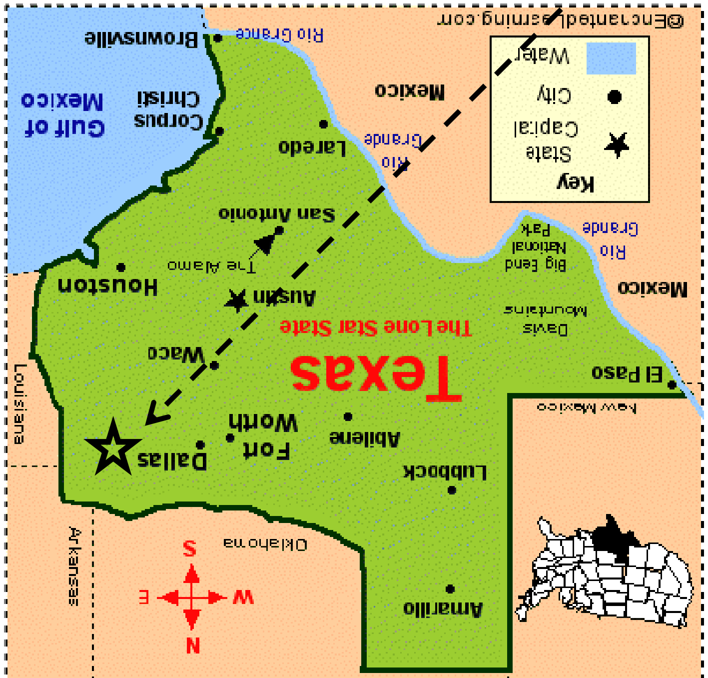
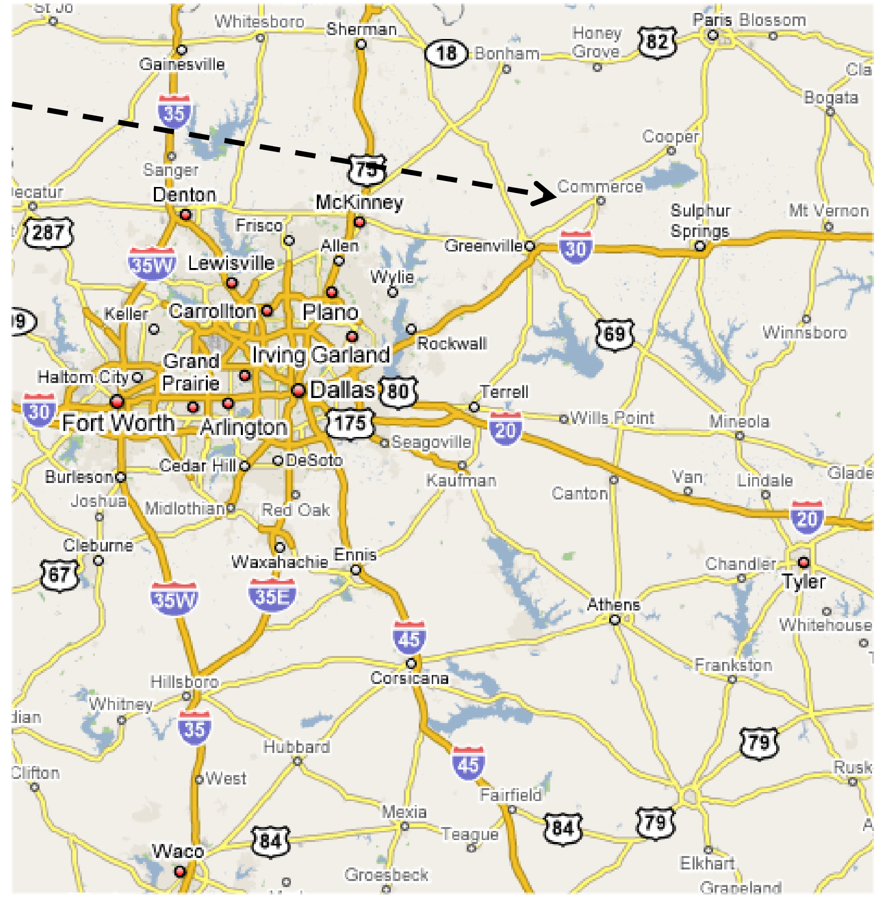
Benchmark calculations of nuclear mass tables

C.A. Bertulani (Texas A&M - Commerce)



As seen from Seattle



Physics – TAMU-Commerce

Mass tables with HFODD (J. Dobaczewski)

http://www.fuw.edu.pl/~dobaczew/hfodd/hfodd.html

1 – Code has ~ 60,000 lines.

