New High-Performance Algorithm for Nuclear Level Densities and Applications

Roman Sen'kov and Mihai Horoi

Physics Department
Central Michigan University

June 21-25, 2010 / Annual UNEDF Collaboration Meeting

◊ **Support from DOE grant DF-FC02-09ER41584 is acknowledged**

Nuclear Level Densities

- need to know nuclear level densities (NLD) for nuclear reactions, astrophysics, and applications
- theories and methods:
  - Fermi Gas Model: combinatorics of single-particle excitations near the Fermi surface. H. A. Bethe, 1936

$$\rho(E,J,\pi) = \frac{1}{2}F(U,J)\rho_{FG}(U), \quad \text{where} \quad U = E - \Delta$$

  - Hartree-Fock-Bogolyubov model: also combinatorics

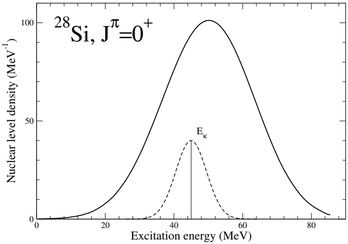
S. Goriely, Nucl. Phys. **A605**, 28 (1996)
Demetriou and Goriely, Nucl. Phys. **A695**, 95 (2001)
S. Goriely, S. Hilaire, and A.J. Koning, Phys. Rev. C **78** 064307 (2008)
Goriely et al., Nucl. Phys. **A773**, 279 (2006); http://www.astro.ulb.ac.be/Html/nld_comb.html

  - Shell Model calculations. Moments Method: describes statistical properties of nuclei

J. B. French and K. F. Ratcliff, Phys. Rev. C**3**, 94 (1971)
S. S. M. Wong, *Nuclear Spectroscopy*, 1986
M. Horoi et al.: PRC **69** 041307(R), (2004); NPA **785**, 142 (2005); PRL **98**, 262503 (2007)

Moments Method. Statistical Spectroscopy

$$\rho(E,\alpha) = \sum_{\kappa} D_{\alpha\kappa} \cdot G(E + E_{gs} - E_{\alpha\kappa}, \sigma_{\alpha\kappa})$$



$\alpha = \{n, J, T_z, \pi\}$ - set of quantum numbers, $G(E,\sigma)$ - Gaussian function

κ - configurations, e.g. 6 particles in *sd* shell:

κ	$d\frac{5}{2}$	$s\frac{1}{2}$	$d\frac{3}{2}$
1	6	0	0
2	5	1	0
3	5	0	1
4	4	2	0
...	...	...	...
15	0	2	4

$D_{\alpha\kappa}$ - number of many-body states with given J that can be built for a given configuration κ

Moments of H for each configuration κ:

$$E_{\alpha\kappa} = \mathrm{Tr}^{(\alpha\kappa)}[H]/D_{\alpha\kappa}$$

$$\sigma^2_{\alpha\kappa} = \mathrm{Tr}^{(\alpha\kappa)}[H^2]/D_{\alpha\kappa} - \left(\mathrm{Tr}^{(\alpha\kappa)}[H]/D_{\alpha\kappa}\right)^2$$

M. Horoi, M. Ghita, and V. Zelevinsky, PRC **69** (2004) 041307(R)

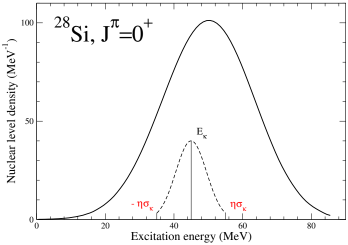
it is important to know the E_{gs} and cut-off parameter η

Moments Method. Statistical Spectroscopy

$$\rho(E,\alpha) = \sum_{\kappa} D_{\alpha\kappa} \cdot G(E + E_{gs} - E_{\alpha\kappa}, \sigma_{\alpha\kappa})$$

$\alpha = \{n, J, T_z, \pi\}$ - set of quantum numbers, $G(E,\sigma)$ - Gaussian function

κ - configurations, e.g. 6 particles in *sd* shell:



κ	$d\frac{5}{2}$	$s\frac{1}{2}$	$d\frac{3}{2}$
1	6	0	0
2	5	1	0
3	5	0	1
4	4	2	0
...	...	...	...
15	0	2	4

