Matrix Computation in Large-Scale Nuclear Structure Calculations

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Collaborators

- LBNL …
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  - James P. Vary

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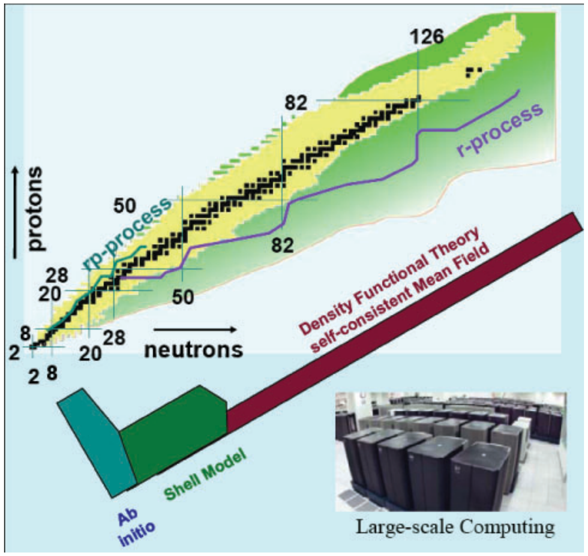
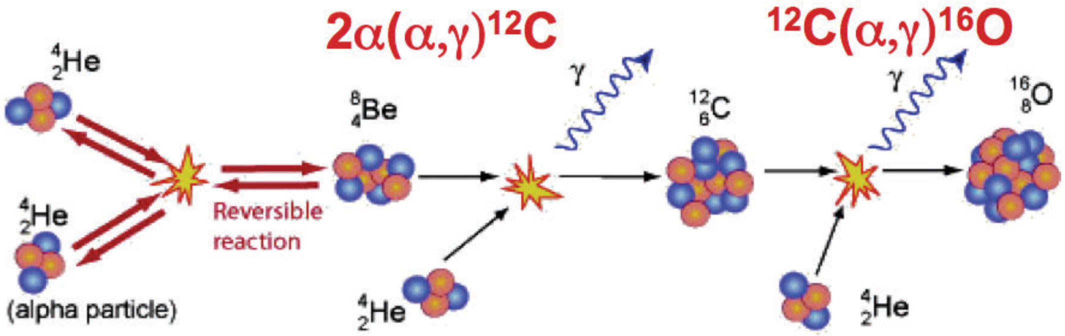
- Calculations done at NERSC and OLCF
  - Part of a nuclear physics INCITE project

Ab initio Nuclear Physics - 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 the fundamental laws of nature?

Ab initio NP - Quantum Many-Body Problem

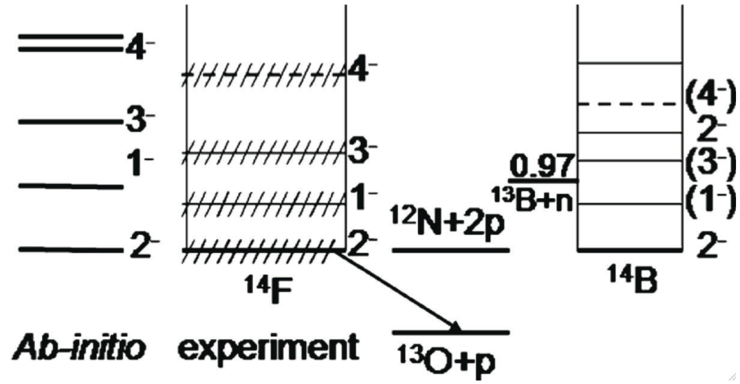
- Eigenvalue problem for wave function $\psi(r_1, \ldots, r_A)$ of A nucleons

