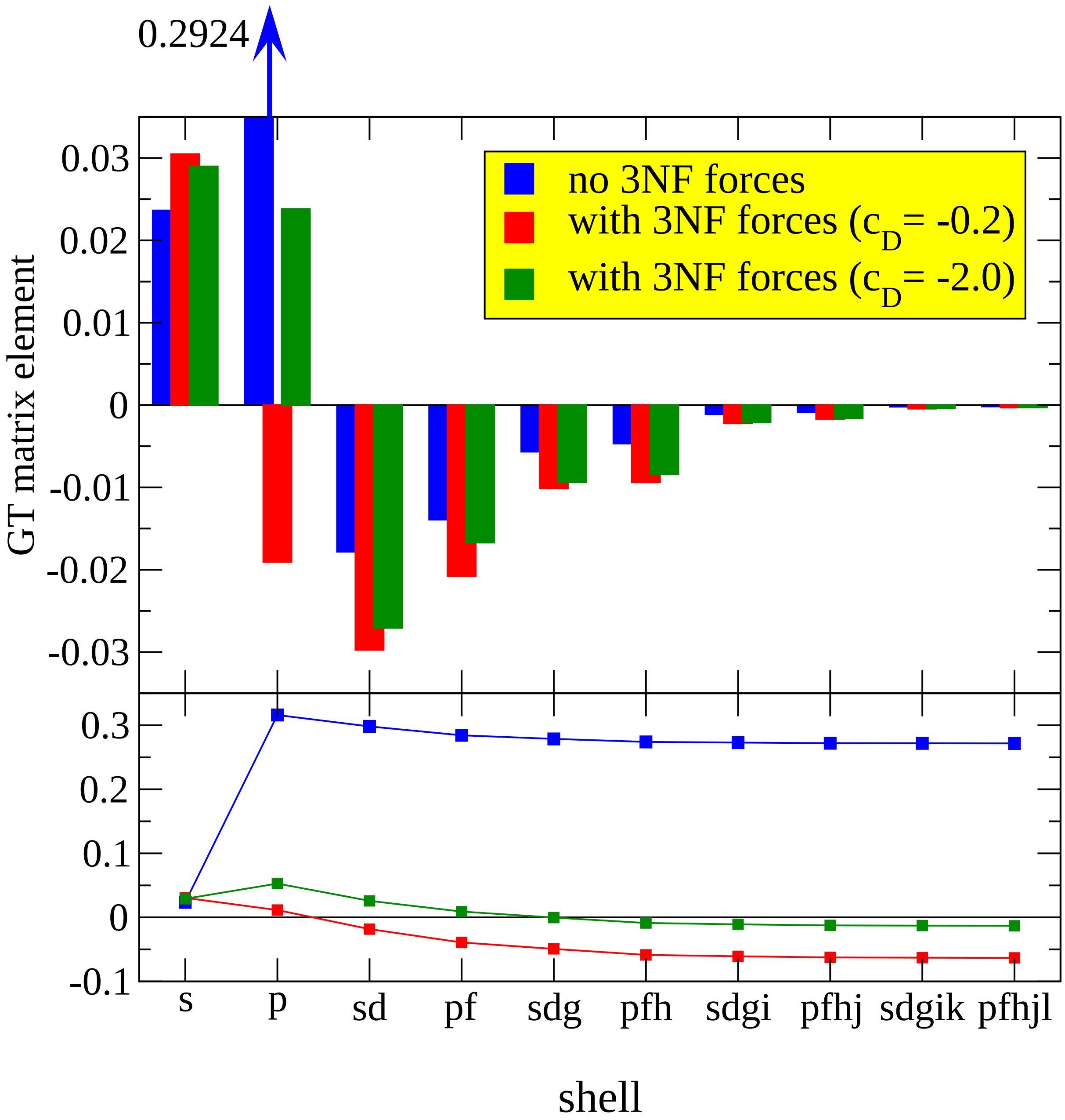
Ab initio structure of Carbon-14 and Nitrogen-14

