

CI approach to complex nuclei and level densities

M. Horoi

with Z. Gao and M. Scott

Department of Physics, Central Michigan University,
Mount Pleasant, Michigan 48859

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1. The main accomplishments since the last meeting
2. Aspects of your science that require high-performance computing
3. Roadmap for the remaining part of Year-3 and Year-4. Sketch of the workplan for Year 5

Publications since the last meeting

- "Angular momentum projected configuration interaction with realistic Hamiltonians,"
Z.-C. Gao and M. Horoi, Phys. Rev. C **79**, 014311 (2009).
- "Parity Dependent Shell Model Level Densities for Nuclear Astrophysics,"
M. Scott and M. Horoi, Proceedings of Science, PoS(NIC-X) 132, 1 (2008).
- "Improved basis selection for the Projected Configuration Interaction method applied to heavy nuclei", Zao-Chun Gao, Mihai Horoi, Y. S. Chen, arXiv:0906.3756.
- "Gamow-Teller transitions to ^{64}Cu measured using the $^{64}\text{Zn}(t,3\text{-He})$ reaction",
G.W. Hitt, R.G.T. Zegers, Sam M. Austin, D. Bazin, A. Gade, D. Galaviz, C.J. Guess,
M. Horoi, M.E. Howard, Y. Shimbara, E.E. Smith, C. Tur, arXiv:0904.3645.
- "Finite Range Gaussian Corrections for Spin- and Parity-Dependent Shell Model Level Density", M. Scott and M. Horoi, in preparation.

Talks since the last meeting

- *Comparison of Nuclear Configuration Interaction Calculations and Coupled Cluster Calculations*, **M. Horoi**, invited talk at the International Symposium on "50 Years of Coupled Cluster Theory", INT Seattle, June 30 - July 2, 2008.
- *Accurate description of the spin- and parity-dependent nuclear level densities*, **M. Horoi**, invited talk at the International Workshop on Statistical Nuclear Physics and its Applications in Astrophysics and Technology, Ohio University, Athens OH, 8-11 July 2008.
- *Parity Dependent Shell Model Level Densities for Nuclear Astrophysics*, International Symposium on Nuclear Astrophysics Nuclei in the Cosmos - IX, Mackinac Island, July 25 - August 1, 2008, **M. Scott** and M. Horoi.
- *New Approaches to Configuration Interaction*, **M. Horoi**, Hokudai-TORIJIN-JUSTIPEN-EFES workshop & JUSTIPEN-EFES-Hokudai-UNEDF meeting, July 21-25, 2008, Hokkaido, Japan.
- *Accurate Nuclear Level Densities for Nuclear Reactions*, **M. Horoi**, Hokudai-TORIJIN-JUSTIPEN-EFES workshop & JUSTIPEN-EFES-Hokudai-UNEDF meeting, July 21-25, 2008, Hokkaido, Japan.
- *Nuclear structure input for nuclear reactions*, **M. Horoi**, International Conference on Interfacing Structure and Reactions at the Center of the Atom, December 1-5, 2008, Queenstown, New Zealand.
- *The Many Facets of the Nuclear CI*, **M. Horoi**, at the UNEDF workshop on Leadership Class CI Codes, San Diego State University, March 11-14, 2009.

M. Horoi et al. :

PRC **67**, 054309 (2003),

PRC **69**, 041307(R) (2004),

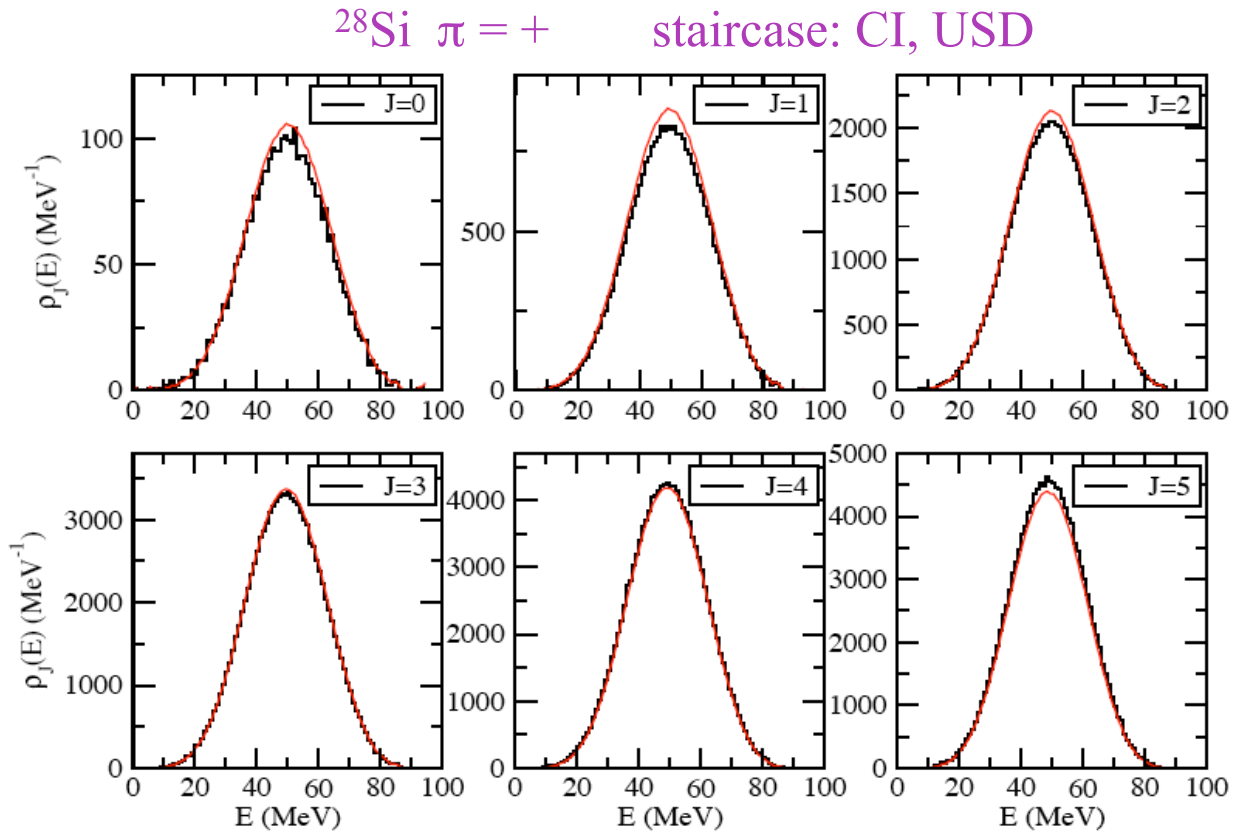
NPA **785**, 142 (2005).

