

Progress with the code NuShellX

Eric McDonald (50% UNEDF, 50% iCER)

Alex Brown

Bill Rae

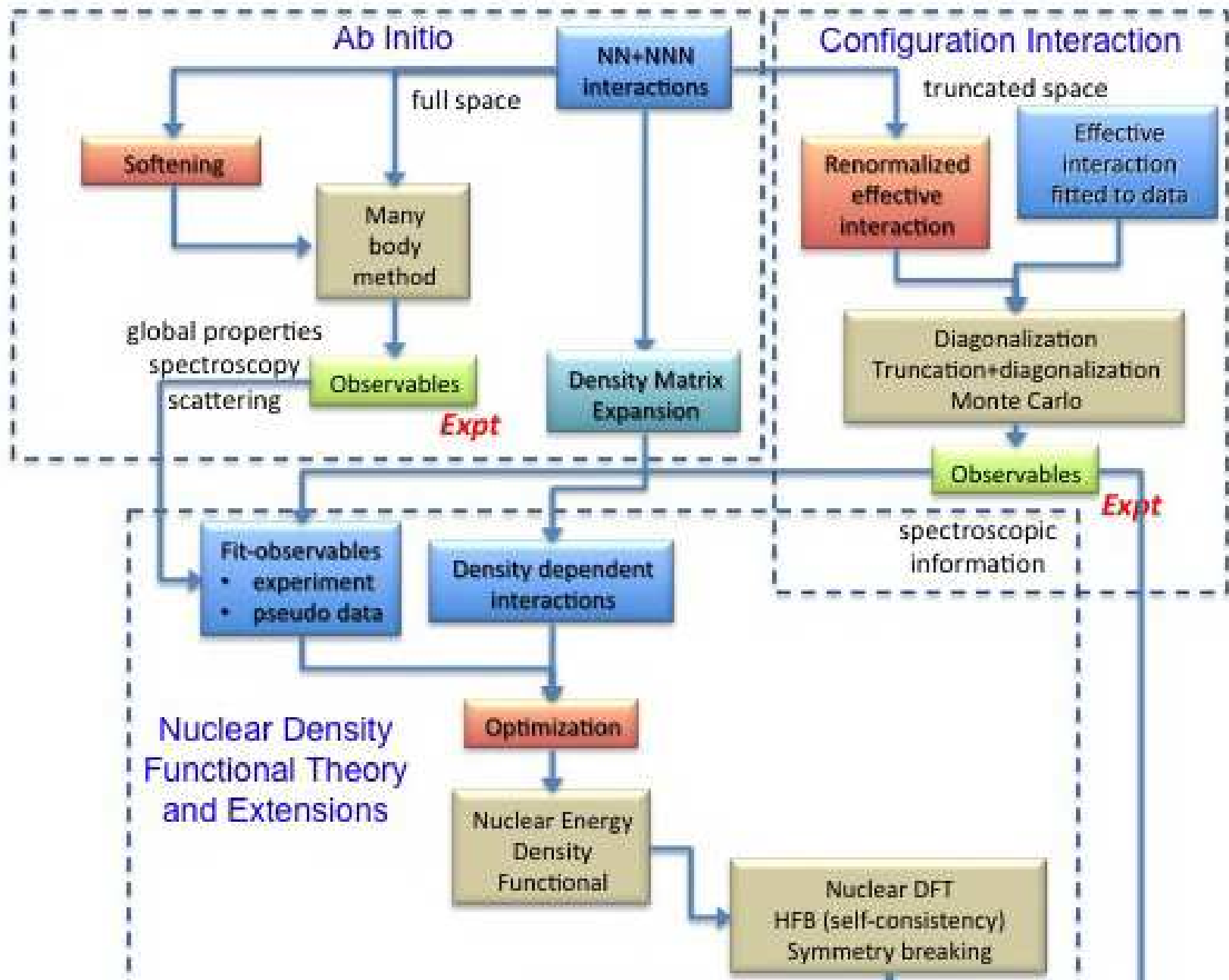
Mihai Horoi

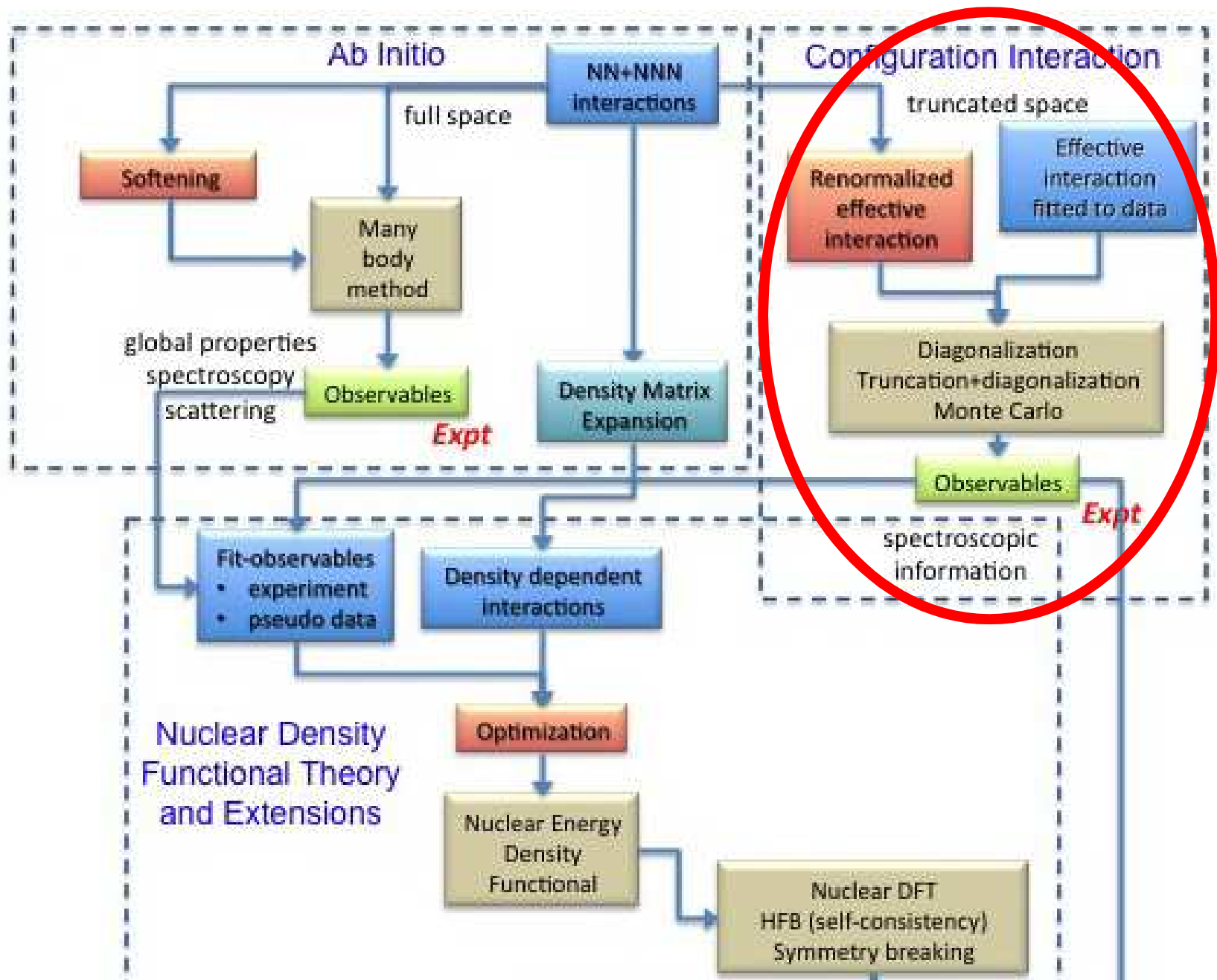
Angelo Signoracci

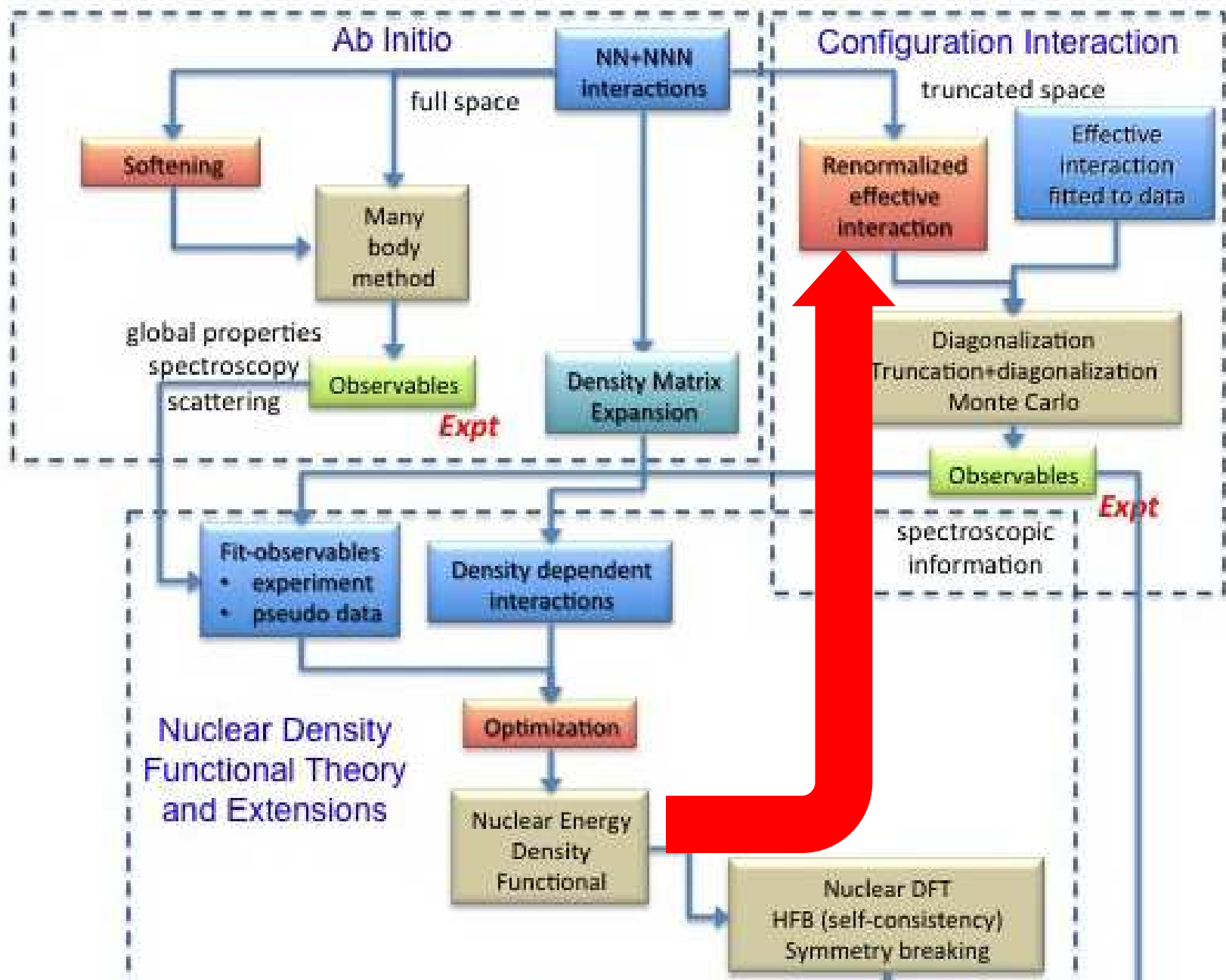
Alexander Litsetsky (summer 2009)

iCER: Institute for Cyber Enabled Research at MSU









NuShellX starts with good-J proton and neutron basis states.
Then a good-J pn basis is generated from vector coupling:

$$| [(J_p, \alpha_p) \otimes (J_n, \alpha_n)] J \rangle$$

Fortran95

OpenMP

The Hamiltonian matrix is obtained “on the fly”