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



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

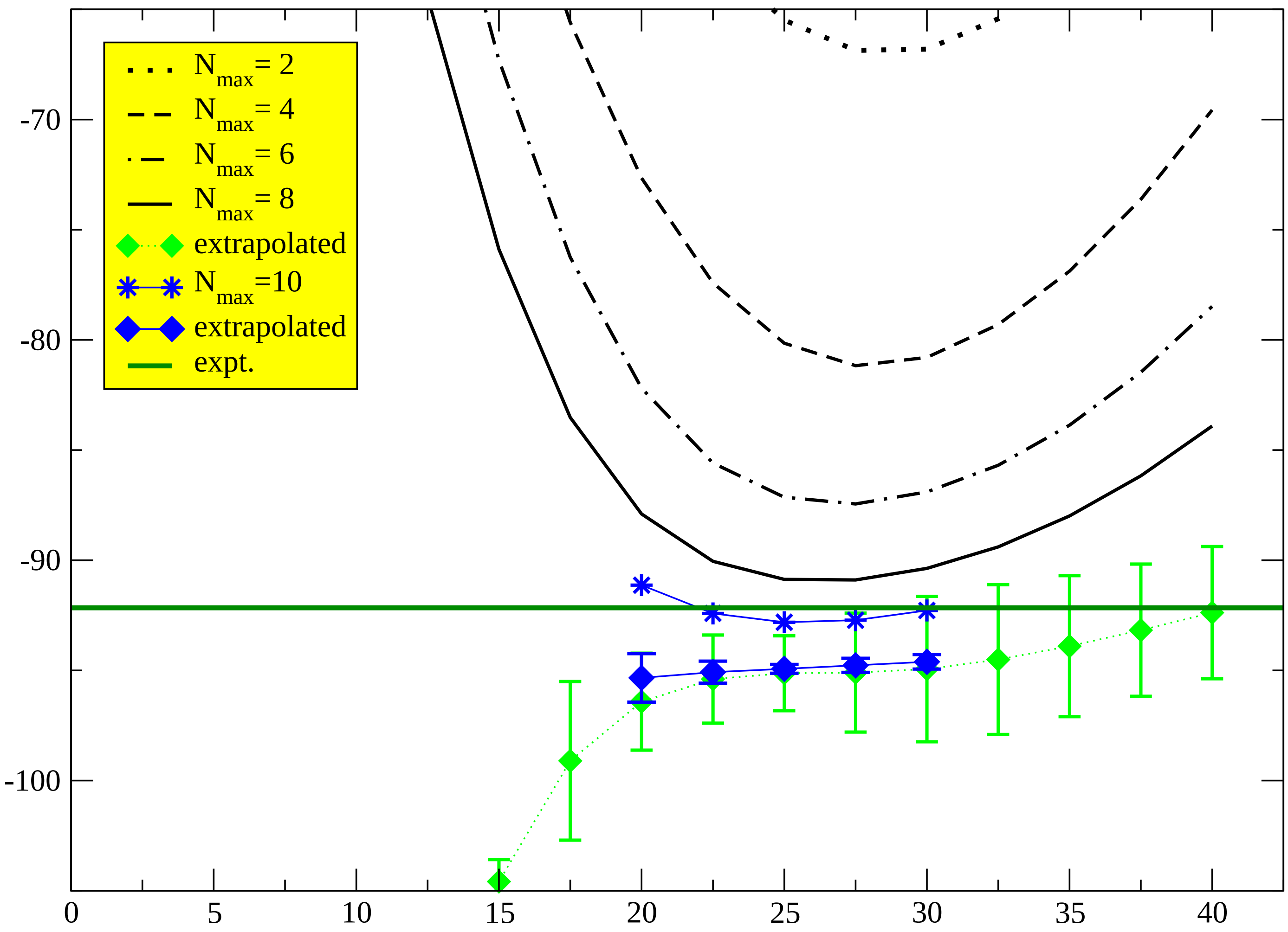
Origin of the anomalously long life-time of ^{14}C