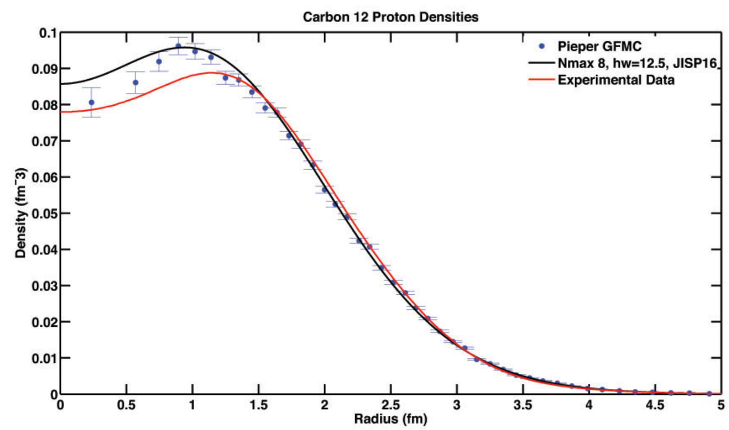
$$\hat{\mathrm{H}}\Psi(r_1,\ldots,r_A) = \lambda\Psi(r_1,\ldots,r_A)$$

with Hamiltonian operator

$$\hat{\mathrm{H}} = \sum_{i<j} \frac{(\vec{p}_i - \vec{p}_j)^2}{2mA} + \sum_{i<j} V_{ij} + \sum_{i<j<k} V_{ijk} + \cdots$$

  - Eigenvalues λ – discrete (quantized) energy levels
  - Eigenvectors: $|\psi(r_1, \ldots, r_A)|^2$ – probability density for finding nucleons 1, …, A at $r_1, \ldots, r_A$.





Ab initio NP – Computational Challenges

- Self-bound quantum many-body problem, with 3*A* 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

Configuration Interaction Methods

- Expand wave function in basis states $\left|\Psi\right\rangle = \sum a_i \left|\psi_i\right\rangle$
- Express Hamiltonian in basis $\left\langle \psi_j \middle| \hat{\mathrm{H}} \middle| \psi_i \right\rangle = H_{ij}$
- Diagonalize Hamiltonian matrix H_{ij}
- Complete basis $\rightarrow$ 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 & corresponding eigenvectors

CI Methods - Basis Space Expansion

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

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

  takes care of anti-symmetrization of nucleons (Fermi-statistics)

- Single-particle basis states
  - eigenstates of SU(2) operators $\hat{L}^2,\hat{S}^2,\hat{J}^2=(\hat{L}+\hat{S})^2,\hat{J}_z$ with quantum numbers $|n,l,s,j,m>$
  - radial wavefunctions: Harmonic Oscillator; Wood--Saxon basis (Negoita, PhD thesis 2010); Gamov, Sturmian, …

CI Methods - Basis Space Expansion

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

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

    - single run gives spectrum
    - Alternatives:
      - LS scheme, Coupled-J scheme, Symplectic basis, …
  - $N_{\max}$ truncation

$$\sum_{k=1}^{A} (2n_{ik} + l_{ik}) \le N_0 + N_{\max}$$

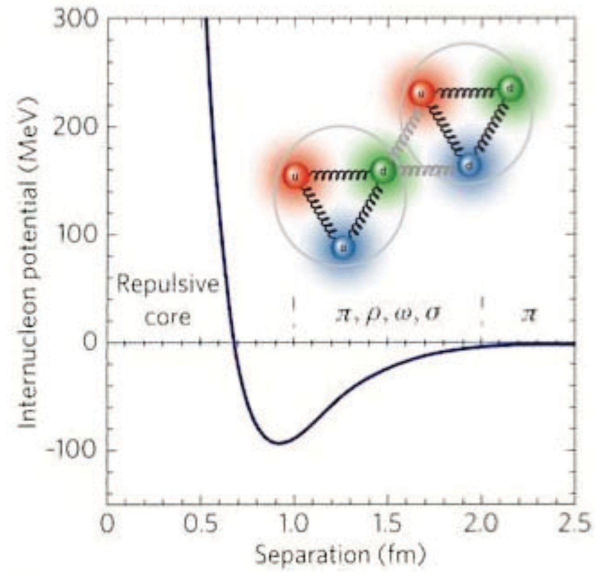
    - alternatives: Monte-Carlo No-Core Shell Model, Importance Truncation, FCI (truncation on single-particle basis only), …