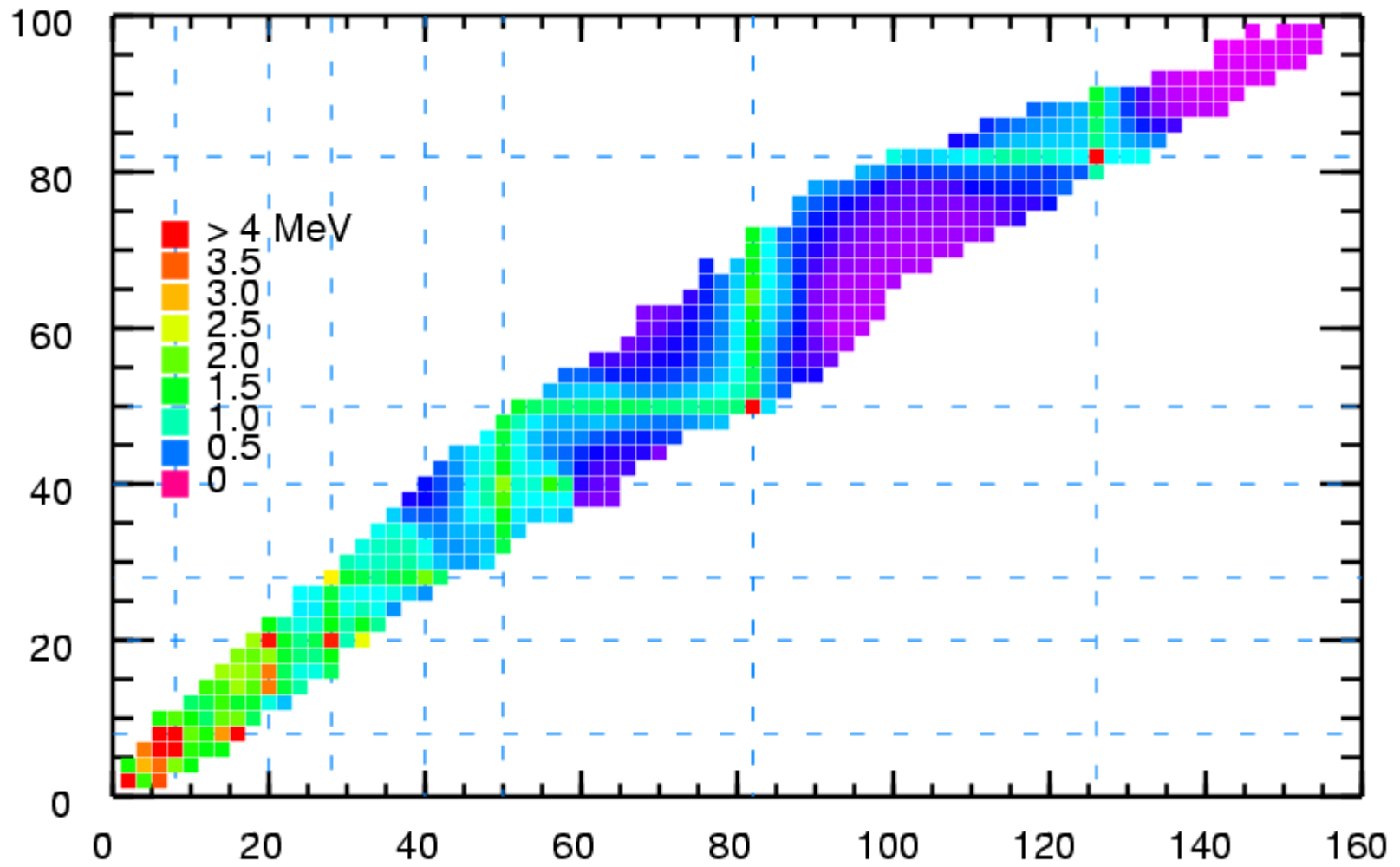
Windows and Linux

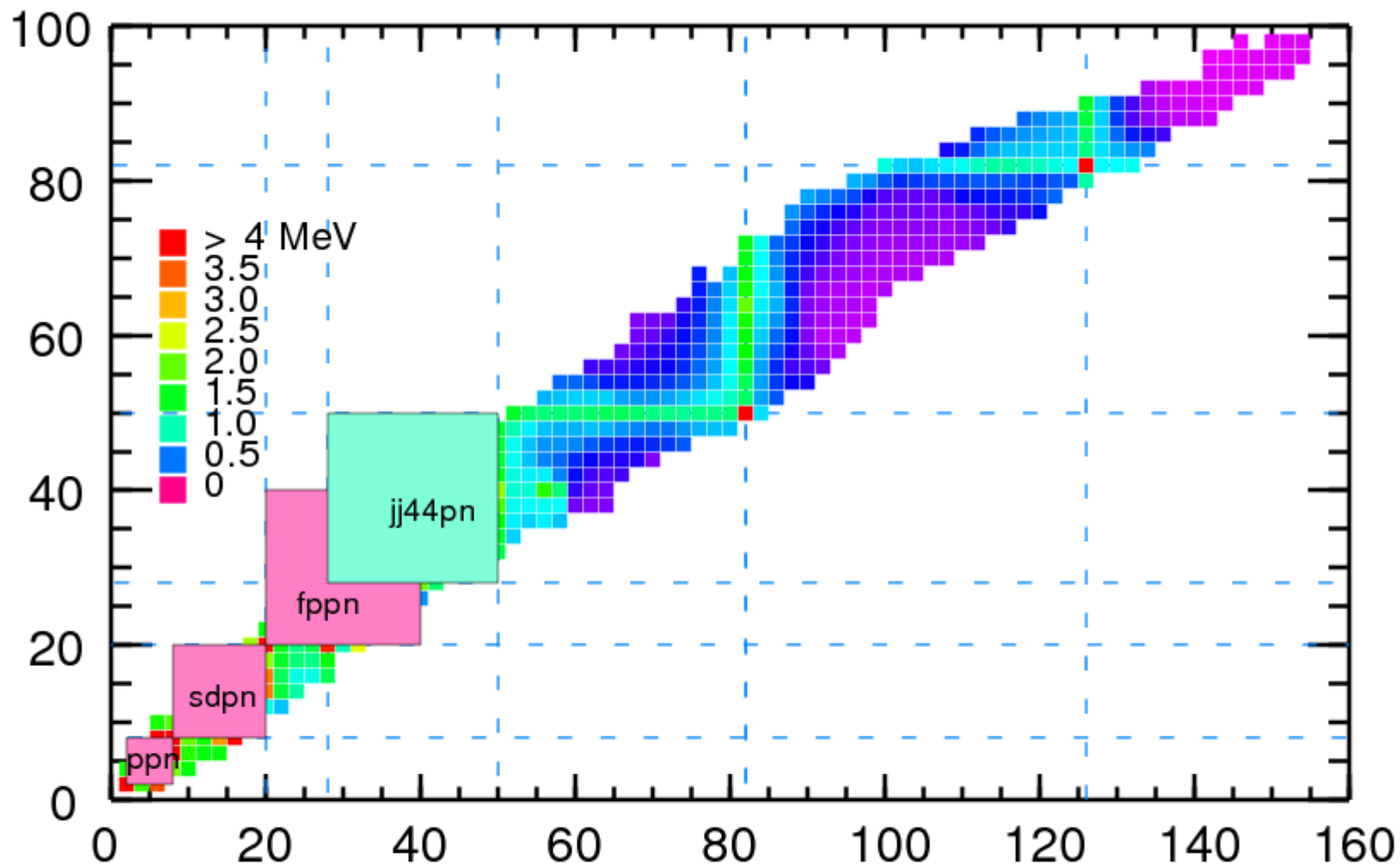
NuShellX@MSU is a set of wrapper codes that makes the program very easy to install and run with standard inputs and outputs.

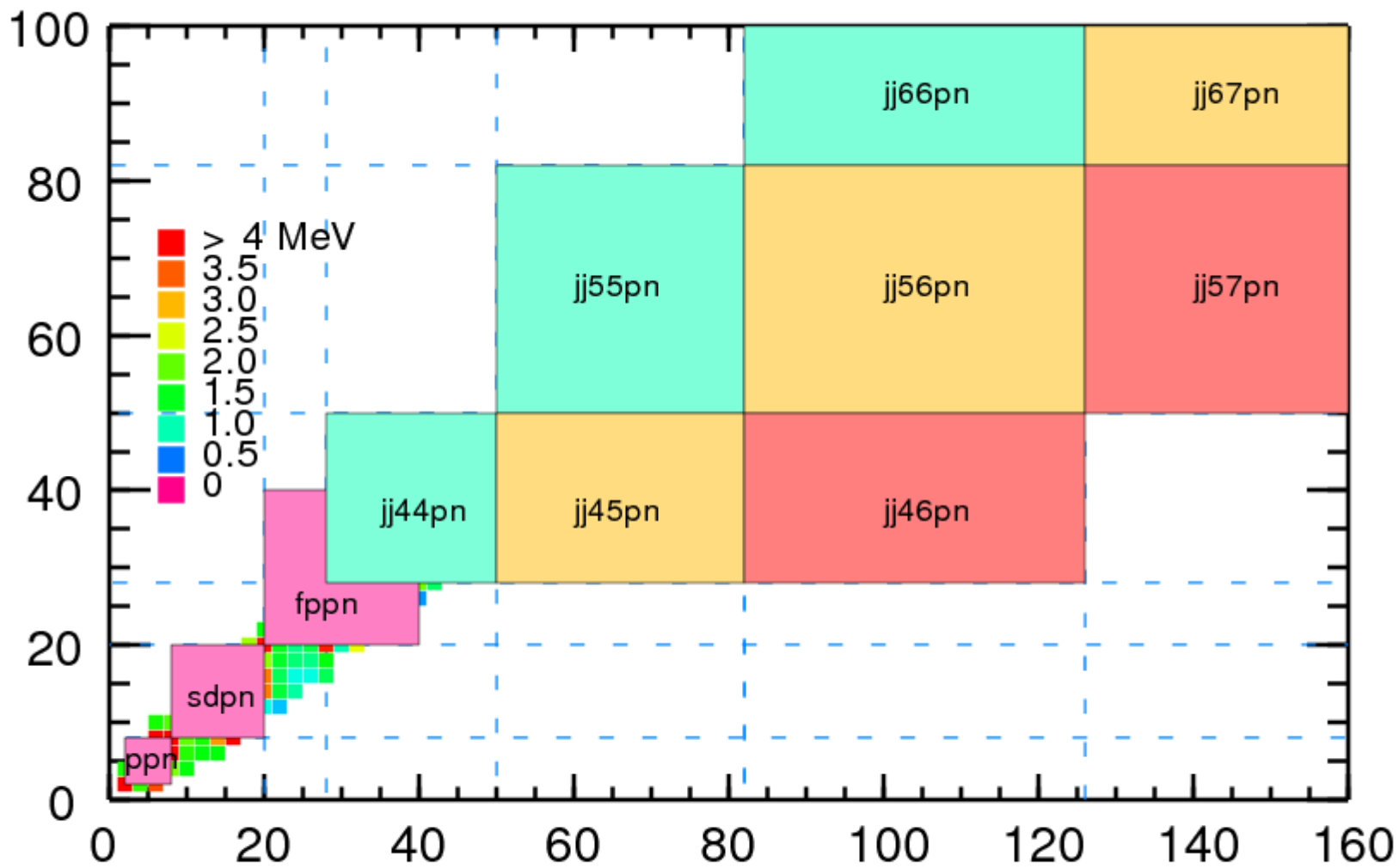
There are many more options that can be accessed by the expert users. The code is open-source so you can make changes.



Energy of first excited 2^+ states







2008-2009 – A stable version compiled with ifort

Summer 2009: Alexander Lisetsky converted the OpenMP part of NuShellX to MPI.

December 2009: A more complete package of programs updated and used for a workshop in Norway.