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

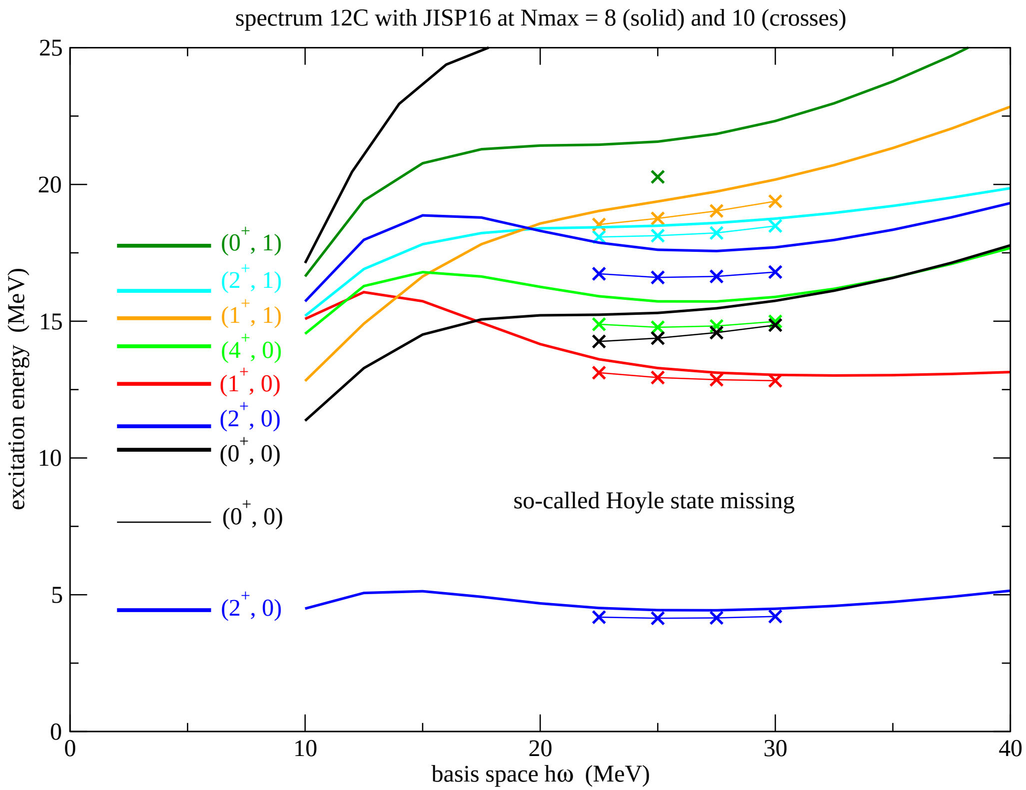
Maris, Vary, Navratil, Ormand, Nam, Dean, PRL106, 202502 (2011)

Results with JISP16 for ^{12}C



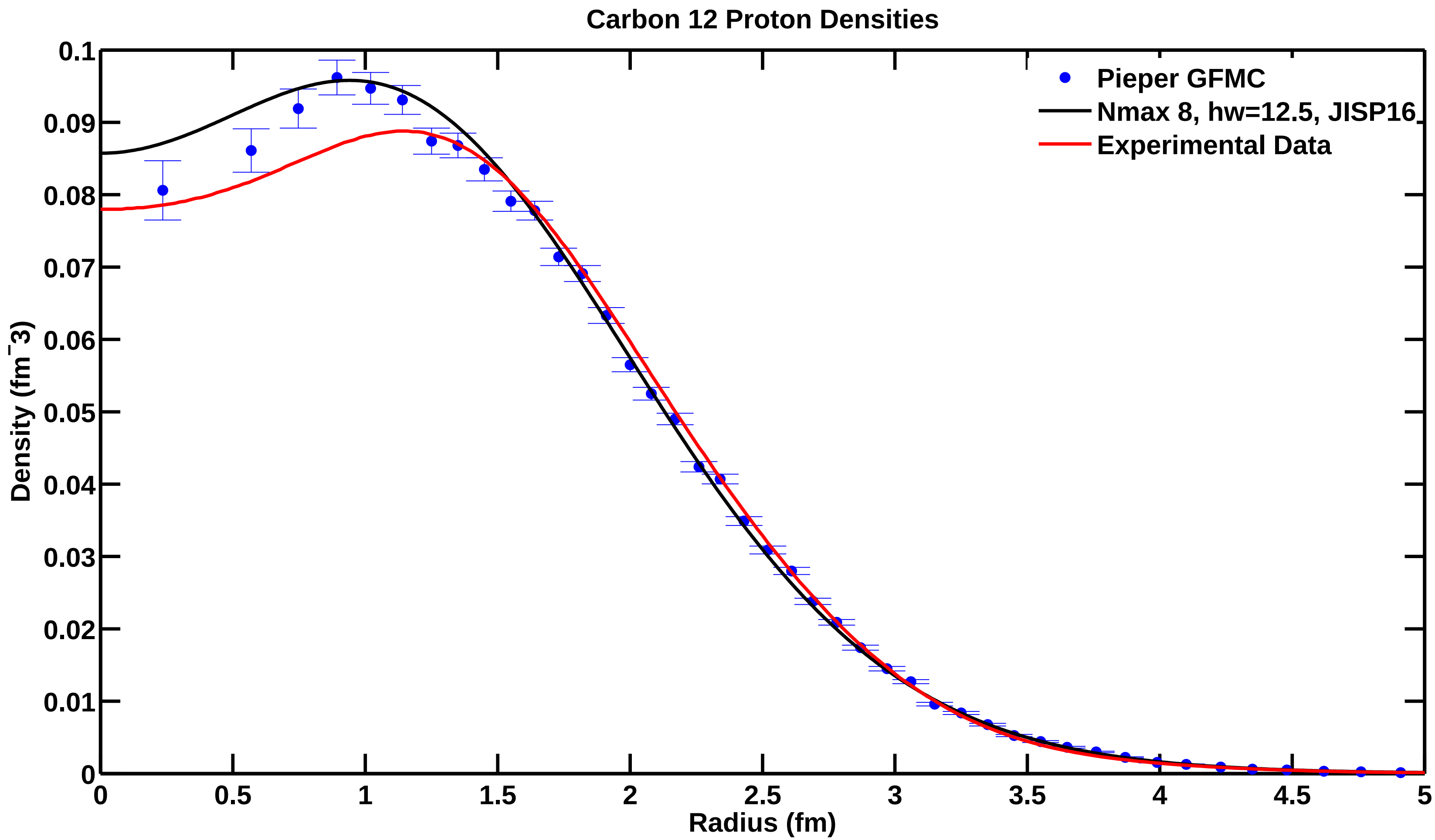
- Calculations for $N_{\text{max}} = 10$ underway (D = 8 billion) using 100,000 cores on JaguarPF (ORNL) under INCITE award