CI Methods - Basis Space Expansion

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

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

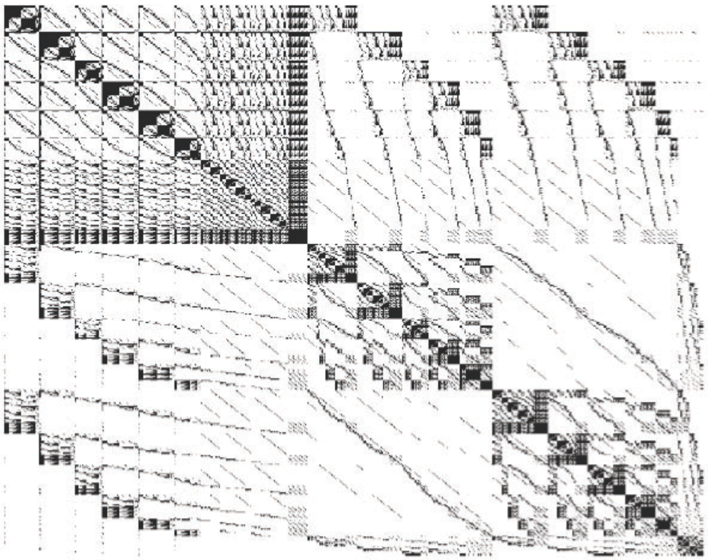
- Pick your favorite potential
  - Argonne potentials: AV8, AV18 (plus Illinois NNN interactions)
  - Bonn potentials
  - Chiral NN interactions (plus chiral NNN interactior
  - …
  - JISP16 (phenomenological nonlocal NN potential)
  - …
  - Obtain from lattice QCD?



CI Methods – Basis Space Expansion

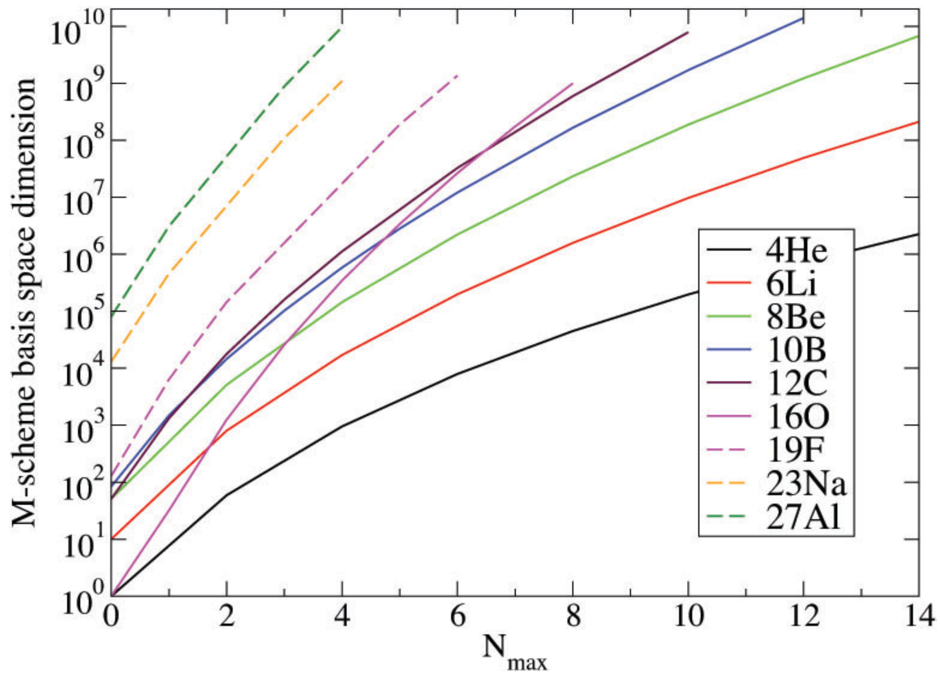
- Expand wave function in basis states $\left|\Psi\right\rangle = \sum a_i \left|\psi_i\right\rangle$
- Express Hamiltonian in basis $\left\langle\psi_j\right|\hat{\mathrm{H}}\left|\psi_i\right\rangle = H_{ij}$
  - large sparse symmetric matrix