$D_{\alpha\kappa}$ - number of many-body states with given J that can be built for a given configuration κ

Moments of H for each configuration κ:

$$E_{\alpha\kappa} = \mathrm{Tr}^{(\alpha\kappa)}[H]/D_{\alpha\kappa}$$

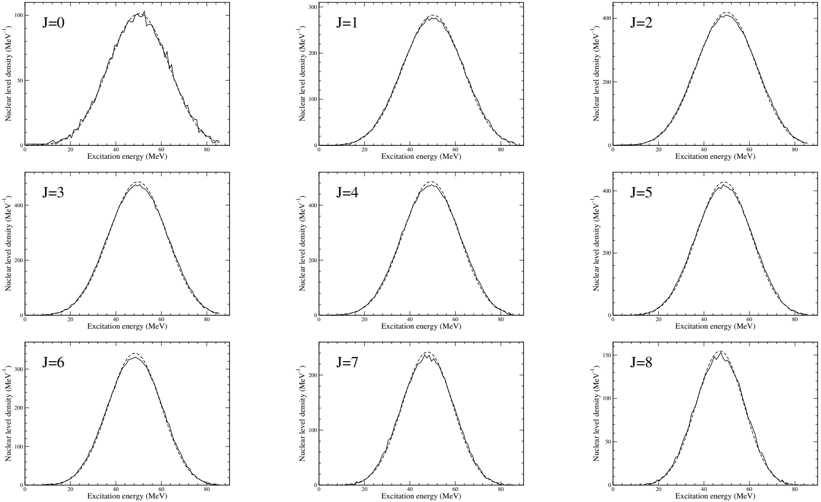
$$\sigma^2_{\alpha\kappa} = \mathrm{Tr}^{(\alpha\kappa)}[H^2]/D_{\alpha\kappa} - \left(\mathrm{Tr}^{(\alpha\kappa)}[H]/D_{\alpha\kappa}\right)^2$$

M. Horoi, M. Ghita, and V. Zelevinsky, PRC **69** (2004) 041307(R)

it is important to know the E_{gs} and cut-off parameter η

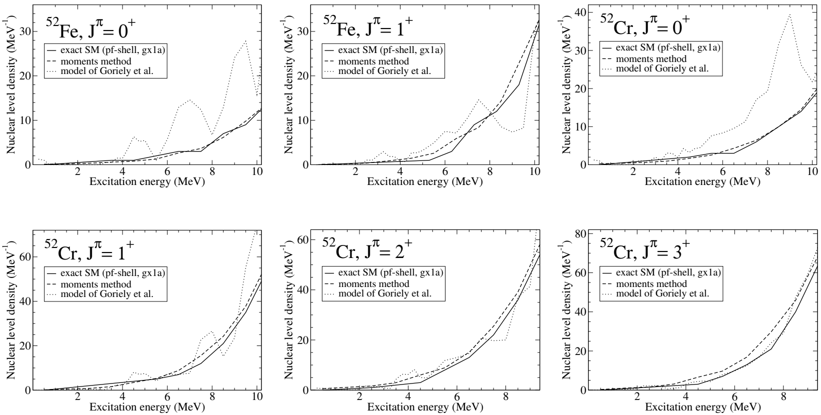
Results for ^{28}Si, parity=+1, various *J*. *sd*-shell

Comparison of nuclear level densities between exact Shell Model (solid line) and Moments Method (dashed line). Cut-off parameter $\eta = 2.8$, USD interaction.



Results for ^{52}Fe, ^{52}Cr, parity=+1, some *J*. *pf*-shell

Comparison of nuclear level densities between exact Shell Model (solid line), Moments Method (dashed line), and HFB method (dotted line). Cut-off parameter $\eta = 2.6$, interaction GXPF1A.