PRL **98**, 265503 (2007)

Configurations: e.g. 8 particles in fp_{g9}

f5	p3	p1	g9	π
8	0	0	0	+
7	1	0	0	+
7	0	0	1	-

preserve rotational invariance and parity



$$\rho(E_x, J, \pi) = \sum_{c \in \text{conf}} D_c(J, \pi) G_{FR}(E, E_c(J), \sigma_c(J))$$

$$E_c(J), \sigma_c(J) \leftarrow \text{Tr}_{SD_c} \langle M | H^q | M \rangle_{SD_c}$$

$$E_x = E - E_{g.s.}$$

$E_c(J), \sigma_c(J)$: computational intensive

$E_{g.s.}$ from CI, PCI, Exponential Convergence Method (PRL **82**, 2064 (1999)), CC, etc.

Configurations can be calculated in parallel by JMOM code

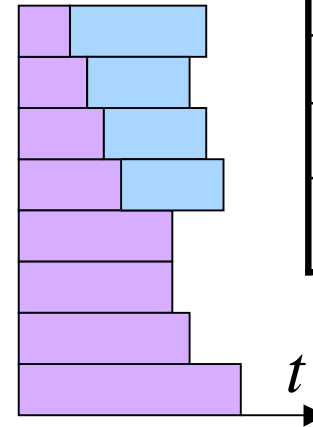
Scaling of the MPI JMOM Code

Domain decomposition: many-body configurations

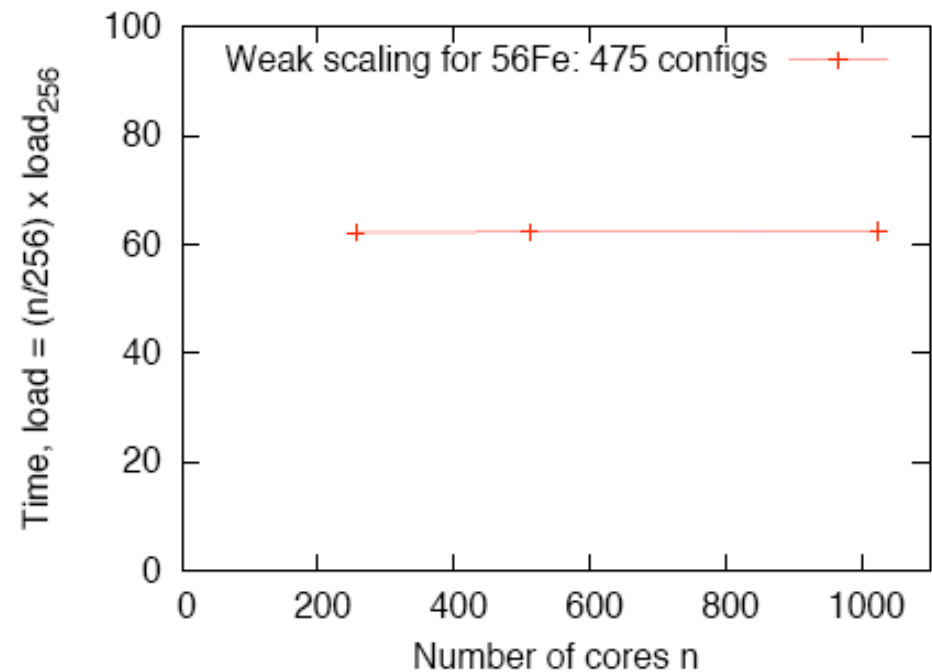
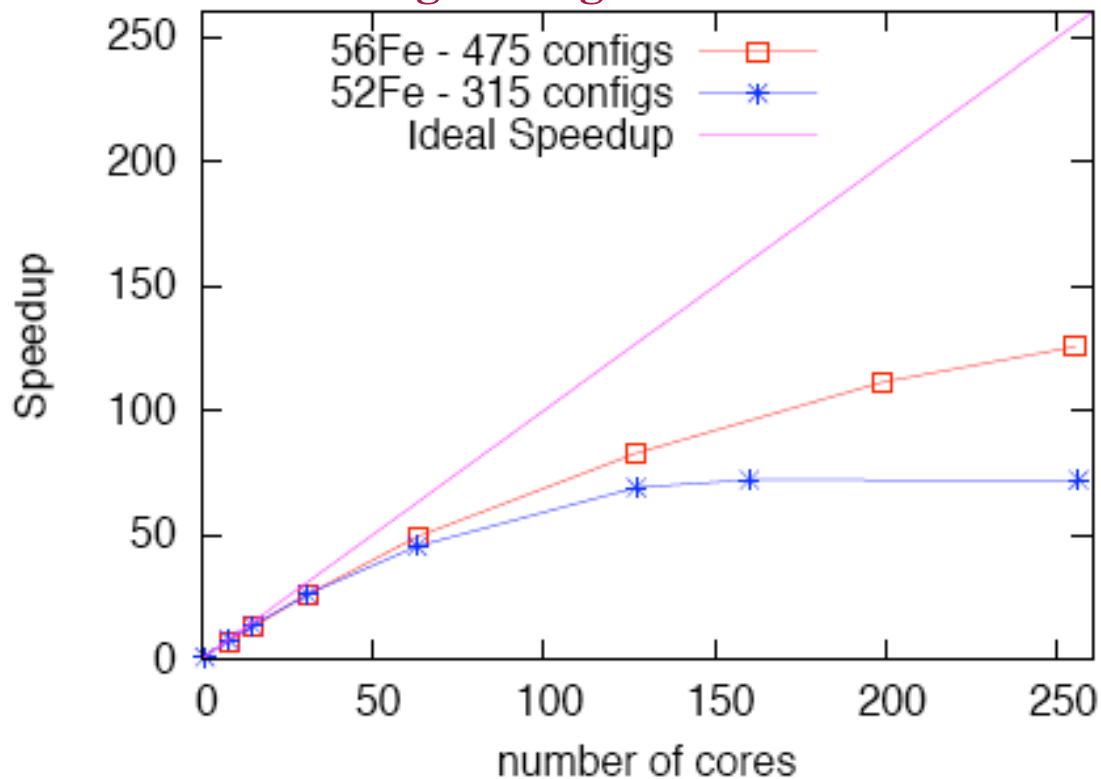
Algorithm: Dynamical Load Balancing

Machine: Franklin/NERSC

Nucleus / model space	Isospin configs	PN - configs
52Fe/pf	315	22028
56Fe/pf	475	51174
64Ge/pfg9/2	3749	2176544