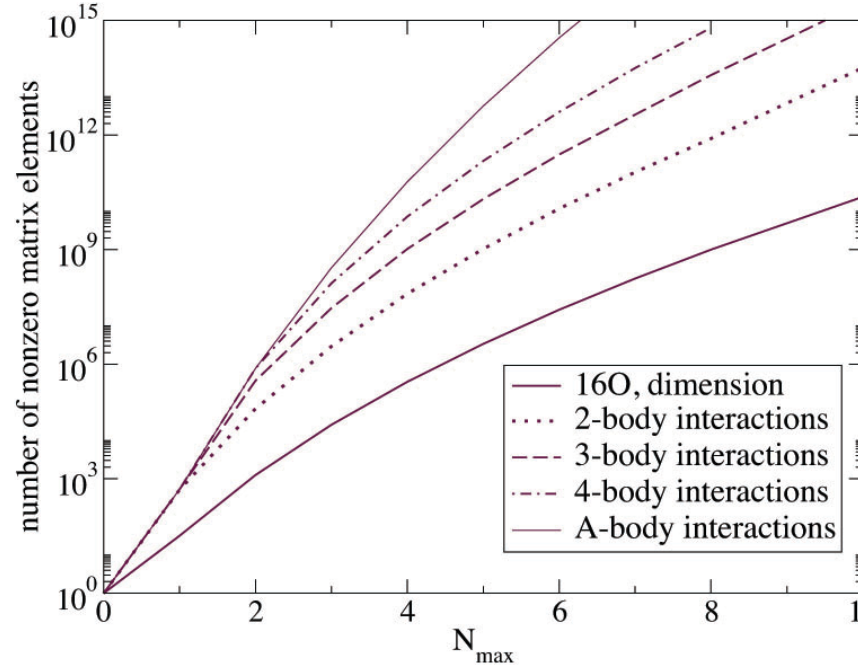
Sparsity Structure for ^{6}Li



- 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 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
- ❑ Extrapolation to infinite basis requires $N_{max} \geq 8$

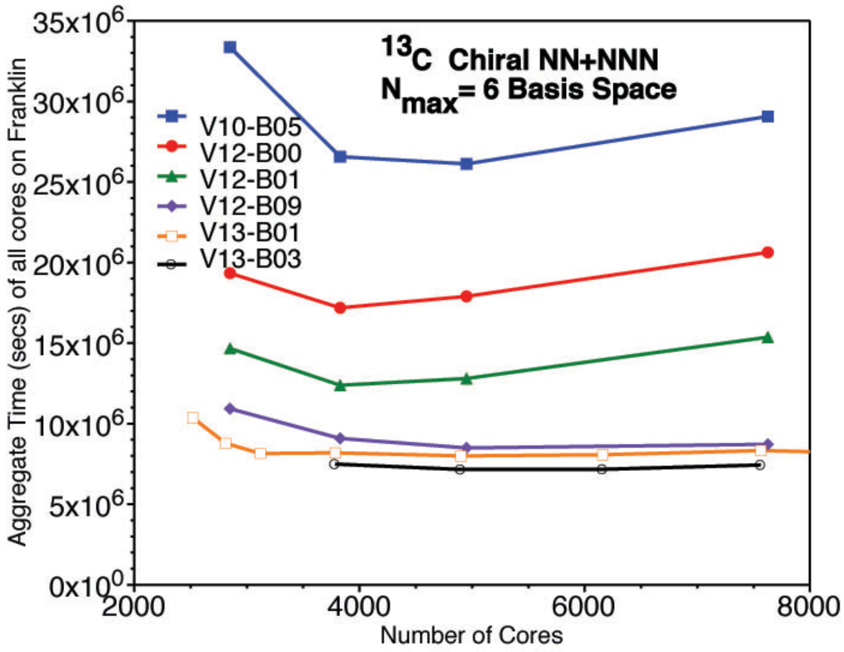
CI Calculations and High Performance Computing

- Hardware
  - individual desktops and laptops
  - local linux clusters
  - DOE NERSC Center at LBNL
    - 17,000,000 CPU hours (ISU collaboration)
  - DOE Leadership Computing Facilities
    - INCITE award - Computational Nuclear Structure (PI: J. Vary, ISU)
    - 20,000,000 CPU hours on Cray XT5 at ORNL
    - grand challenge award at Livermore (Jurgenson, 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

MFDn Performance Over Past 4 Years

- updated from Sternberg, Ng, Yang, Maris, Vary, Sosonkina, Le, "Accelerating Configuration Interaction calculations for nuclear structure", presented at SC08.