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



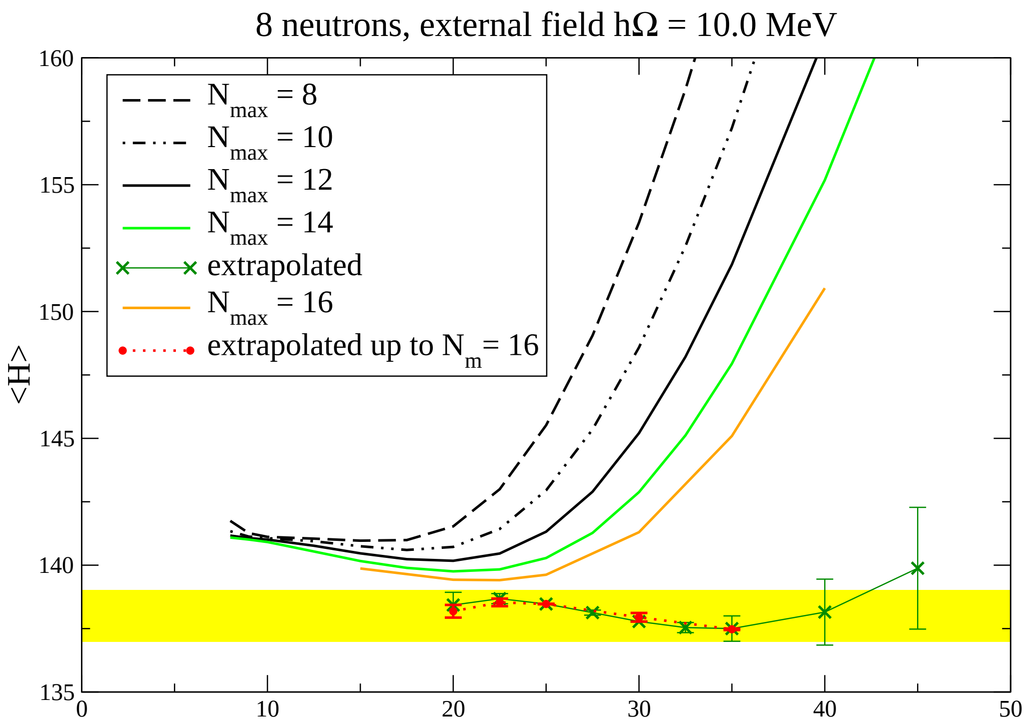
- GFMC: AV18 + IL7, on BlueGene/P using 131,072 cores (INCITE)
  "More scalability, Less pain", Lusk, Pieper, and Butler, SciDAC review 17, 30 (2010)
- JISP16 density at $N_{\text{max}} = 8$, $\hbar\omega = 12.5$ MeV