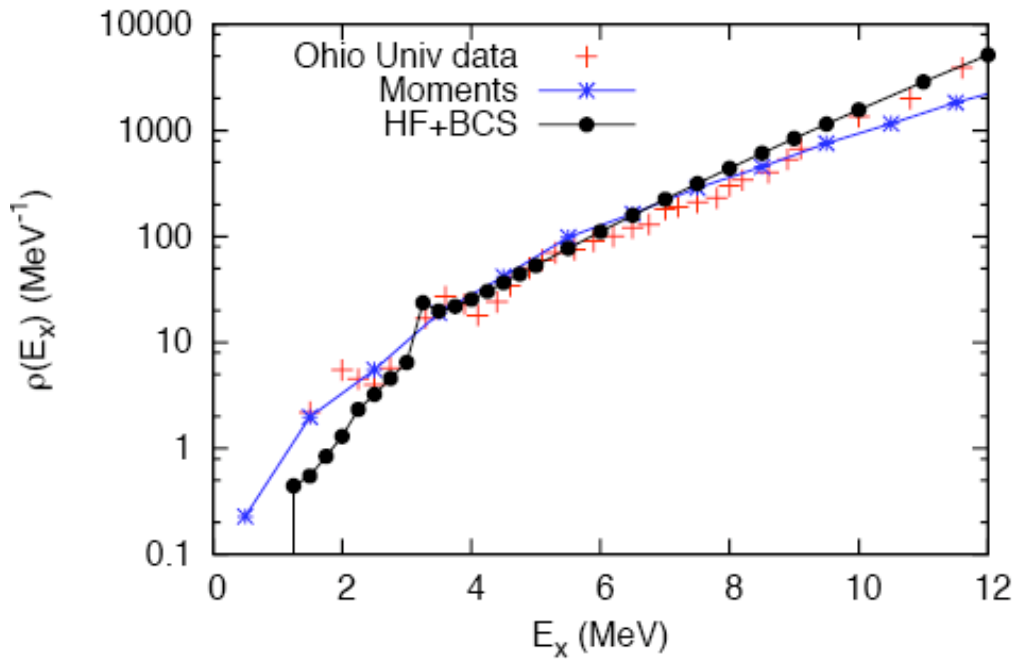


Strong scaling

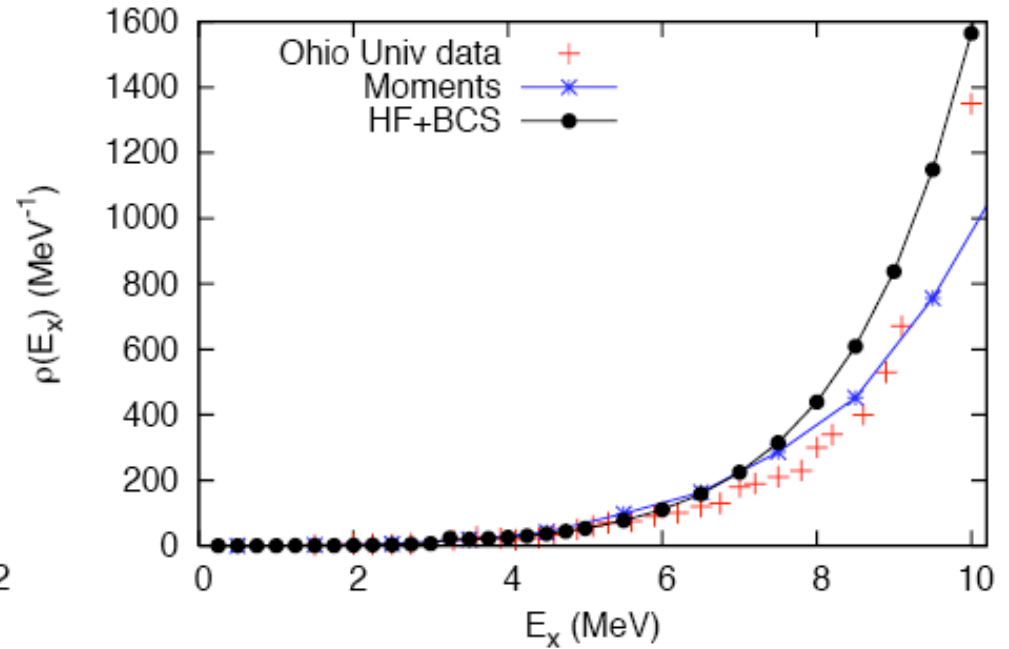


NLD of ^{56}Fe : CI, Moments, HF+BCS

Level density: ^{56}Fe



Level density: ^{56}Fe



Ohio data: PRC **74**, 014314 (2006)

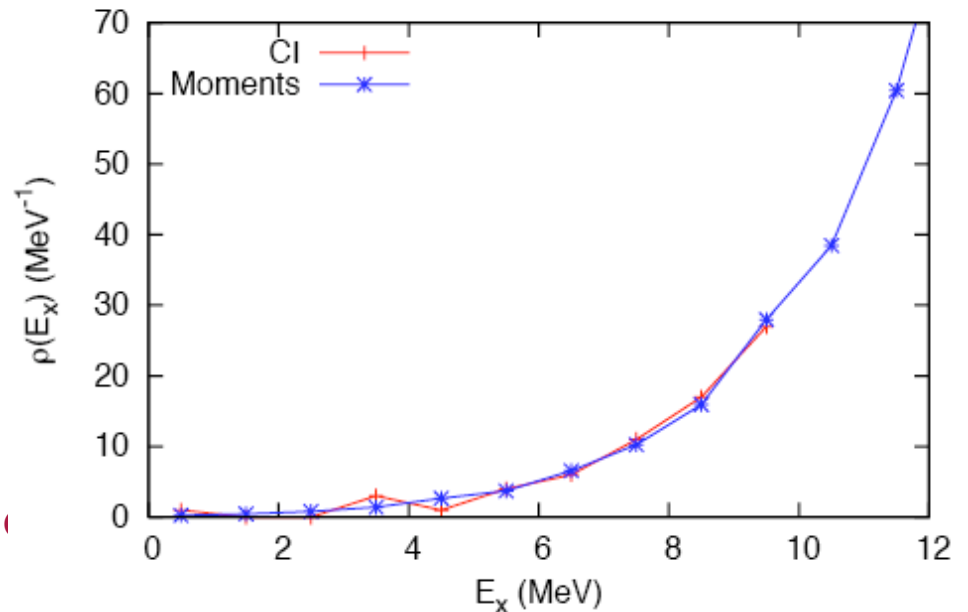
HF+BCS: $\rho_{HF+BCS}(U)$

- Demetriou and Goriely, Nucl. Phys. **A695** (2001) 95.
- <http://www-astro.ulb.ac.be/Html/nld.html>