  - ^{13}C chiral N3LOc 2- and 3-body interactions
  - Dimension 38×10^6
  - # nonzero m.e. 56×10^{10}
  - memory for matrix: 5 TB
  - size input 3 GB
  - Version 13-B03: hybrid MPI and OpenMP (Jan. 2011)



Total-J Computation

- Sometimes it is necessary to compute the eigenstates of the nuclear Hamiltonian matrix for a specific angular momentum (J).
  - E.g., investigating nuclear level densities or evaluating scattering amplitudes

- A possible solution is to compute a large number of eigenpairs. Then determine with eigenpairs correspond to the desirable J value.
  - Expensive … because of the cost computing a large number of eigenpairs with the knowledge that some of them will be discarded anyway.

- A better approach is needed.
  - Want to project the problem into a smaller subspace that captures the same information.
  - Solve the smaller problem to extract the projected eigenvectors.
  - Then extract the corresponding eigenvectors of the original Hamiltonian.

Total-J Computation

- Question: How to find the appropriate subspace?

- Useful to consider the total angular moment squared operator K, which has the property that $HK = KH$.
- For a fixed J value, $\lambda = J(J+1)$ is an eigenvalue of K.
- If Z is an invariant subspace associated with λ, then it is also invariant under H.
- Eigenvalues of $G = Z^T HZ$ are also eigenvalues of H, associated with a specific J.
- If V contains the eigenvectors of G, then ZV contains the desired eigenvectors of H.

- The problem is to compute the eigenvectors of K corresponding to the eigenvalue $\lambda = J(J+1)$.