HFB Data: Goriely et al., Nucl. Phys. **A773**, 279 (2006); http://www.astro.ulb.ac.be/Html/nld_comb.html

^{64}Ge and ^{68}Se, $pf + g\frac{9}{2}$ shell. Guessing the ground state energies

$$E_{gs}(pf + g9/2) = E_{gs}(pf) - \Delta E$$

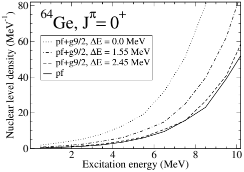
^{64}Ge:

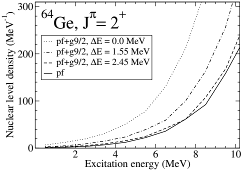
$E_{gs}(pf) = -304.25$ MeV

$\Delta E = 0; 1.55; 2.45$ MeV

J-Dim $\sim 10^7$ for *pf*

$\sim 10^{12}$ for *pfg9*





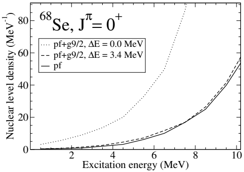
^{68}Se:

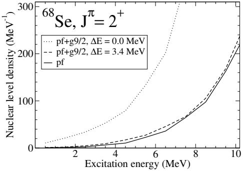
$E_{gs}(pf) = -353.1$ MeV

$\Delta E = 0; 3.4$ MeV

J-Dim $\sim 10^8$ for *pf*

$\sim 10^{12}$ for *pfg9*





Results:

$E_{gs}(pfg9, {}^{64}\text{Ge}) = -306.7$ MeV, $\quad E_{gs}(pfg9, {}^{68}\text{Se}) = -356.5$ MeV

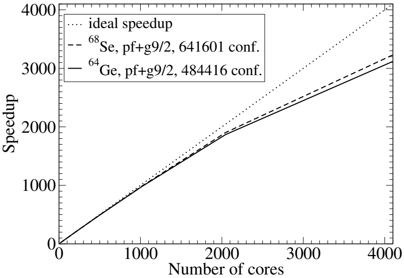
Scaling of the MPI Moments Method Code

Speedup $= T_1/T_n$,
n - number of cores
T_n - calculation time with n cores
(ideally $T_n = T_1/n$)

Domain decomposition: many-body configurations

Algorithm: Dynamically Load Balancing

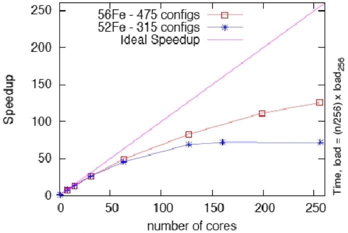
Machine: Francline/NERSC



at number of cores $\sim$ 2000 the calculation time T is about 1 min!!!

advantages of the P-N formalism:

Nucleus, model space	Isospin config.	P-N config.
^{52}Fe, *pf*	315	22028
^{56}Fe, *pf*	475	51174
^{64}Ge, *pfg*9	3749	484416



Removal of the center-of-mass spurious states

Lawson method

$$H \to H' = H + \beta \left[\left(H_{CM} - \frac{3}{2}\hbar\omega \right) \frac{A}{\hbar\omega} \right]$$

D.H. Gloekner and D.R. Lawson, Phys. Lett. B **53**, 313 (1974)

Recursive method

3D-Harmonic oscillator:

$$\mathcal{N}_{pure}(A, K\hbar\omega) = \mathcal{N}_{tot}(A, K\hbar\omega) - \sum_{K'=1}^{K} \mathcal{C}_{K'} \mathcal{N}_{pure}(A, (K - K')\hbar\omega)$$

$$\mathcal{N}_{pure}(A, 0\hbar\omega) = \mathcal{N}_{tot}(A, 0\hbar\omega), \quad \mathcal{C}_{K'} = (K' + 1)(K' + 2)/2$$

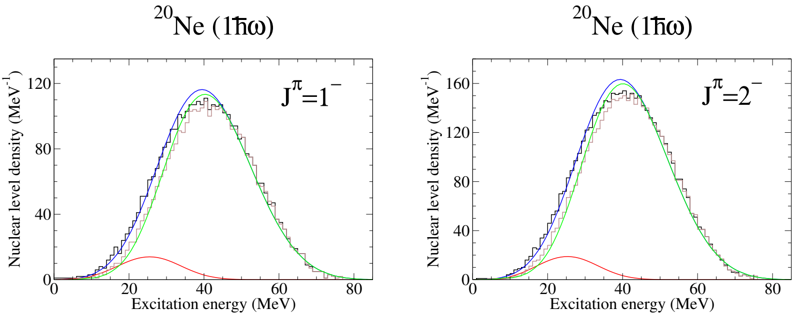
P. Van Isacker, Phys. Rev. Lett. **89**, 262502 (2002)