<http://www.nsl.msue.edu/~brown/BrownNorway/Norway.html>

It includes:

- 1) Full linux version (with ifort)
- 2) Wrapper: connection to table of isotopes to automatically generate figures with a comparison between experiment and theory.
- 3) Wrapper program (ham) that combines EDF (Skyrme for now) with renormalized NN (Morten Hjorth-Jensen's programs) to provide an starting input for a CI Hamiltonian based on a "core nucleus" and a "model space" (initial defaults like skxtb, n3lo, vlowk and 2nd order core-polarization for NN)

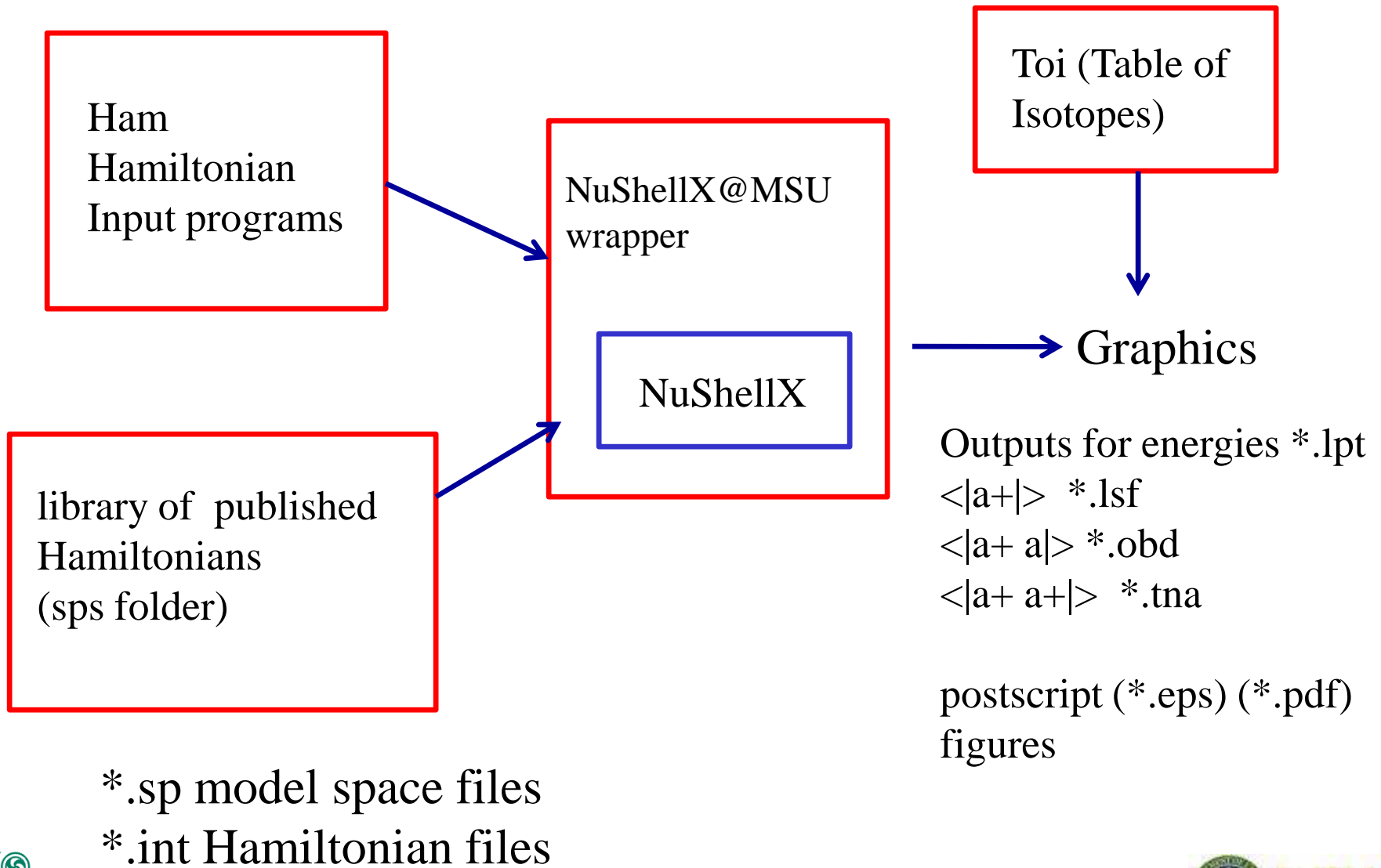
2010: Eric McDonald started (50% UNEDF, 50% iCER)

Done: NuShellX with the PGI compiler so we have a more portable code
- in particular for NERSC etc.

With OpenMP best on a machine like Euclid with many (48) cores.

year 4 deliverable: Improve the scalability of the CI code NuShellX to
hundreds of cores.





```
euclid.nerisc.gov - euclid - SSH Secure Shell
File Edit View Window Help
[Icons: Save, Print, Find, Home, Undo, Redo, Copy, Paste, Delete, Insert, Help, etc.]
Quick Connect Profiles
UW PICO 5.04 File: cr48.ans
-----
lpe, 0 ! option (lpe or lan), neig (zero=10)
fp ! model space (*.sp) name (a8)
n ! any restrictions (y/n)
gxia ! interaction (*.int) name (a8)
 24 ! number of protons
 48 ! number of nucleons
 0.0,16.0, 1.0, ! min J, max J, del J
 0 ! parity (0 for +) (1 for -) (2 for both)
-----
st ! option
█
```

Example for a very small case

^{48}Cr $J=0$ (pf shell)