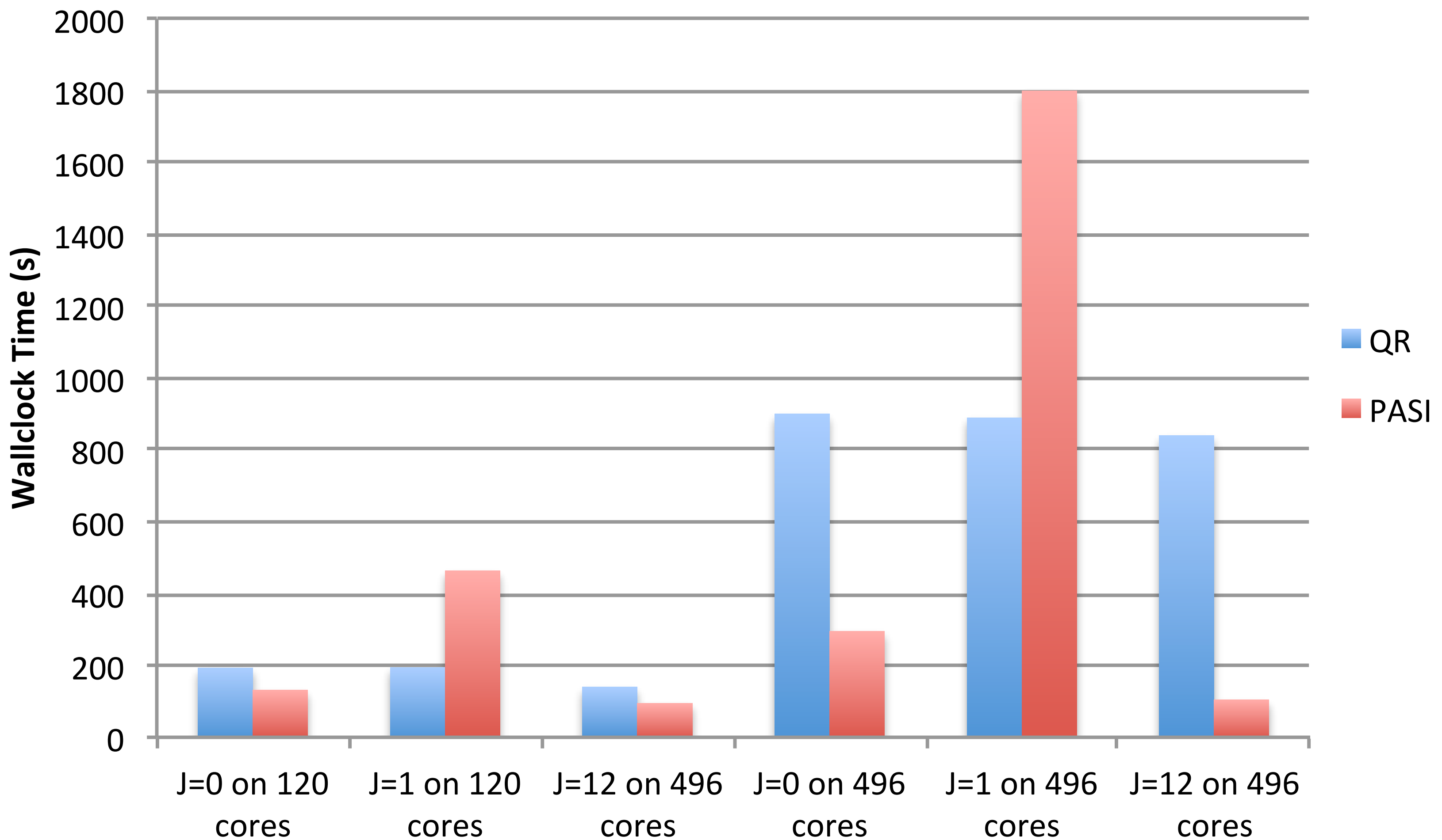
Total-J Computation

- Computing the eigenvectors of K …
  - Bad news: K is as large as the Hamiltonian H.
  - Good news: K can be "organized" so that it has a nice block diagonal structure.
    - Z also has a block "diagonal" form.

- Have investigated 3 ways to compute the eigevectors of K …
  - Shift-invert Lanczos applied to $(K - a\, I)^{-1}$, where a is close to J(J+1).
  - QR factorization applied to $(K - \lambda\, I)$.
  - Polynomial accelerated subspace iteration: apply Lanczos to $p(K)$, where $p(\omega)$ is a polynomial that assumes a max value at $\omega = \lambda$ and much smaller values elsewhere.

Some Numerical Results

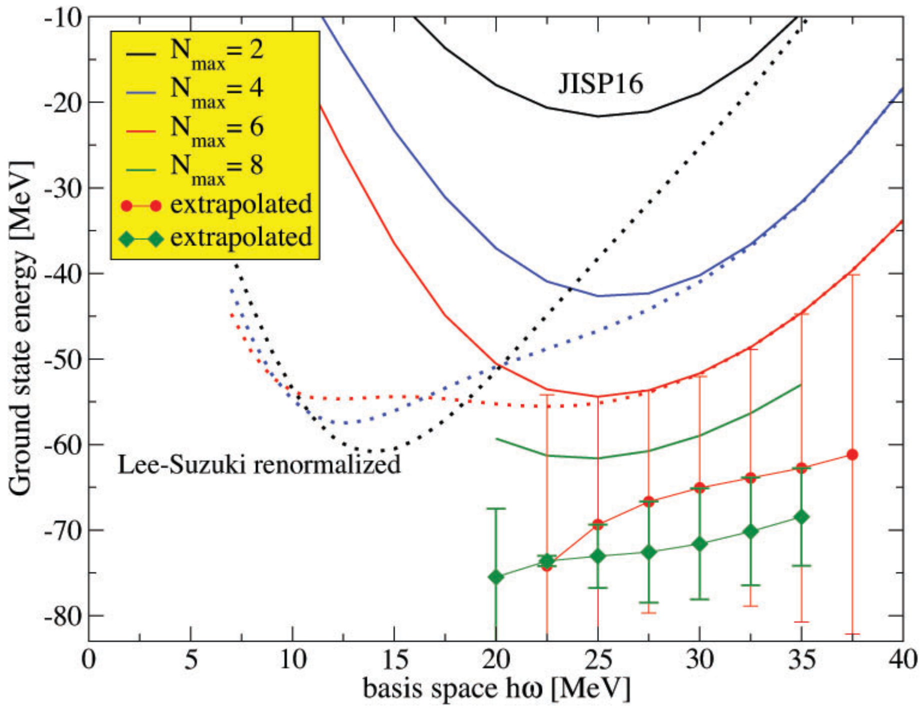
- Comparing QR and polynomial subspace iteration