Nuclear level density:

$$\rho^{(0)}(E, J, K) = \rho(E, J, K) - \sum_{K'=1}^{K} \sum_{J_{K'}=J_{min}}^{K, step\ 2} \sum_{J'=|J-J_{K'}|}^{J+J_{K'}} \rho^{(0)}(E, J', K - K')$$

M. Horoi and V. Zelevinsky, Phys. Rev. Lett. **98**, 262503 (2007)

Example: ^{20}Ne, (s-p-sd-pf)-model space, $1\hbar\omega$



, are shell model calculations with $\beta = 0$ and $\beta = 4$,

, , - moments method: ρ, $\rho^{(0)}$, and $\delta\rho = \rho - \rho^{(0)}$

$$J = 1: \quad \rho^{(0)}(E, 1, 1\hbar\omega) = \rho(E, 1, 1\hbar\omega) - \sum_{J'=0}^{2} \rho(E, J', 0\hbar\omega)$$

$$J = 2: \quad \rho^{(0)}(E, 2, 1\hbar\omega) = \rho(E, 2, 1\hbar\omega) - \sum_{J'=1}^{3} \rho(E, J', 0\hbar\omega)$$

NLD and Hauser-Feshbach

talys 1.2 : www.talys.eu

NLD-M1

ldmodel 1: Constant temperature + Fermi gas model

ldmodel 2: Back-shifted Fermi gas model

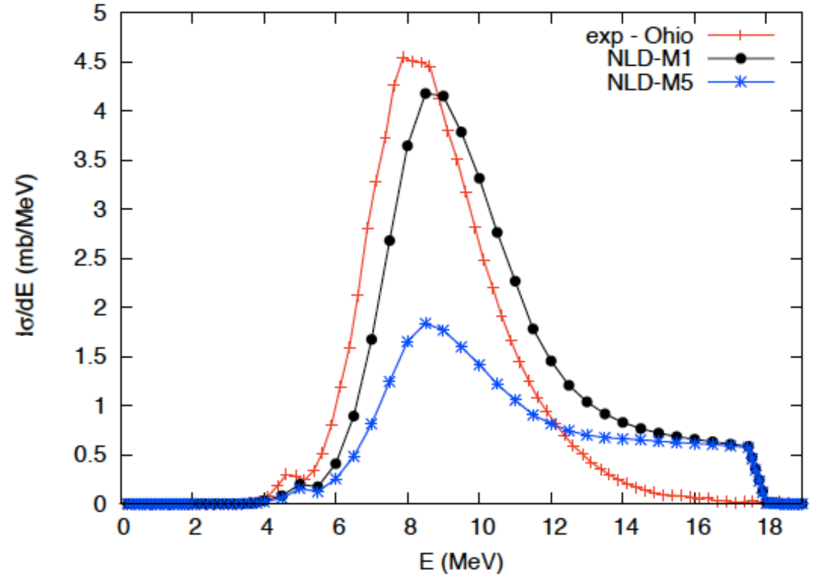
ldmodel 3: Generalised superfluid model

ldmodel 4: Microscopic level densities from Goriely's table

ldmodel 5: Microscopic level densities from Hilaire's table

NLD-M5

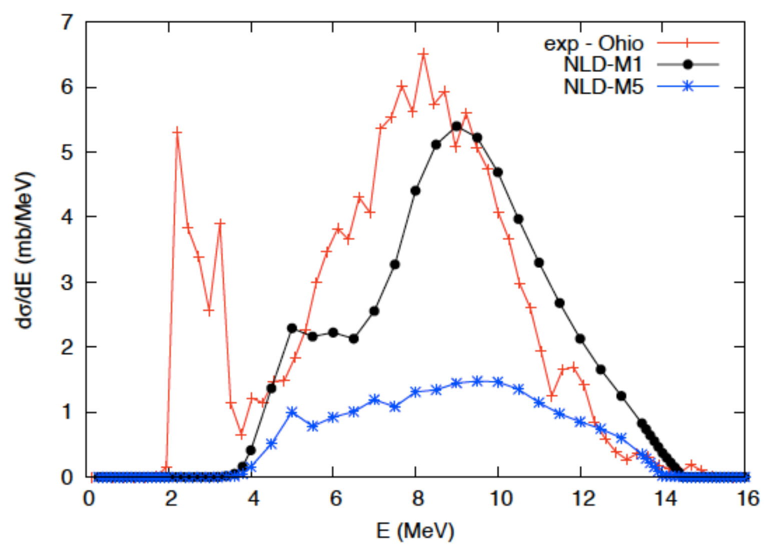
Exp – Ohio: A. Voinov et al., PRC **76**, 044602 (2007)