M-scheme dimension = 1,963,461

J-scheme dimension = 41,355

16 threads on Euclid

10 eigenstates with 1 keV accuracy

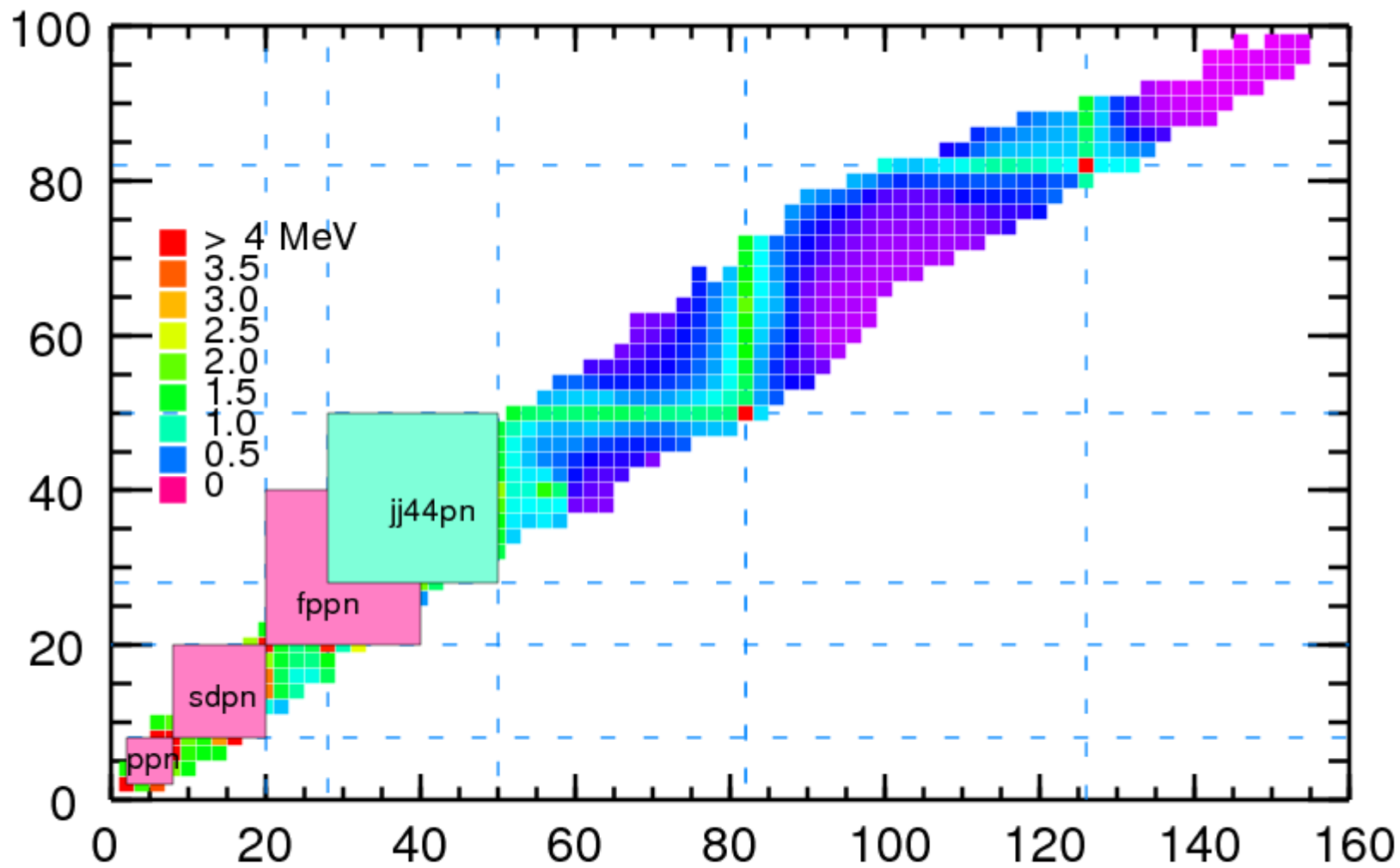
takes about 10 seconds

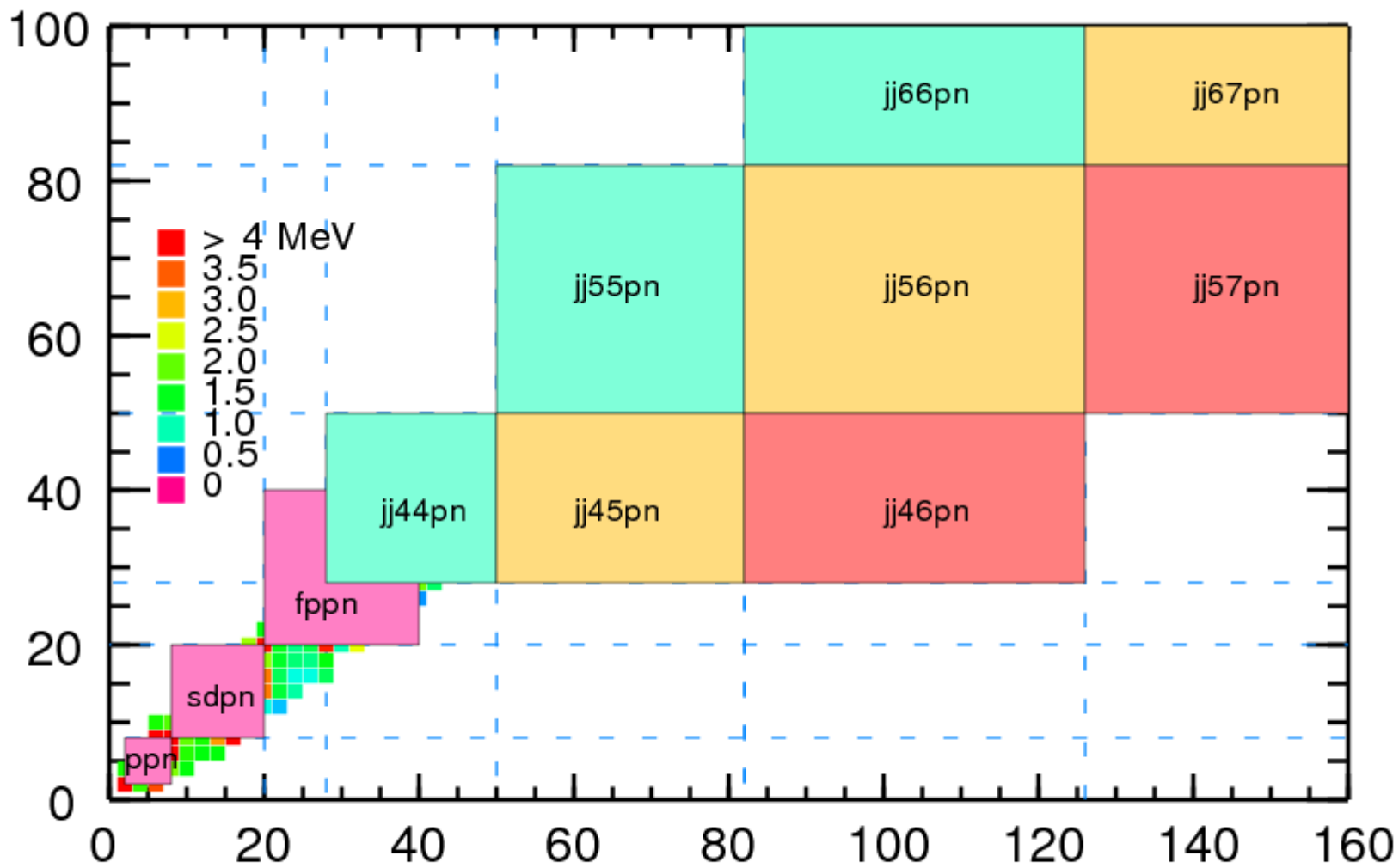
Presently used for J-scheme dimensions up to about 100,000,000

Up to about 400 levels for a given J.

Most nuclear structure experiments at the NSCL require the use of NuShellX for comparison to theoretical expectations.