Validating ab-initio DME/DFT calculations

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

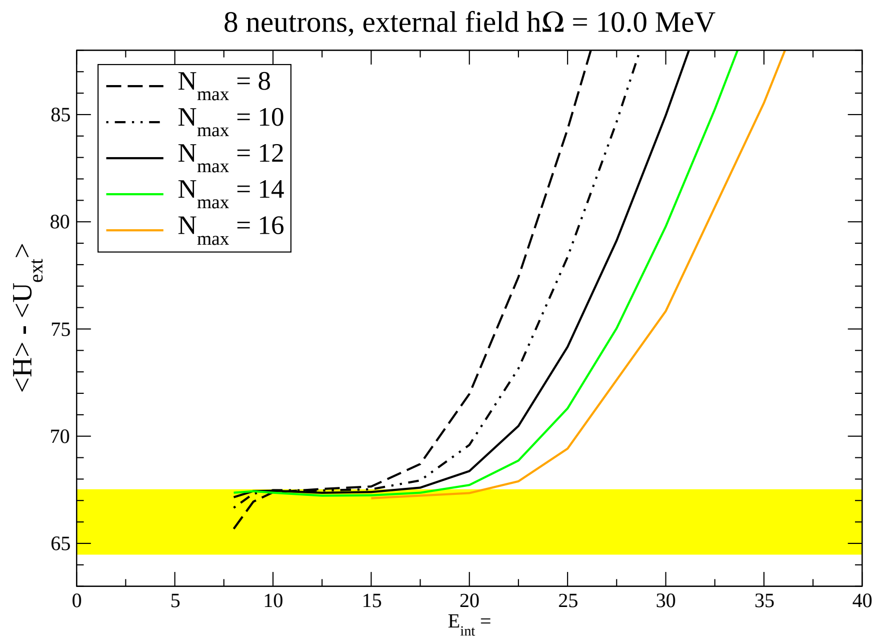
- Simple model for interaction
  - Minnesota potential
- Ab-initio NCFC calculations for neutrons in H.O. potential
  - including numerical error estimates on all 'observables'
- DFT using same NN interaction as NCFC
  - Hartree–Fock
  - Density Matrix Expansion, Hartree–Fock
  - Density Matrix Expansion, 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

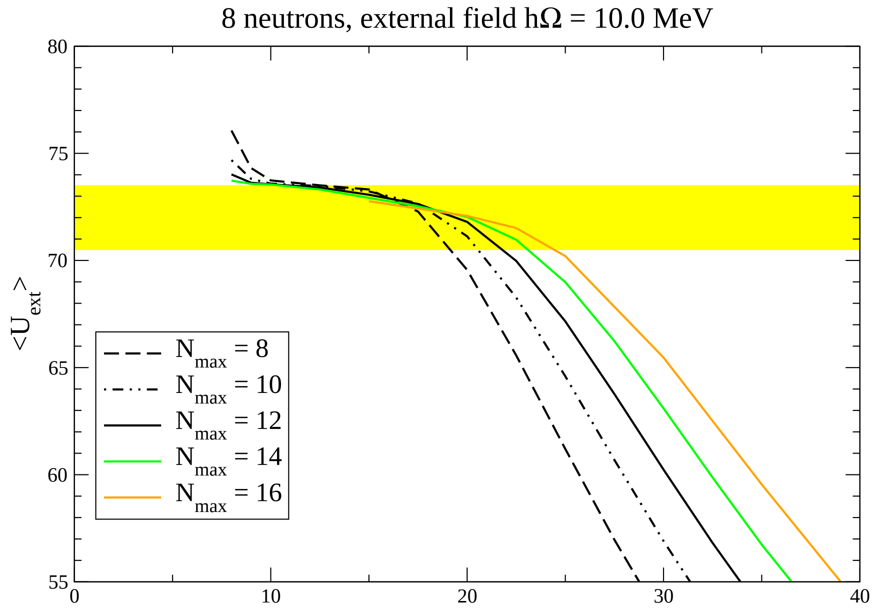
Minnesota potential – total energy



- 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 – external and internal energy