$\leftarrow {}^{58}Fe({}^{3}He,\alpha){}^{57}Fe$

$\theta = 150^0$

$E_{{}^3He} = 10.0\ MeV$



$\leftarrow {}^{59}Co(d,\alpha){}^{57}Fe$

$\theta = 150^0$

$E_d = 7.5\ MeV$

Comparison with Moments Densities

talys 1.2 : www.talys.eu

NLD-M1

ldmodel 1: Constant temperature + Fermi gas model

ldmodel 2: Back-shifted Fermi gas model

ldmodel 3: Generalised superfluid model

ldmodel 4: Microscopic level densities from Goriely's table

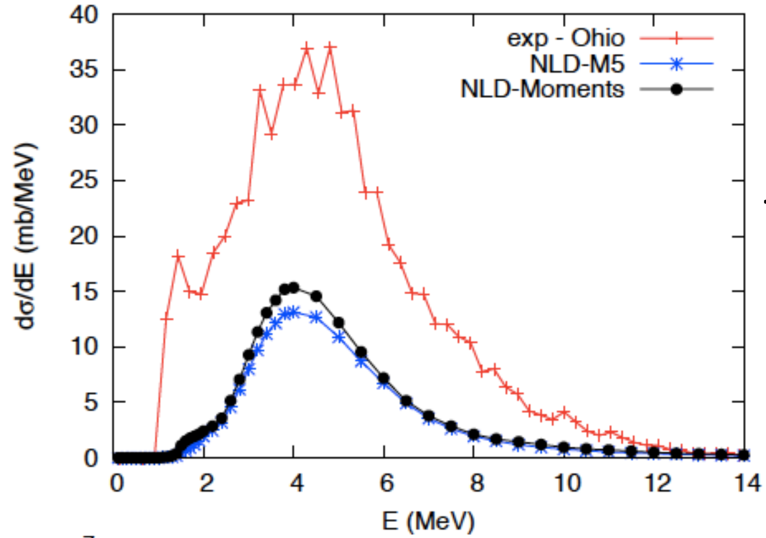
ldmodel 5: Microscopic level densities from Hilaire's table

NLD-M5

Interface:

Moments table -> Hilaire's table

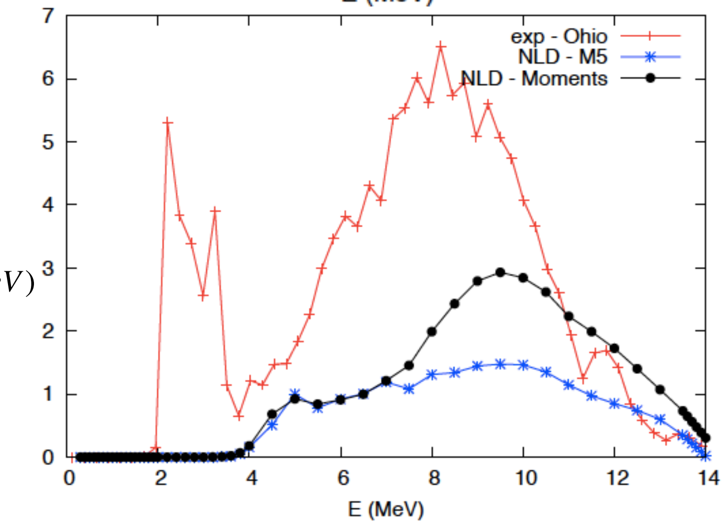
Exp – Ohio: A. Voinov et al., PRC **76**, 044602 (2007)