HFB+Combinatorial: $\rho(E_x, J, \pi)$

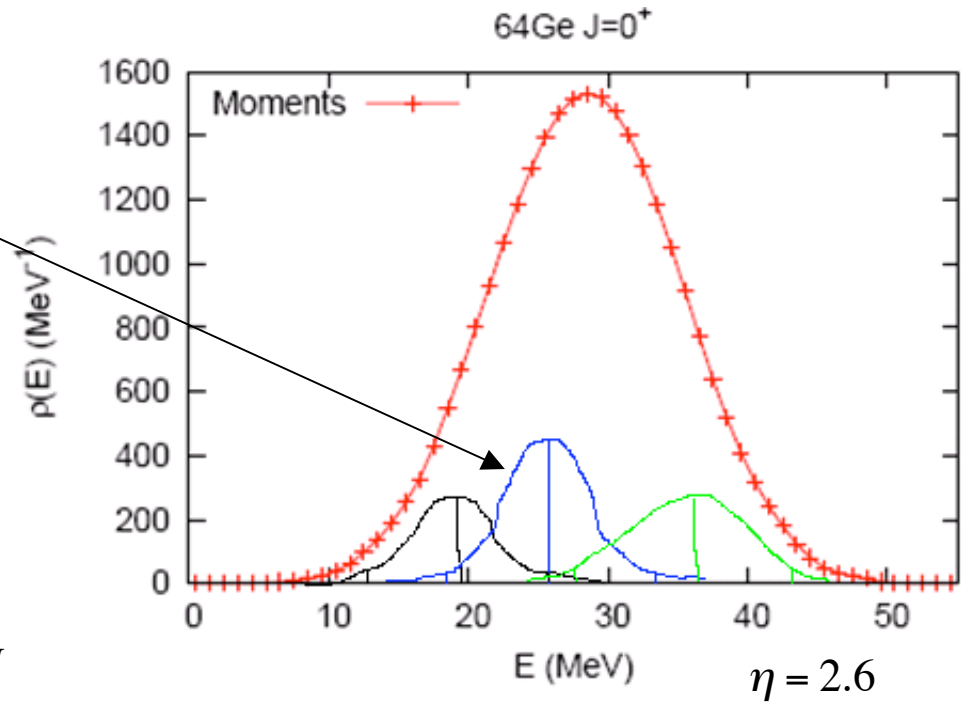
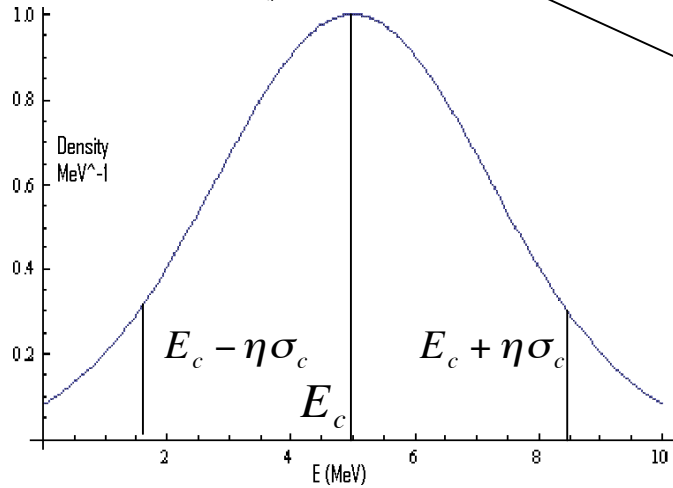
- S. Hilaire and S. Goriely, Nucl. Phys. **A779** (2006) 63
- http://www-astro.ulb.ac.be/Html/nld_comb.html

Level density: $^{56}\text{Fe}, J=0$

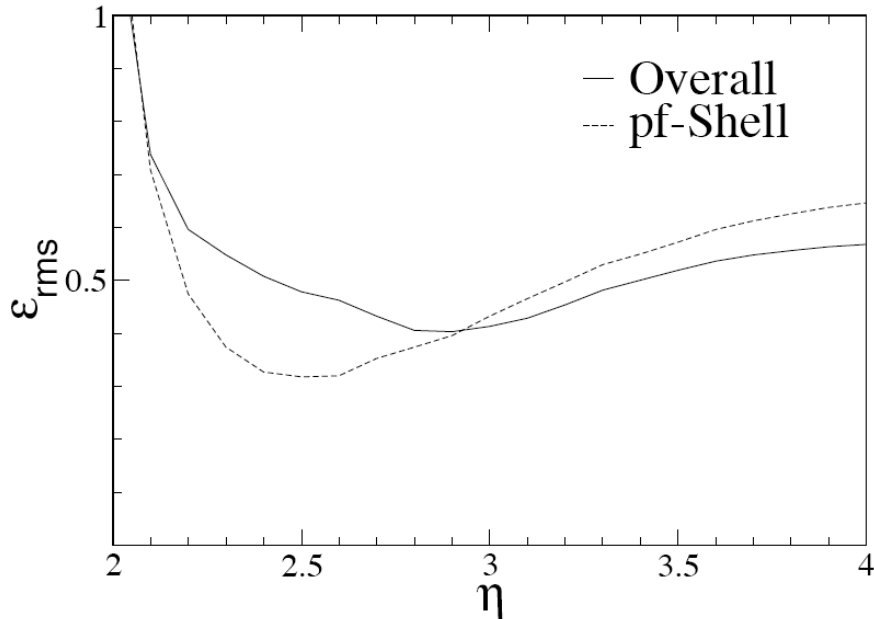


Study of Errors

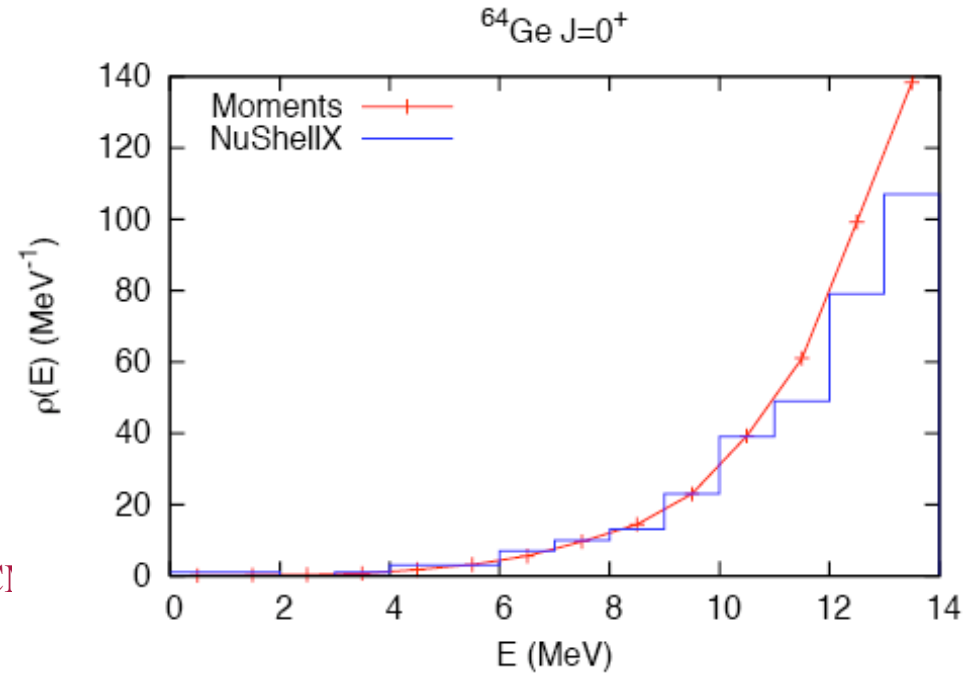
$$\rho(E_x, J, \pi) = \sum_{c \in \text{conf}} D_c(J, \pi) G_{FR}(E, E_c(J), \sigma_c(J))$$



$$\epsilon_{rms} = \exp \left[\sqrt{\frac{1}{N} \sum_i \left(\ln \frac{\rho_i^{MOM}}{\rho_i^{CI}} \right)^2} \right] - 1 \quad \text{error relative to CI}$$