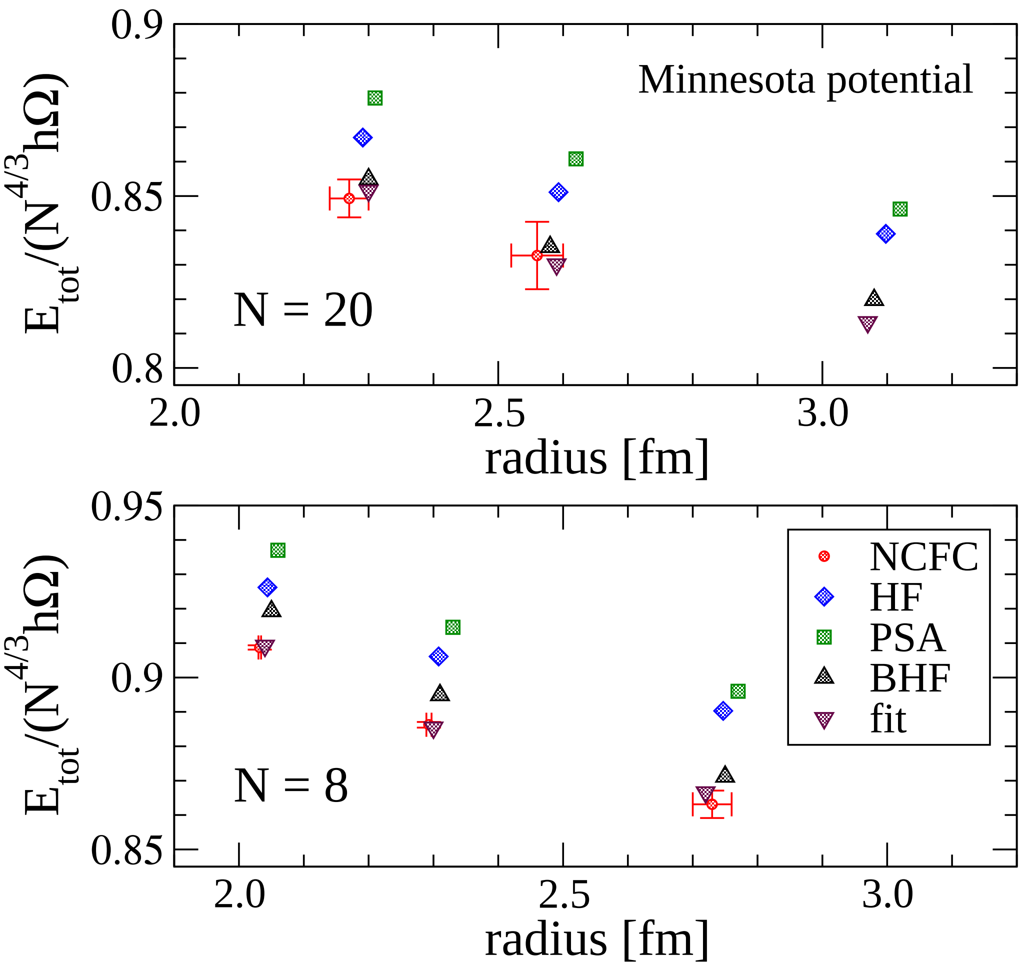




- Neither internal energy nor $\langle U_{\text{ext}} \rangle$ converge monotonically
- Exponential extrapolation not applicable
- Numerical error estimates based on convergence trend
- H.O. external field: radius $\langle r^2 \rangle$ proportional to $\langle U_{\text{ext}} \rangle$

Minnesota potential – Total energy vs. radius

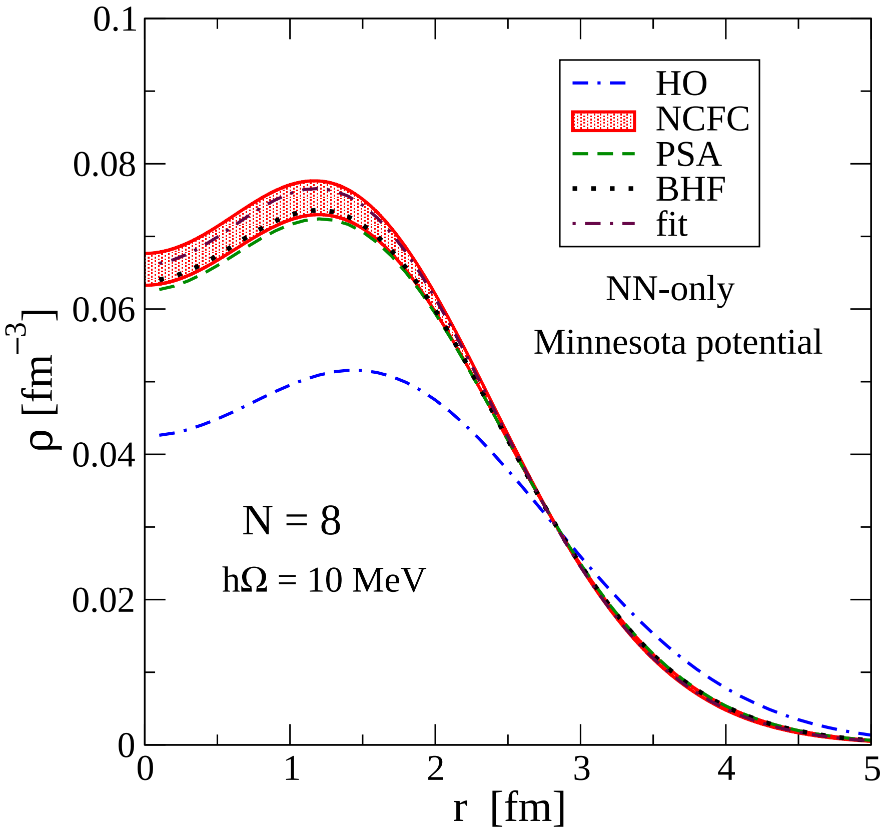
Bogner, Furnstahl, Kortelainen, Maris, Stoistov, Vary, arXiv:1106.3557