$\leftarrow {}^{58}Fe({}^{3}He, p)^{60}Co$

$\theta = 150^0$

$E_{^3He} = 10.0\ MeV$



$\frac{d\sigma}{dE}\ (mb/MeV)$

$\leftarrow {}^{59}Co(d, \alpha)^{57}Fe$

$\theta = 150^0$

$E_d = 7.5\ MeV$

NLD: reaction rates

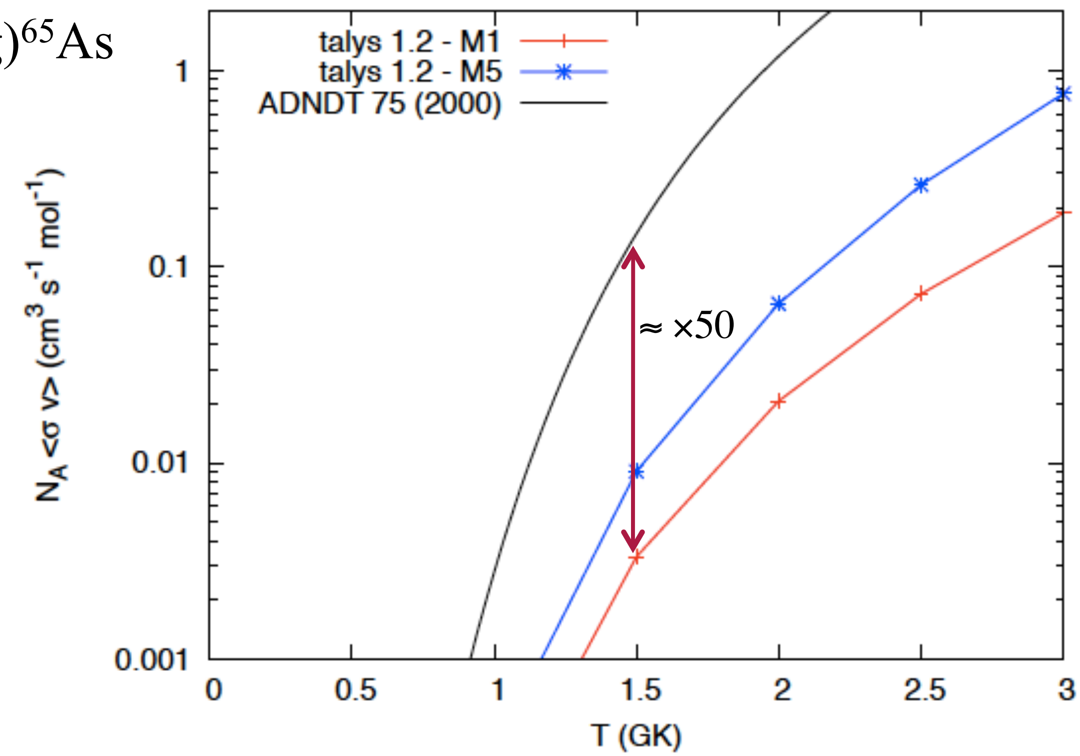
talys 1.2 : www.talys.eu

Rauscher & Thielemann ADNDT **75**, 1 (2000)

$$N_A\langle\sigma v\rangle^*_{\alpha\alpha'}(T) = \left(\frac{8}{\pi m}\right)^{1/2}\frac{N_A}{(kT)^{3/2}\,G(T)}\int_0^\infty\sum_\mu\frac{(2I^\mu+1)}{(2I^0+1)}\times \sigma^\mu_{\alpha\alpha'}(E)E\exp\left(-\frac{E+E^\mu_x}{kT}\right)dE,$$

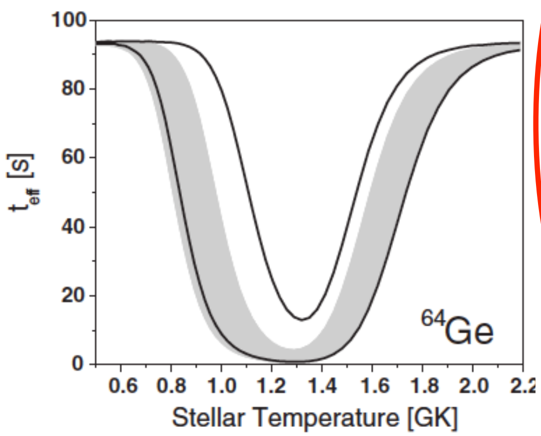
$$G(T)=\sum_\mu(2I^\mu+1)/(2I^0+1)e^{-E_x^\mu/kT}\rightarrow\sum_{I,\pi}\int(2I^\pi+1)/(2I^0+1)\rho(E_x,I,\pi)e^{-E_x/kT}dE_x$$