Scientific Discovery - Unstable Nucleus ^{14}F

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

  - Dimension 2×10^9
  - # nonzero m.e. 2×10^{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 14B: 86 ± 4 MeV agrees with experiment 85.423 MeV

Predictions for ^{14}F Confirmed by Experiments

Theory published PRC: Feb. 4, 2010

Physics Letters B 692 (2010) 307–311

Contents lists available at ScienceDirect

Physics Letters B

www.elsevier.com/locate/physletb

Experiment published: Aug. 3, 2010

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

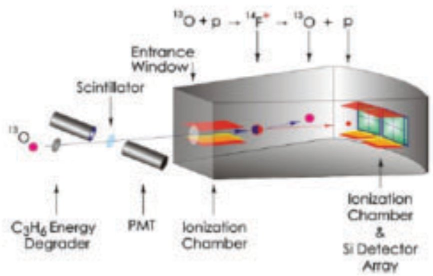


Fig. 1. (Color online.) The setup for the ^{14}F experiment. The "gray box" is the scattering chamber. See explanation in the text.

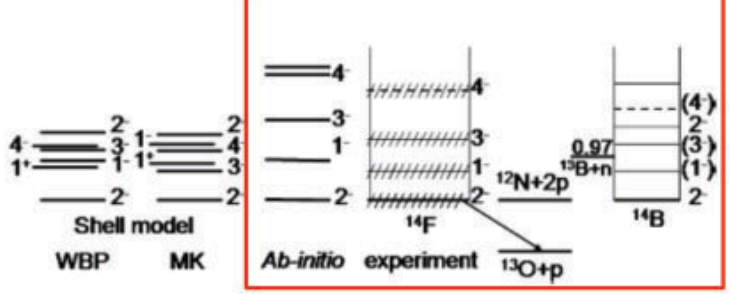


Fig. 6. ^{14}F level scheme from this work compared with shell-model calculations, ab-initio calculations [3] and the ^{14}B level scheme [16]. The shell model calculations were performed with the WBP [21] and MK [22] residual interactions using the code COSMO [23].

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

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

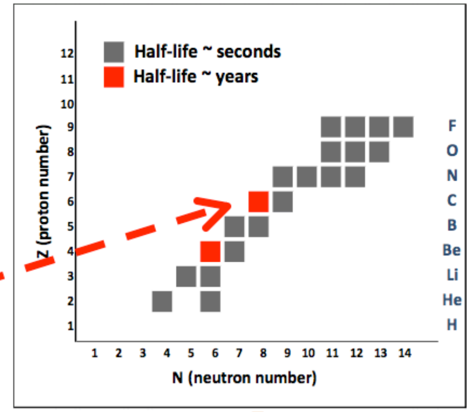
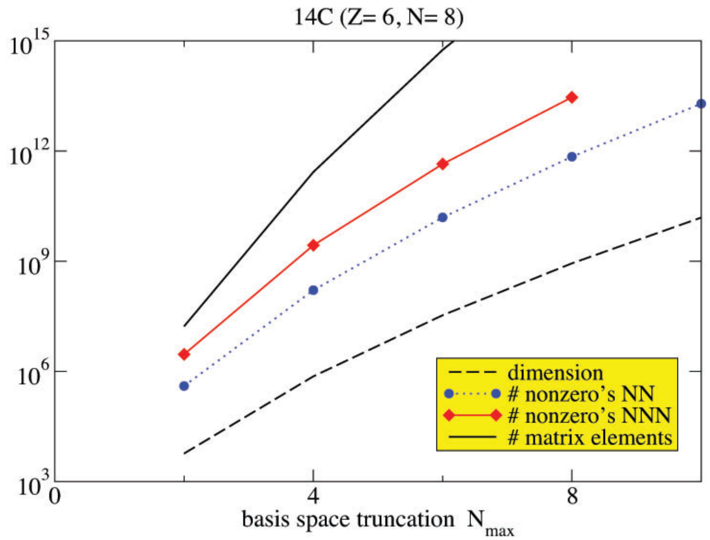