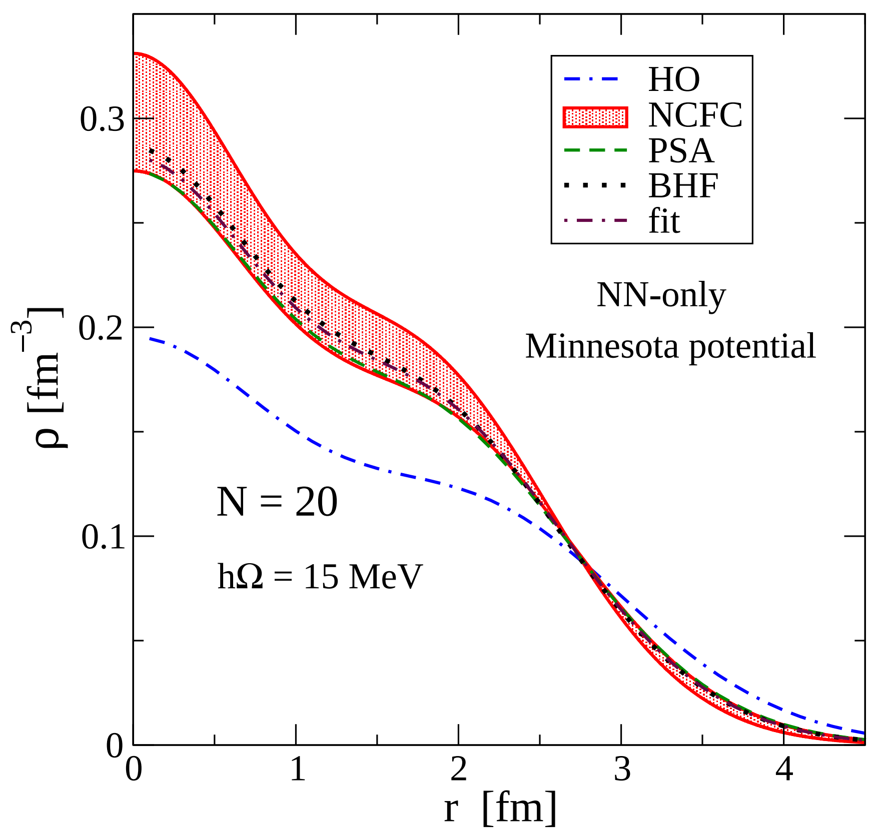


- Neither HF nor DME/PSA HF in agreement with NCFC
- DME BHF close to NCFC
- Fit with volume term and surface term can reproduce NCFC data

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

Physics projects in progress

- Comparison of neutron drop results with different interactions and different methods (w. Joe Carlson, Stefano Gandolfi, Steve Pieper)
- Analysis of convergence behavior and dependence on infrared and ultraviolet cutoffs (w. Sid Coon, Bira van Kolck)
- Evaluation of binding energies, spectra, and select static and transition observables of Be-isotopes w. JISP16
- Evaluation of densities as well as select static and transition observables of narrow states in Li-isotopes w. JISP16 (w. Chase Cockrell, PhD student)
- Evaluation of static and transition one-body density matrices and electroweak amplitudes from the SM and, together, evaluate the ^{12}C$(\nu, \nu')^{12}$C cross section needed for long-baseline neutrino mixing experiments (w. Harry Lee)
- Chiral 2- and 3-body runs for A = 7 through 12 (w. Erik Jurgenson, Petr Navratil, Dick Furnstahl)