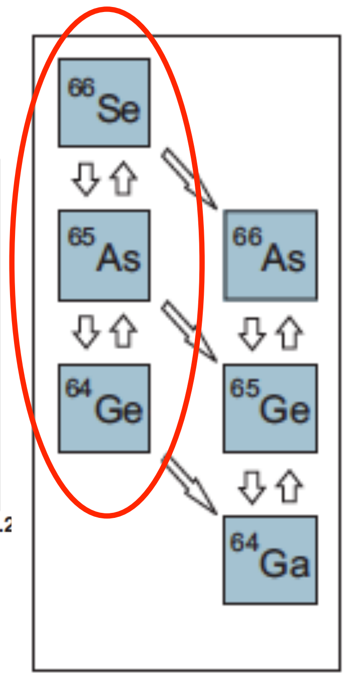
$^{64}Ge(p,g)^{65}As$



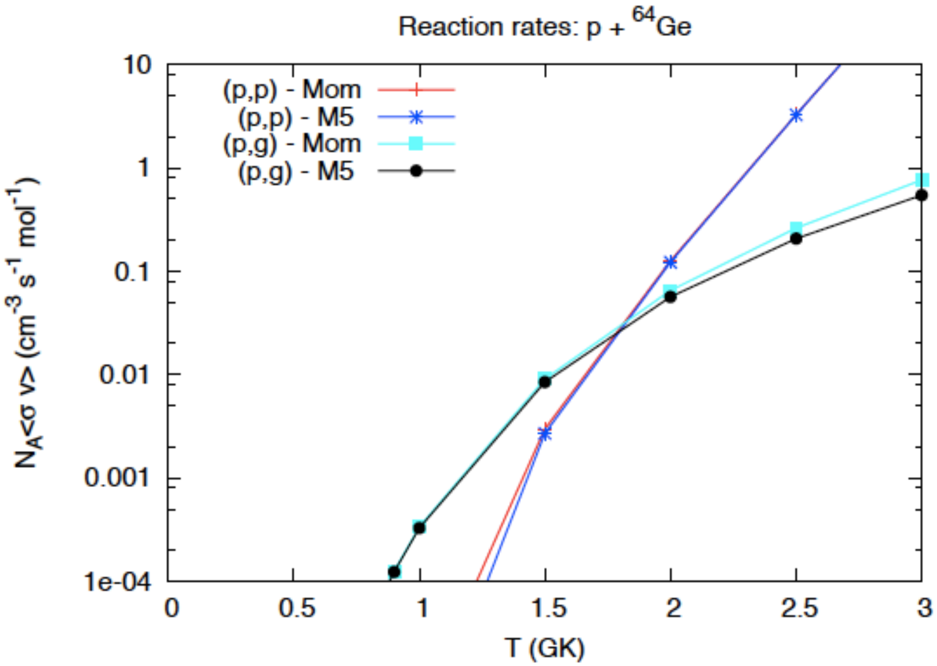
Comparison with Moments Densities

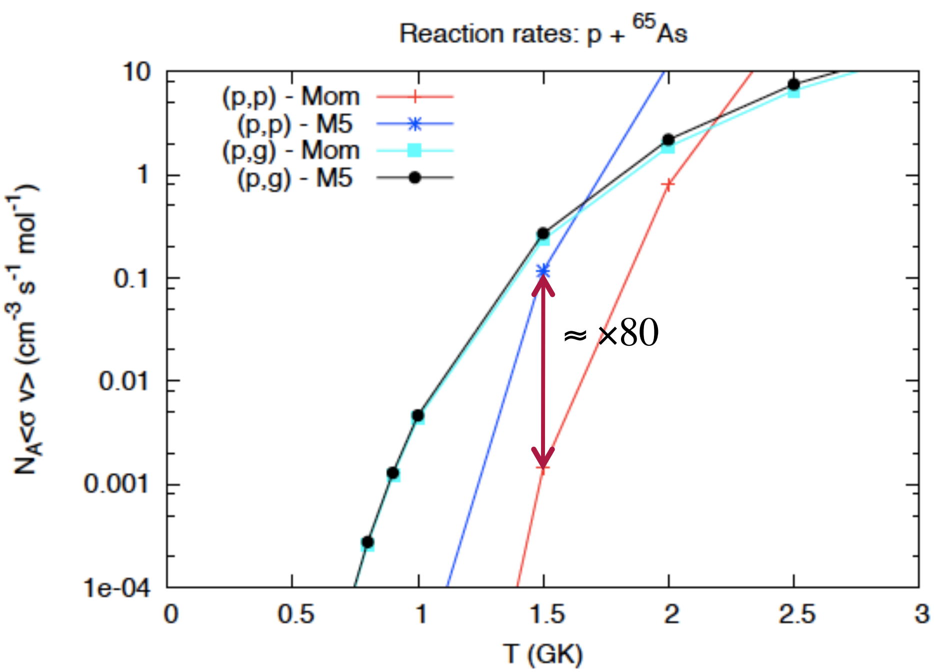
Is ^{64}Ge a "waiting-point" nucleus in the rp-process path?