M. Horoi CI



Improved PCI basis selection

General Structure of PCI basis
(Basis states are deformed Slater determinants)

Choice of $|\kappa_i, 0\rangle$

Main Idea: Minimize S_n

$$S_n = \sum_{i=1}^n \lambda_i$$

$$Ax_i = \lambda_i Bx_i$$

$$\mathbf{A} = \begin{pmatrix} H_{11} & H_{12} & \dots & H_{1n} \\ H_{21} & H_{22} & \dots & H_{2n} \\ \dots & \dots & \dots & \dots \\ H_{n1} & H_{n2} & \dots & H_{nn} \end{pmatrix}, \mathbf{B} = \begin{pmatrix} N_{11} & N_{12} & \dots & N_{1n} \\ N_{21} & N_{22} & \dots & N_{2n} \\ \dots & \dots & \dots & \dots \\ N_{n1} & N_{n2} & \dots & N_{nn} \end{pmatrix}$$

$$H_{ij} = \langle i | HP_{MK}^I | j \rangle \quad N_{ij} = \langle i | P_{MK}^I | j \rangle$$

$$|i\rangle = |\kappa_i, 0\rangle \quad |j\rangle = |\kappa_j, 0\rangle$$

$$\left\{ \begin{array}{ll} 0p - 0h, & np - nh \\ |\kappa_1, 0\rangle, & |\kappa_1, j\rangle, \dots, \\ |\kappa_2, 0\rangle, & |\kappa_2, j\rangle, \dots, \\ \dots & \dots \\ |\kappa_N, 0\rangle, & |\kappa_N, j\rangle, \dots \end{array} \right\}$$