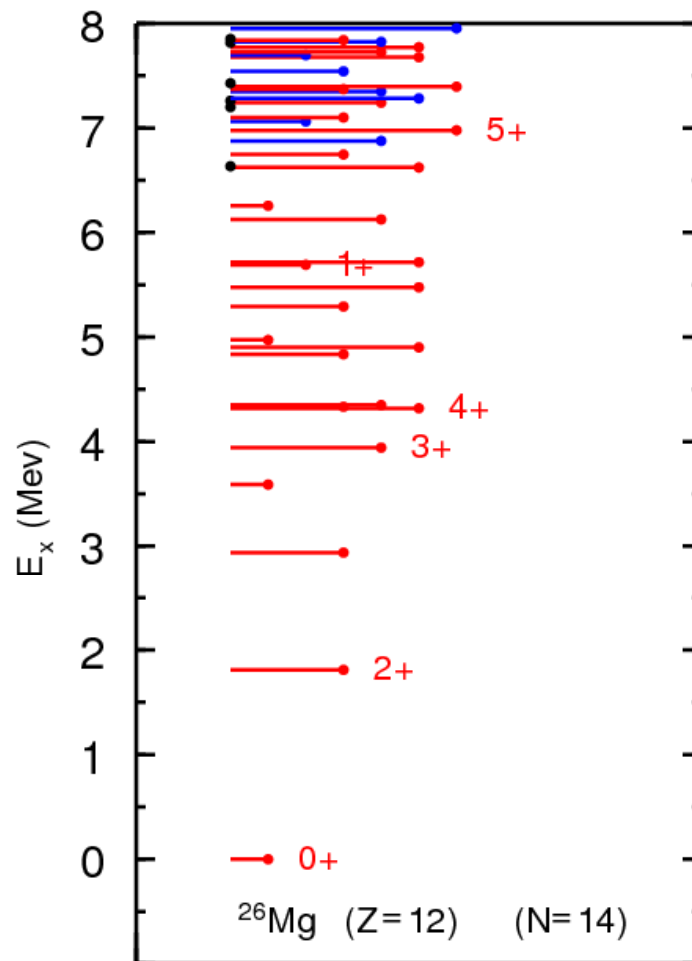
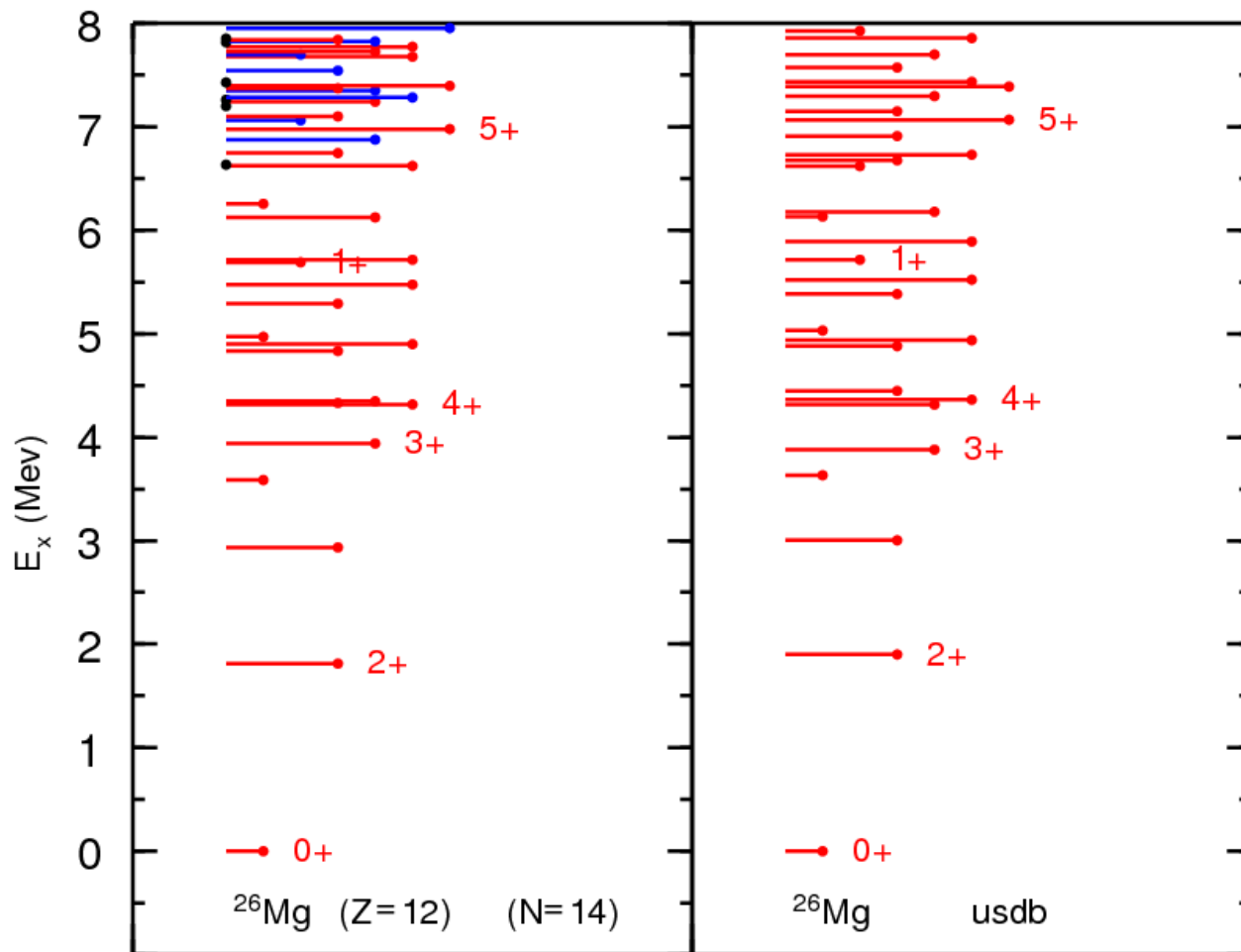


Figure generated from Toi program with experiment from