More physics projects in progress

- Investigation of realistic basis functions
  - small improvement in convergence of E_{gs} Wood–Saxon basis (Negoita, PhD thesis, journal paper in preparation)
  - flexible radial wavefunction (w. Mark Caprio)
- Ab-initio calculations of level densities at fixed J (w. Esmond Ng, Chao Yang, Hasan Metin Aktulga)
- Ab-initio reactions using J-matrix methods (w. Andrey Shirokov, Sasha Mazur)
- Description of (broad) resonances in finite H.O. basis (w. Andrey Shirokov, Sasha Mazur)
- ^{6}He proton scattering (w. Charlotte Elster and Steve Weppner)
- Benchmarking NC-MCSM (w. Abe, Otsuka, Shimizu, Utsuno)
- Benchmarking SU(3)-based CI code
  - PetaApps, PI Jerry Draayer
  - SU(3)-based CI code: Tomas Dytrych

Ab initio deliverables – to be done

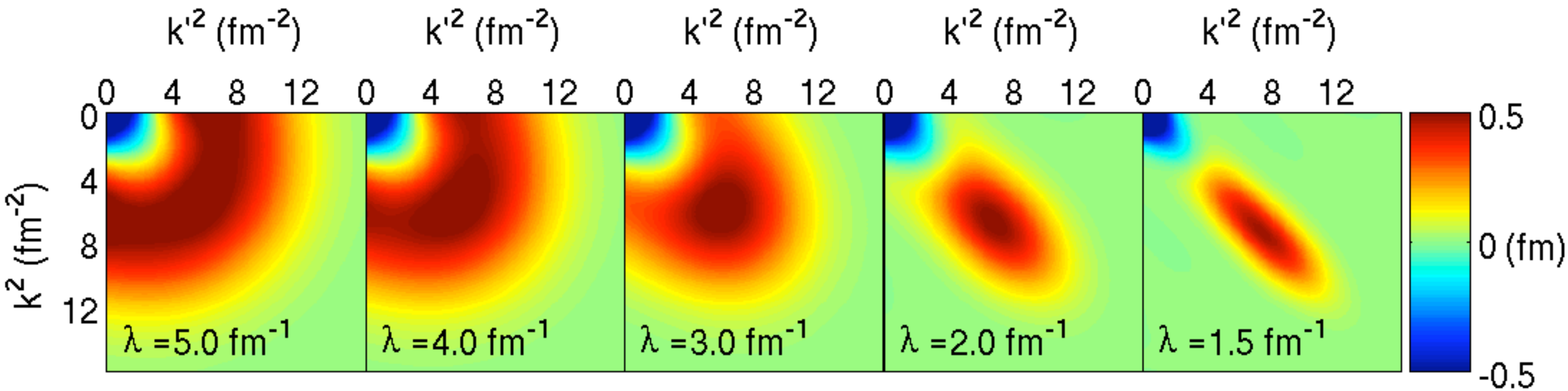
- MFDn Version 13
  - axially deformed HO external fields
  - general spherical (e.g. WS) external fields
  - code documentation, publication of MFDn?
  - integrate python script for MFDn with other scripts
- MFDn – Total-J
  see next talk (Hasan Metin Aktulga)
- Set of neutron properties for DFT/DME communities
  - JISP16, up to about 40 neutrons
    (paper in preparation)
  - additional neutron drop calculations
    (e.g. deformed HO/WS external field,
    SRG-evolved chiral 2- and 3-body forces, . . .)
    as needed/requested
- Set of nuclei in external fields for DFT/DME communities
  - which nuclei, which interactions, which external fields?

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
  - Monte-Carlo Shell Model — Otsuka et al, PPNP47, 319 (2001)
  - No-Core Monte-Carlo Shell Model
    Abe, Maris, Otsuka, Shimizu, Utsuno, Vary, in preparation
    - 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
  - Importance Truncation — Roth, Phys. Rev. C79, 064324 (2009)
    - reduce basis dimension by order of magnitude
    - many-body states single Slater Determinants in M-scheme

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}
  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

Outlook to future work

- Code development in collaboration with CS/AM
  - Investigate alternative eigensolver, block algorithms
  - Database and work-flow management system
    - including upstream and downstream codes
  - MFDn Version 14
    - improve load-balancing and scalability
    - improve single-processor performance
  - MFDn – Total-J
  - Integrate MFDn and SU(3) and Sp(3R) code
  - Four-body interactions
  - Importance truncation
- Physics
  - Explore sd-shell
  - Four-body interactions (induced or 'bare')
  - Reactions