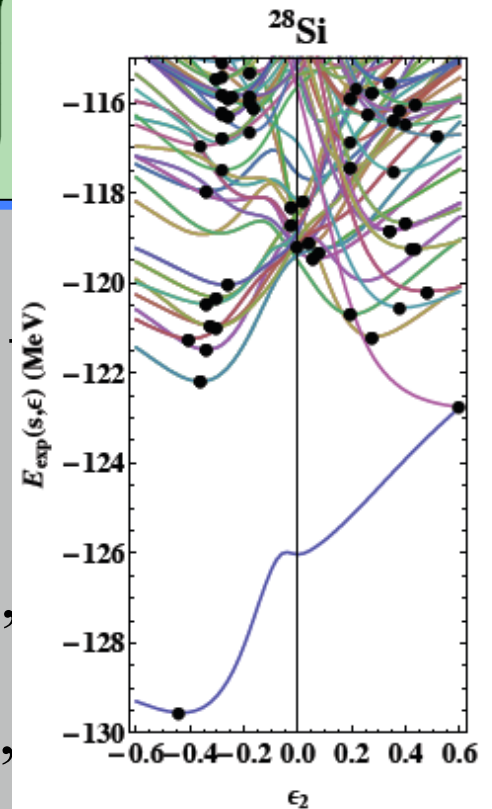
Choice of $|\kappa_i, j\rangle$

$$\Delta E = \frac{1}{2} (E_0 - E_j)$$

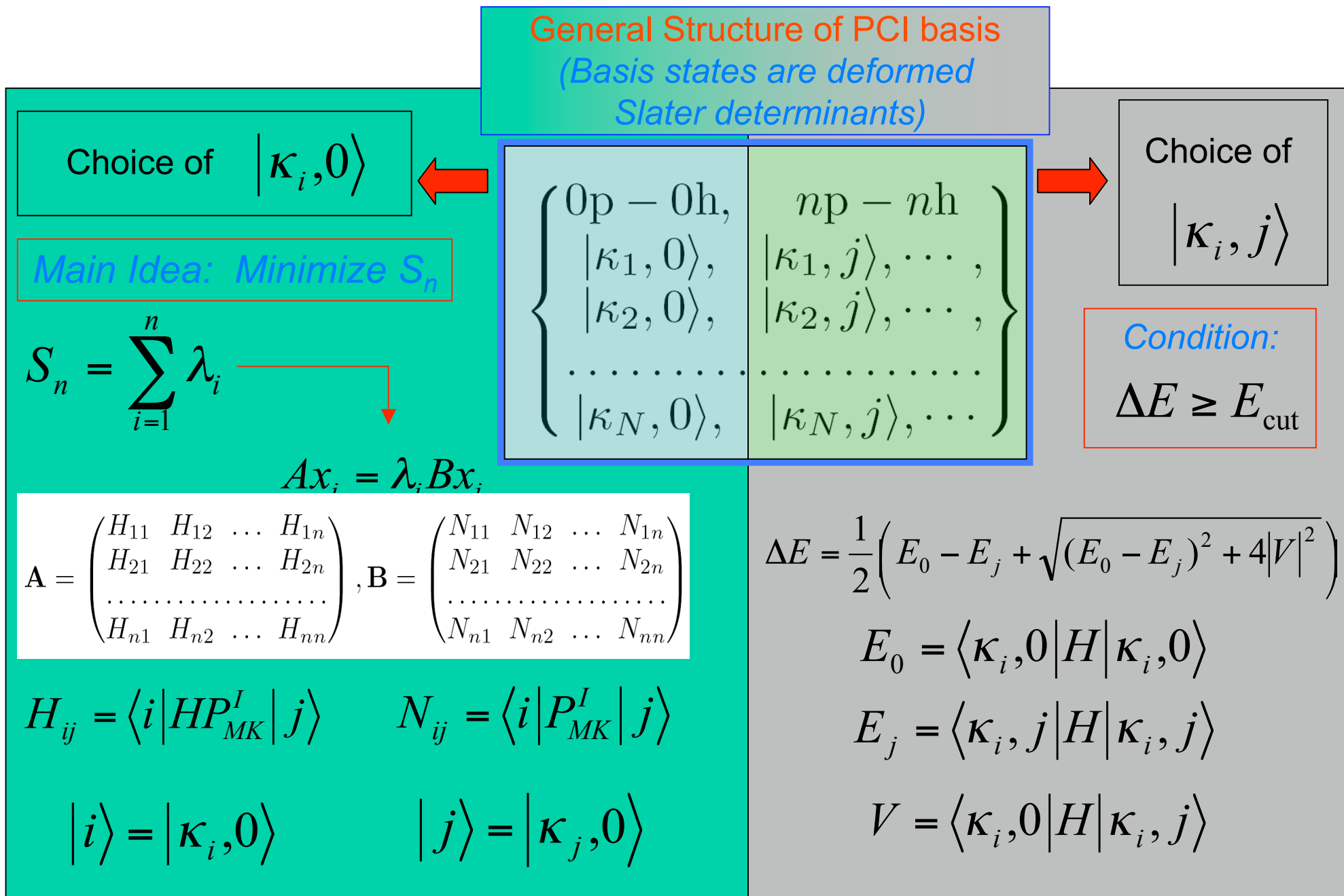
$$E_0 = \langle \kappa_i$$

$$E_j = \langle \kappa_i,$$

$$V = \langle \kappa_i,$$



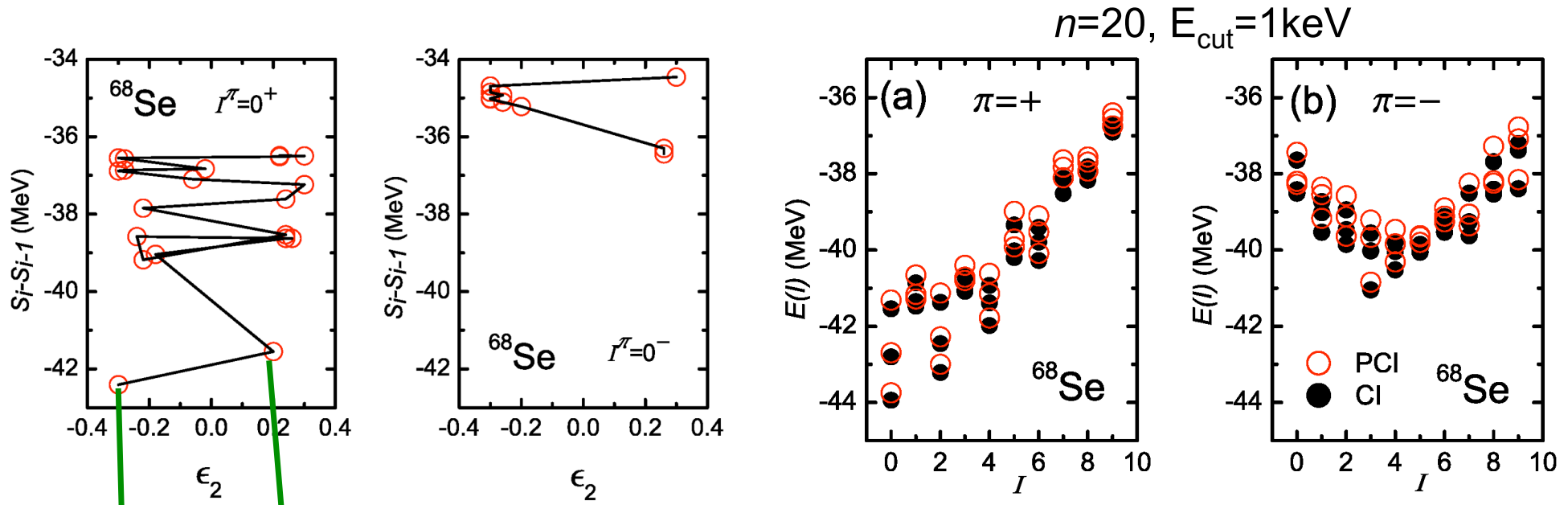
Improved PCI basis selection



^{68}Se

Interaction taken from:

K. Kaneko, M. Hasegawa, and T. Mizusaki, Phys. Rev. C 70, 051301(R) (2004).



Conclusions:

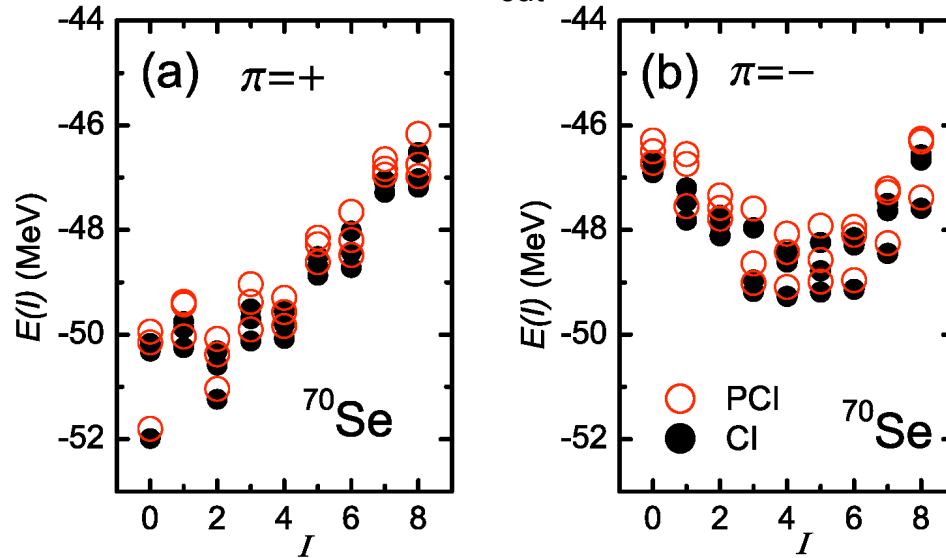
- 1, The physics of shape coexistence in ^{68}Se can be clearly seen from the PCI basis.
- 2, With new method of basis selection the PCI energies are very close to those of full CI for both positive parity and negative parity states.

Interaction taken from:

K. Kaneko, M. Hasegawa, and T. Mizusaki,
Phys. Rev. C 70, 051301(R) (2004).

^{70}Se

$n=20, E_{\text{cut}}=1\text{keV}$



Time of calculation:

Full CI: 20 cpu days for each I^π
PCI: 1-2 cpu days for each I^π

TABLE I: PCI Dimensions compared with those of full CI for ^{70}Se

Spin (I)	$\pi = +$		$\pi = -$	
	PCI	CI	PCI	CI
0	3665	6.7×10^6	4497	6.7×10^6
1	4735	2.0×10^7	4431	2.0×10^7
2	4369	3.2×10^7	4284	3.2×10^7
3	4799	4.2×10^7	4778	4.2×10^7
4	4384	5.0×10^7	4476	5.0×10^7
5	4714	5.5×10^7	4284	5.5×10^7
6	4246	5.8×10^7	4636	5.8×10^7
7	4505	5.9×10^7	4159	5.9×10^7
8	4125	5.7×10^7	4056	5.7×10^7