the table of isotopes



Experiment ^{26}Mg Theory

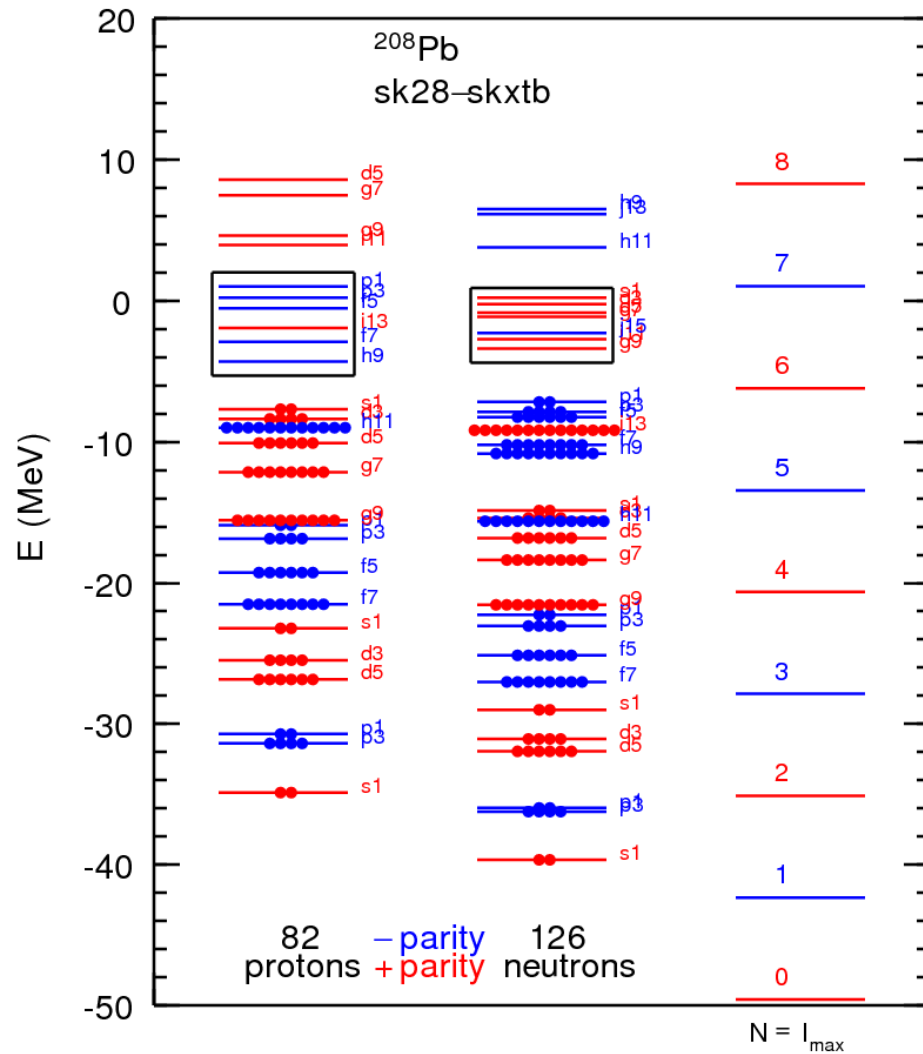
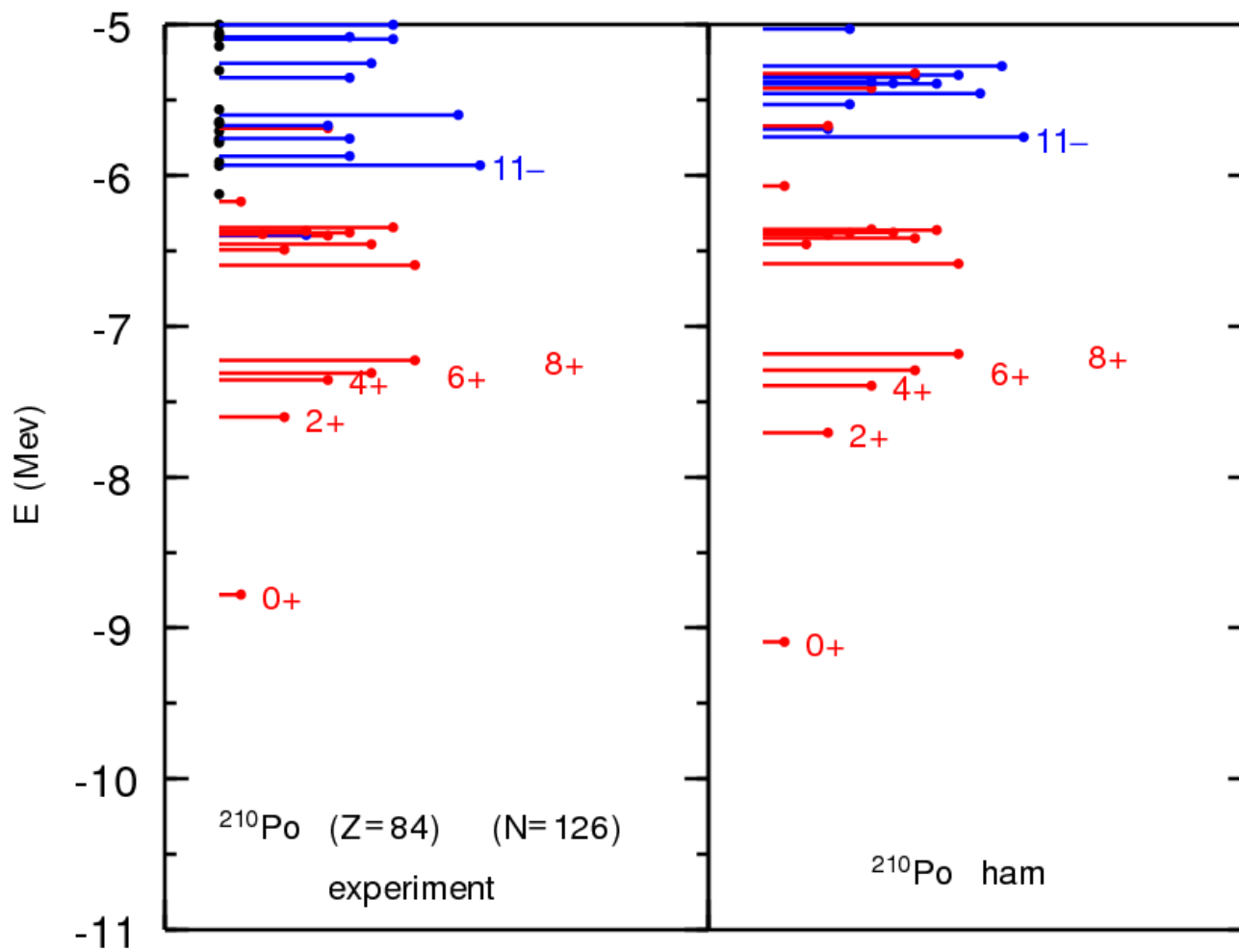