From P. Shury et al., PRC 75, 055801 (2007)





Deliverable for year 4

- new algorithm for Moments Method in the proton-neutron formalism was developed. it is about a **few thousands** times faster compared to the previous one
- the code is parallelized and was tested using 4,000 processors
- **breakthrough** in NLD calculations. we can now calculate the spin- and parity- dependent nuclear level densities for model spaces with *m*-scheme dimensions of order of $10^{16} - 10^{18}$, i.e. $\sim$ 2 major shells
- can use the Moments Method to predict the ground state energies
- some applications to the nuclear reactions were made
- preliminary algorithm of removal of the contribution of center-of-mass spurious states

Publications

- *Improved basis selection for the Projected Configuration Interaction method applied to heavy nuclei,* Z. Gao, M. Horoi, and Y.S. Chen, Phys. Rev. C **80**, 034325 (2009).
- *A High-Performance Algorithm to Calculate Spin- and Parity-Dependent Nuclear Level Densities*, R. Senkov and M. Horoi, arXiv:1004.5027, submitted to Phys. Rev C, (2010).
- *Improved Accuracy Moments Method for Spin-Dependent Shell Model Nuclear Level Densities*, M. Scott and M. Horoi, submitted to Europhys. Lett. (2010).

Presentations

- *Novel Computational Aspects of the Shell Model Nuclear Level Densities and Reaction Rates*, M. Horoi, invited talk at RIKEN, Saitama, Japan, May 20, 2010
- *New Approaches for Shell Model Level Densities and Reaction Rates,* M. Horoi, invited talk at University of Tokyo, May 20, 2010.
- *Novel High Performance Computational Aspects of the Shell Model Approach for Medium Nuclei,, M. Horoi,* invited talk at the 6th ANL/MSU/JINA/INT FRIB Theory Workshop, "Computational Forefront in Nuclear Theory: Preparing for FRIB,", ANL March 25, 2010.
- *Progress and problems with projected basis CI*, M. Horoi, invited talk at the Leadership Class CI codes workshop, San Diego State University, March 12, 2010.
- *A Performant Algorithm to Calculate Spin- and Parity-Dependent Nuclear Level Densities*, R. Senkov and M. Horoi, APS April Meeting, February 15, 2010.
- *Spin- and Parity-Dependent Nuclear Level Densities for rp-Process Nuclei*, M. Horoi, invited talk at the National Superconducting National Lab, MSU, October 22, 2009.
- *Spin- and Parity-Dependent Shell Model Nuclear Level Densities for Medium-Mass Nuclei, M. Scott and M. Horoi, DNP/APS Fall Meeting, Big Island, HI, October 13-17, 2009.*

Plans for year 5

- finalize the algorithm of removal of the contribution of center-of-mass spurious states
- calculate NLD for large model spaces, e.g. 2 major shells
- need of effective interaction, consider schematic interaction
- calculate more reaction rates in the rp-process path

Defining the cut-off parameter η

f_{err} is an error factor:

$$f_{err} = \exp\left(\sqrt{\frac{1}{N_i}\sum_{i=1}^{N_i} \ln^2\left[\frac{\rho_{mm}(E_i)}{\rho_{sm}(E_i)}\right]}\right) - 1$$

$\rho_{sm}(E)$ - Shell Model density

$\rho_{mm}(E)$ - Moment Method density

$\eta^* = 2.6 \div 2.8$