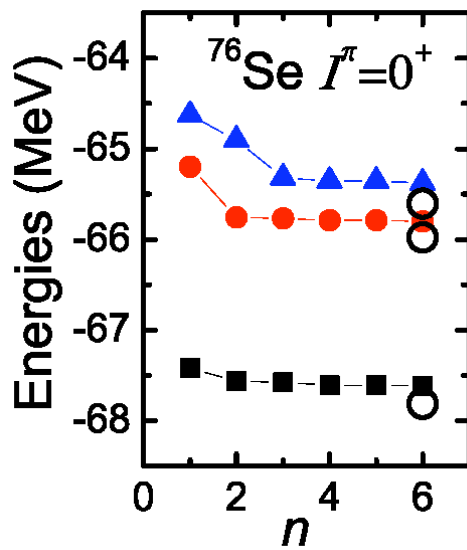
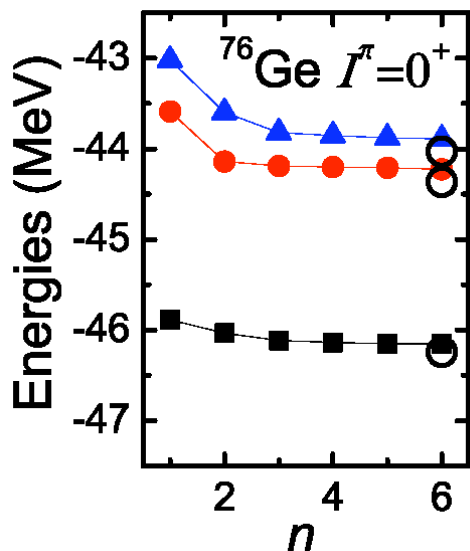
Conclusion:

Both PCI dimensions and times are much smaller than those for full CI.

Zao-Chun Gao, Mihai Horoi, Y. S. Chen, arXiv:0906.3756

Double beta decay nuclei

^{76}Ge and ^{76}Se



Interaction taken from:

K. Kaneko, M. Hasegawa, and T. Mizusaki,
Phys. Rev. C 70, 051301(R) (2004).

Conclusion:

Good approximations for the low-lying 0^+ states of ^{76}Ge and ^{76}Se have been obtained with very small bases.

Goal:

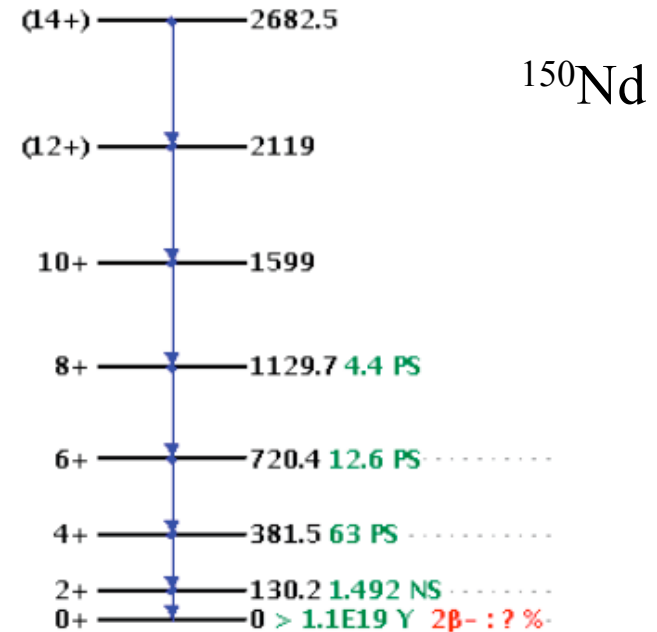
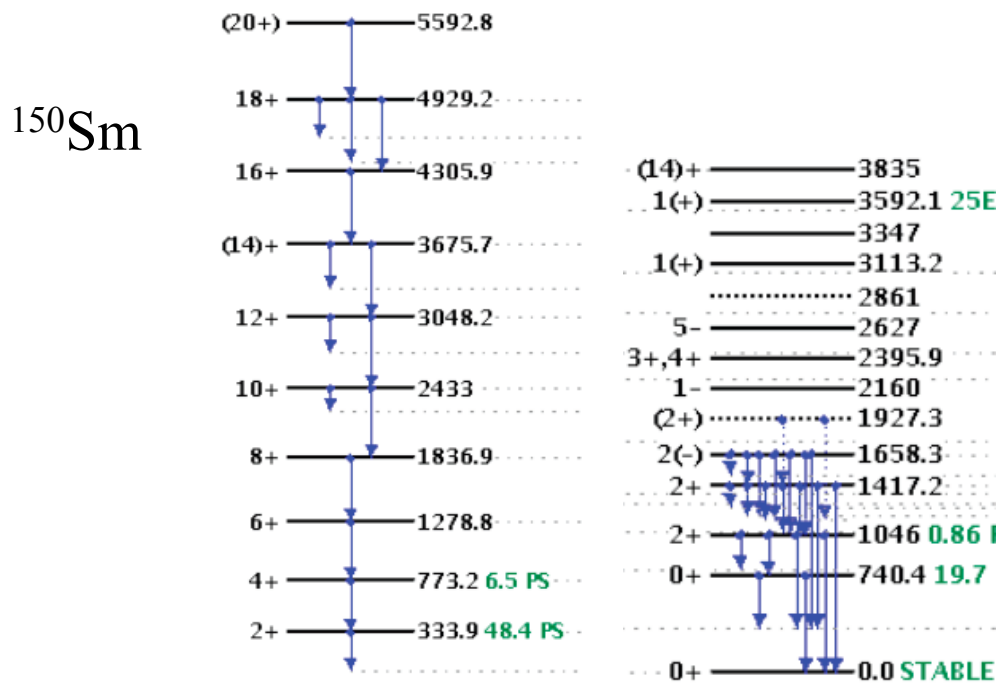
Try to use PCI to calculate the ground states of ^{150}Nd and ^{150}Sm

	^{76}Ge	^{76}Se
n	6	6
PCI_dim	561	647
$E_{\text{PCI}}(\text{MeV})$	-46.155	-67.618
$E_{\text{CI}}(\text{MeV})$	-46.241	-67.814
$E_{\text{PCI}}-E_{\text{CI}}(\text{MeV})$	0.086	0.196

Two $0\nu\beta\beta$ decay cases

- $^{76}\text{Ge} \rightarrow ^{76}\text{Se}$
- fp-g $9/2$ valence space
- p,n: 0f $7/2$ 0f $5/2$ 1p $3/2$ 1p $1/2$ 0g $9/2$
- ^{76}Ge : dim 1,296,156,991,047
- ^{76}Se : dim 18,333,463,355,503

- $^{150}\text{Nd} \rightarrow ^{150}\text{Sm}$
- p: 0g $7/2$ 1d $5/2$ 1d $3/2$ 2s $1/2$ 0h $11/2$
- n: 1f $7/2$ 1f $5/2$ 0h $9/2$ 2p $3/2$ 2p $1/2$ 0i $13/2$
- ^{150}Nd : dim 222,314,413,121,622
- ^{150}Sm : dim 32,199,157,066,956



Status of the Year 3 Project

- The **PCI** code was **extended to two major shells**, and the selection of the deformed basis was significantly improved. $pf+g_{9/2}$ calculations were performed for ^{64}Ge , which shows coexistence between oblate and triaxial deformations, and compared with truncated CI calculations.
- The **extended PCI** code was successfully used in the $f_{5/2}pg_{9/2}$ model space using effective interactions that includes octupole terms. Se isotopes 68 to 76 were studied. ^{76}Se is important for the double beta decay of ^{76}Ge . **Both parities were successfully calculated and compared with the full CI results.**
- The **Moments code** was used to calculate nuclear level densities (NLD) for **several nuclei around the rp-process** waiting-point nuclei ^{64}Ge and ^{68}Se . Some of the **results were compared** with the exact NLD results obtained with the new J-scheme code **NuShellX**.
- The **Moments code** was **successfully parallelized** and benchmarked on Franklin/NERSC. It clearly shows good strong scaling up to 256 processing elements (PEs) and very good weak scaling up to 1024 PEs.