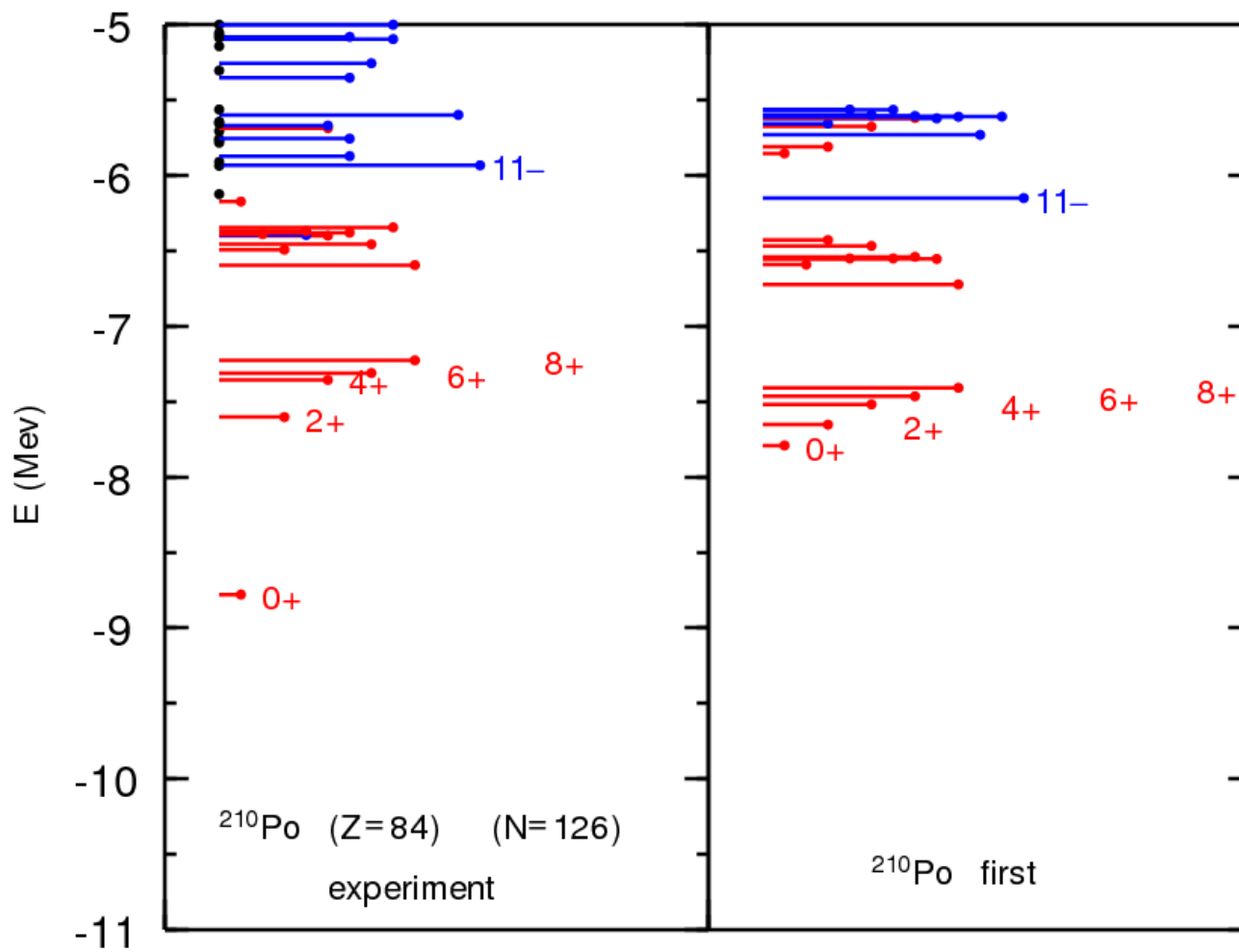
Figure generate by Hamiltonian program



^{210}Po

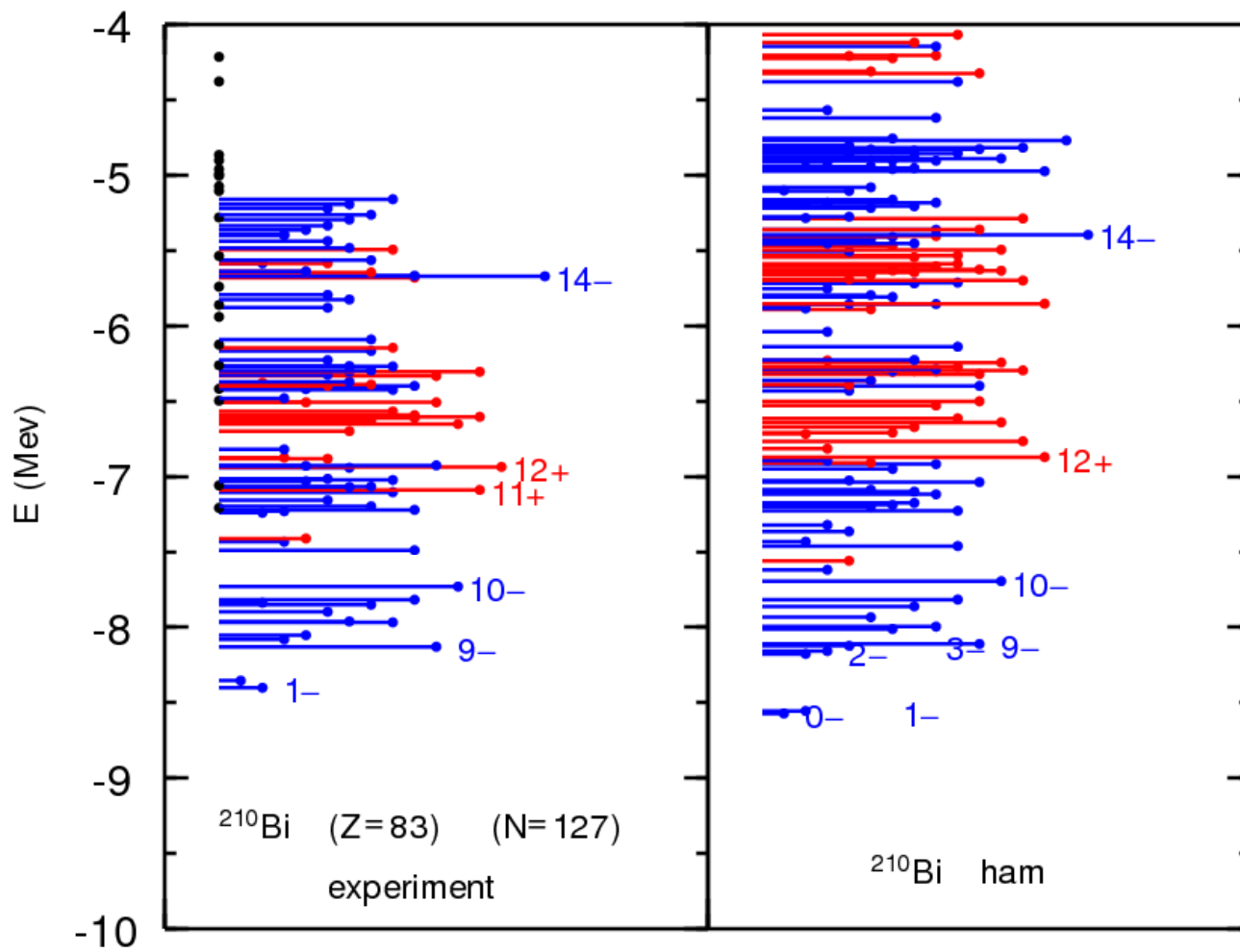
Skyrme (Skxmb) +
 V_{lowk} N3LO (second order)





^{210}Po

Skyrme (Skxmb) +
 V_{lowk} N3LO (first order)



^{210}Bi

euclid.nersc.gov - euclid - SSH Secure Shell

File Edit View Window Help

Quick Connect Profiles

UW PICO 5.04 File: na230.deo

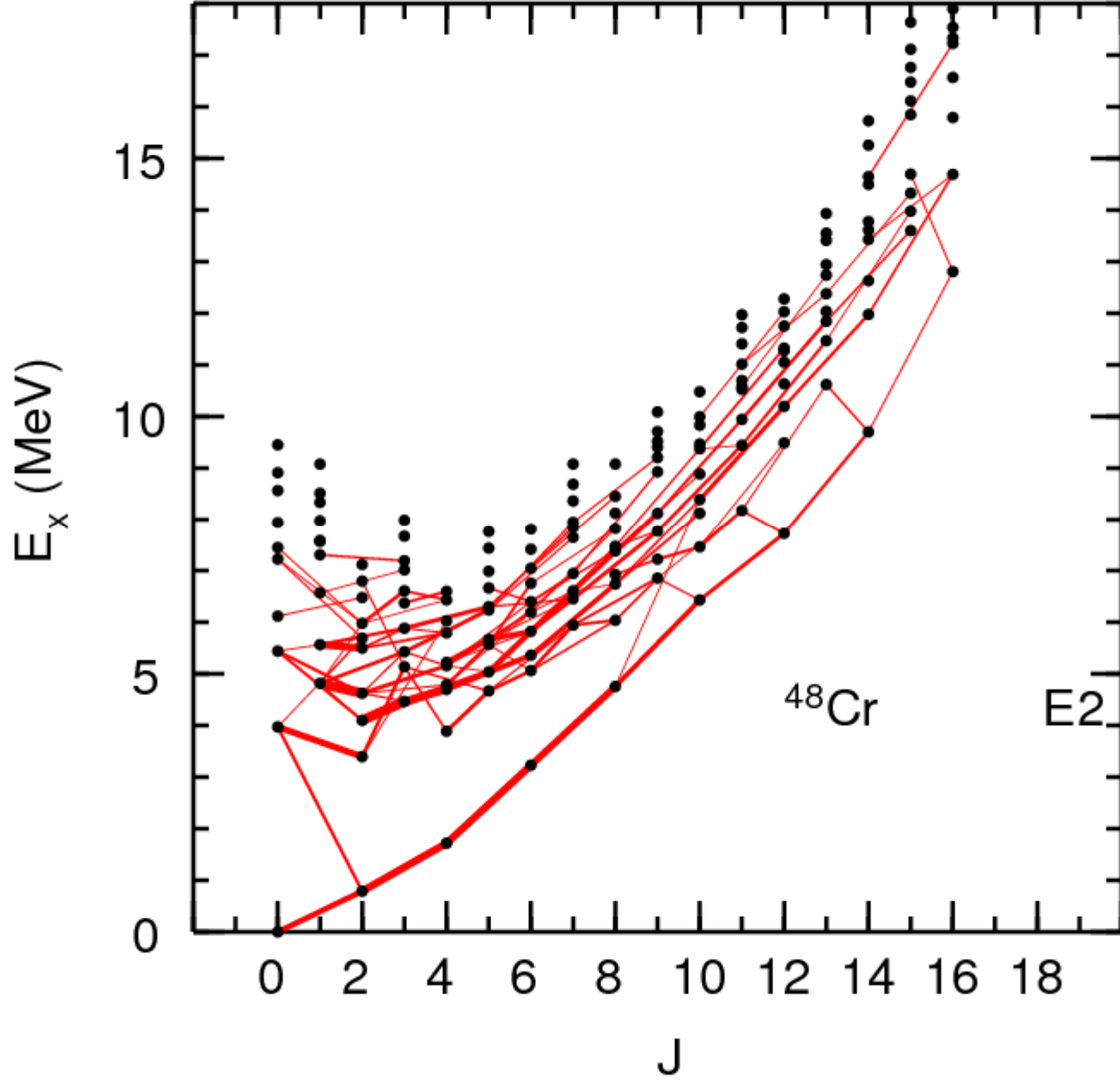
```

! model space = sd
! interaction = usdb
! e_p = 1.500
! e_n = 0.500
! g_sp = 5.586
! g_sn = -3.826
! g_lp = 1.000
! g_ln = 0.000

```

Ei (MeV)	Ji	ni	tau (psec)	T_(1/2) (psec)	M1 moment (u_N)	Q moment (e^2 fm^2)	
0.000	3/2+	1	0.000000	0.000000	2.097	11.83	-----
	Ef	Jf	nf	BR	del	B(M1)	B(E2)
0.399	5/2+	1	2.356305	1.633273	2.749	-2.50	-----
	Ef	Jf	nf	BR	del	B(M1)	B(E2)
0.000	3/2+	1	100.0000	-0.06	0.3780E+00	0.1332E+03	
2.169	7/2+	1	0.031591	0.021897	2.451	-12.45	-----
	Ef	Jf	nf	BR	del	B(M1)	B(E2)
0.000	3/2+	1	8.6893	999.00	0.0000E+00	0.4675E+02	
0.399	5/2+	1	91.3107	-0.23	0.2809E+00	0.6968E+02	
2.173	1/2+	1	0.057436	0.039811	1.061	0.00	-----
	Ef	Jf	nf	BR	del	B(M1)	B(E2)
0.000	3/2+	1	97.8102	0.16	0.9198E-01	0.6975E+01	
0.399	5/2+	1	2.1898	999.00	0.0000E+00	0.1771E+02	





2010-2011 with Eric McDonald

- 1) Improve the thick-restart version of Lanczos.
- 2) Port OpenMP parallelization to CUDA.
- 3) Test and optimize MPI and MPI/OpenMP versions.
- 4) Understand scalability barriers in NuShellX to enable most effective use of CUDA and leadership-class machines.

Goal is to make the calculation for one J state as fast as possible –
for J-scheme dimensions up to 10^9 (one billion)

To be combined with parallel options for many J and many nuclei.
For a given model space typically 10×200