Chart of light nuclei that decay via beta emissions

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

- compare e.g. *β* decay $^6He(0^+) \rightarrow {}^6Li(1^+)$
  - half-life $\tau_{1/2}$ = 806.7 ± 1.5 msec
  - Gamow-Teller transition B(GT) = 4.71
  - good agreement between ab-initio calculations and experiment
    - Vaintraub, Barnea, Gazit, arXiv:0903.1048 [nucl-th]

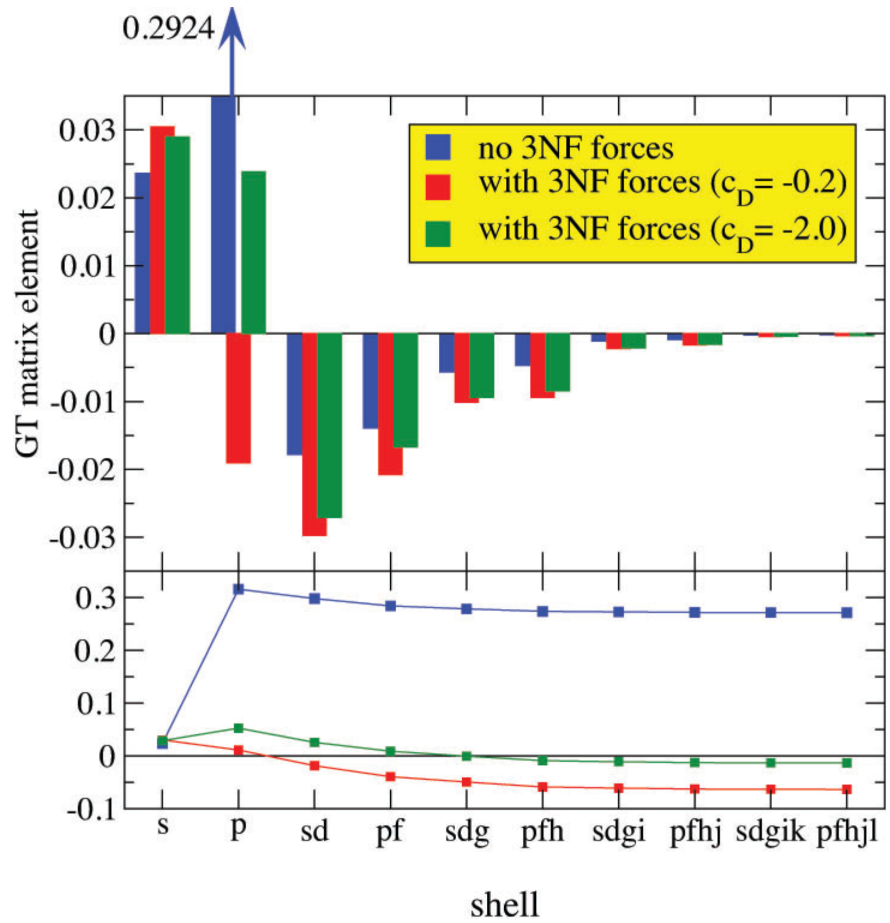
Ab initio Structure of ^{14}C - Role of 3-body Forces



- 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

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)



Concluding Remarks

- We have worked with nuclear physicists to improve their nuclear structure calculation code, which enables them to do calculations that they were not able to do previously.
  - Subsequently used the code to make scientific discoveries
- More to do …
  - Algorithmic improvements
  - New methodologies
  - Scalability
  - New physics – heavier nuclei
- Main challenge: large-scale matrix computation
  - Particularly solution of large sparse eigenvalue problems
  - Opportunities to collaborate nuclear physicists

Concluding Remarks

- Other Applications involving linear algebra problems
  - Nonlinear eigenvalue problems in accelerator modeling, materials sciences, chemical sciences, …
  - AMR, linear solvers, nonlinear solvers in land-ice modeling
  - Linear solvers in fusion sciences, earth sciences, …

- More other applications …
  - Power network simulation
  - Extreme climate events
  - Image analysis (in biological sciences)
  - Cybersecurity