Roadmap for rest of Year 3 and Year 4

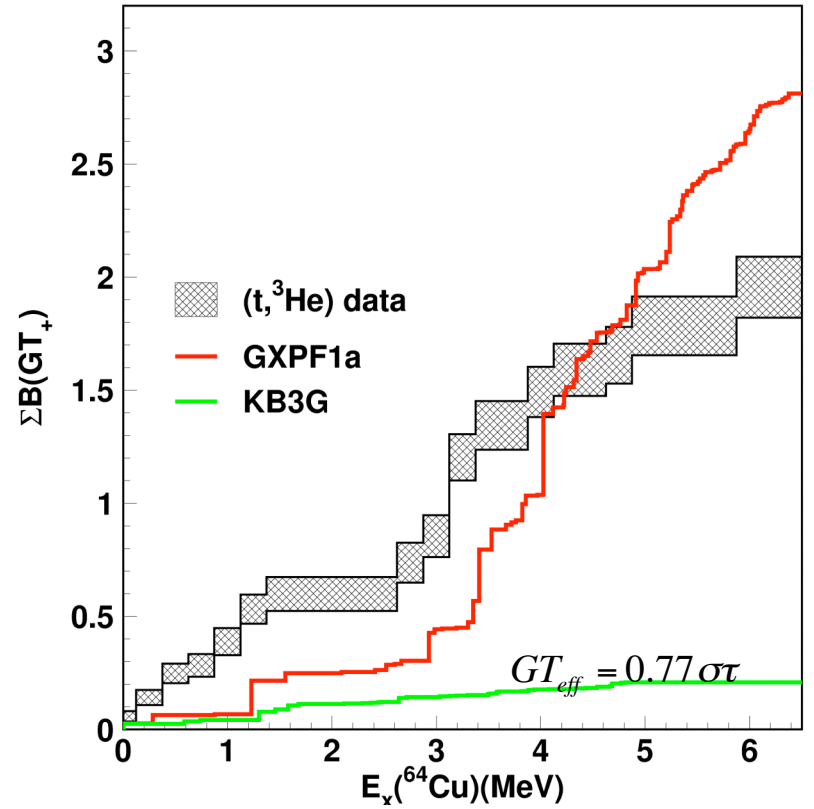
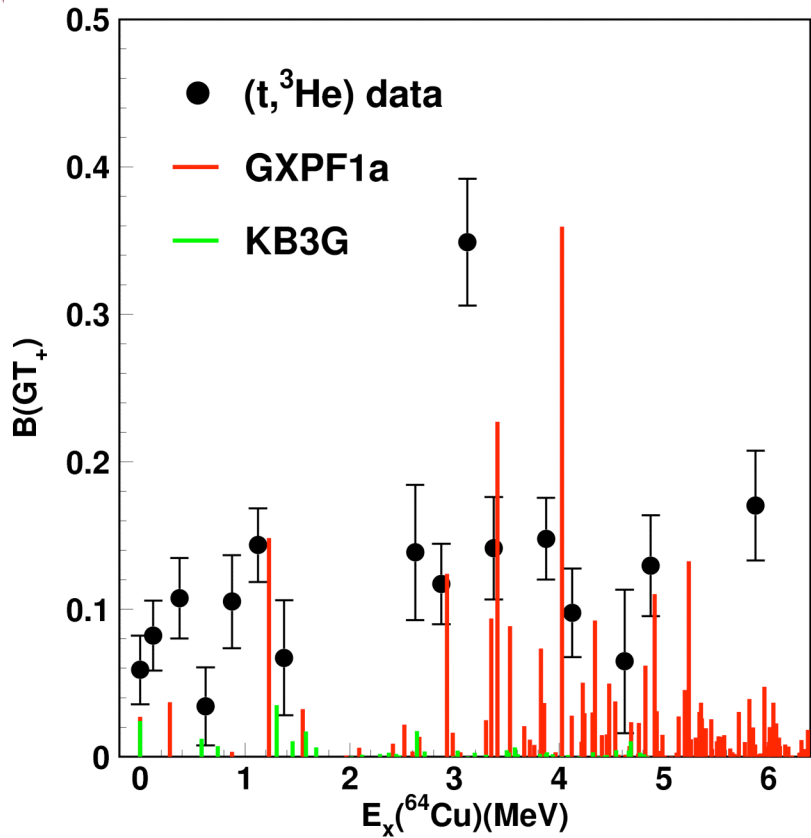
- We are on track with the year 3 plan. Most of the work was done, and we are in the process of publishing the results.
- No reaction rates using the moments NLD were calculated so far. We will initially try to use talys code for some initial testing using mixed input.
- A clear path to make the Moments code scale to tens or/and hundreds of thousands of cores using PN configurations was identified and it will be further pursued in Year 4. The entire code has to be rewritten.
- In Year 4 we will continue to improve the scalability of NuShellX to hundreds of cores and compare its exact results with the results of PCI and NLD/Moments.
- We will continue to improved the projection techniques to get better estimations for the energy of the yrast states necessary for level density.

High-performance computing requirements:

The new PN version of the Moments code will require special treatment to passing the effective interaction to tens or/and hundreds of thousands of cores. Have to decide: parallel I/O, broadcasting, or/and sharing on multi-core nodes.

Roadmap for Year 5

- A first shot to double beta decay (DBD) of ^{150}Nd .
- Calculate the DBD matrix elements for the ^{76}Ge decay in pf+g valence space; estimate the contribution of the partner spin-orbit states.
- Improve the efficiency of the PN NLD/Moments code and calculate NLDs for heavier nuclei in the rp-path; interface NLDs with nuclear reaction codes.



180 1^+ states in ^{64}Cu : NuShellX – no truncations
 M-scheme dim = 187M

$$M_{GT}^{2\nu}(0^+) = \sum_k \frac{\langle 0_f \| \sigma \tau^- \| 1_k^+ \rangle \langle 1_k^+ \| \sigma \tau^- \| 0_i \rangle}{E_k + E_0}$$

M. Horoi et al., arXiv:0904.3645, submitted to PRC

UNEDF Pack Forest
 June 24, 2009

M. Horoi CI