2 - HFB, h.o. expansion, breaks all self-consistent symmetries, and t-symmetry.

3 - Includes t-odd terms in Skyrme functional.

4 – Large continuum space included

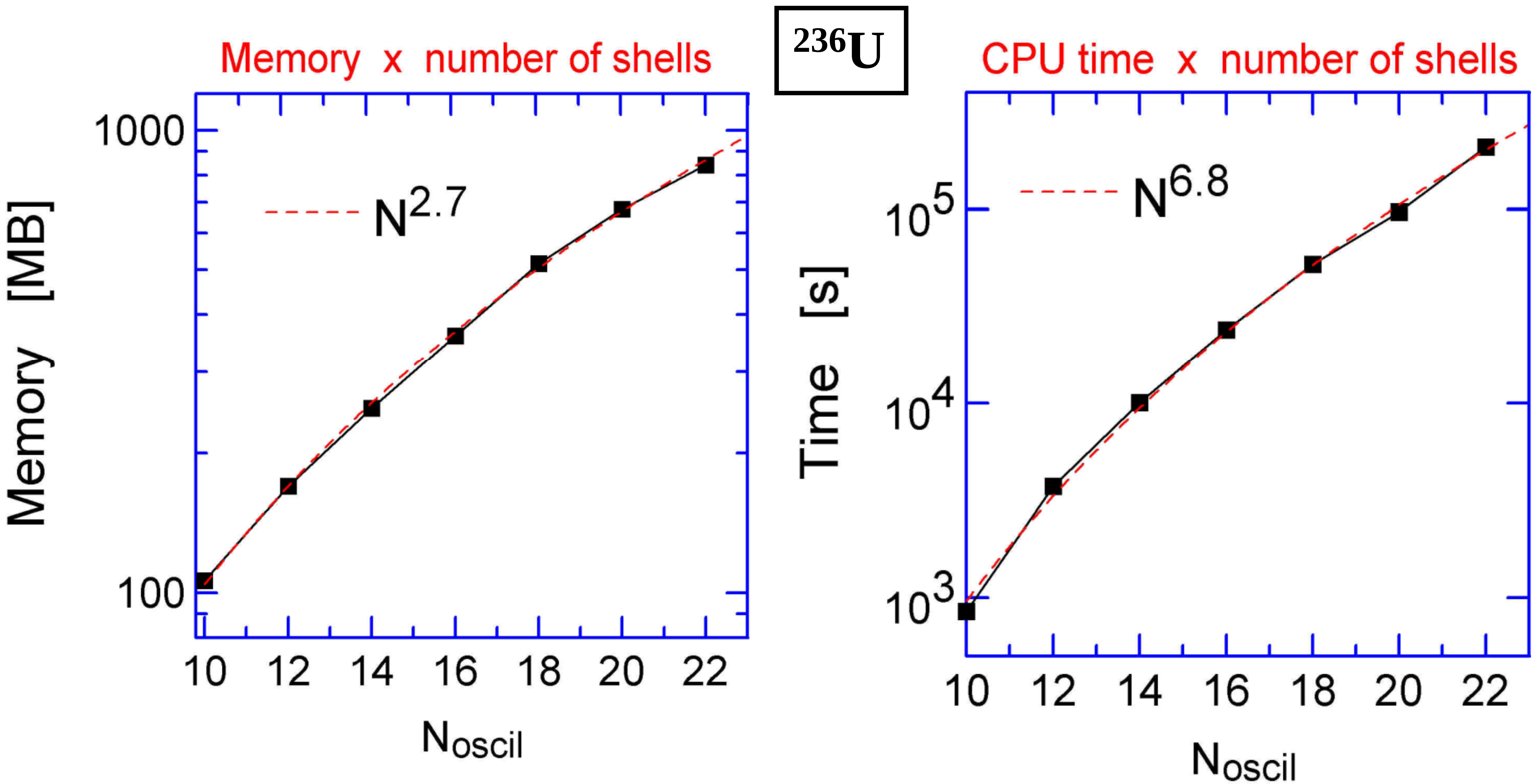
5 - Blocking and Lipkin-Nogami (LN) implemented recently by J. Dobaczewski.

Blocking still has convergence problems.

6 – People involved: Nazarewicz, Stoitsov, Schunck (ORNL), Dobaczewski (Poland), More, Sarich (Argonne), Bertulani (Tamu-Commerce)

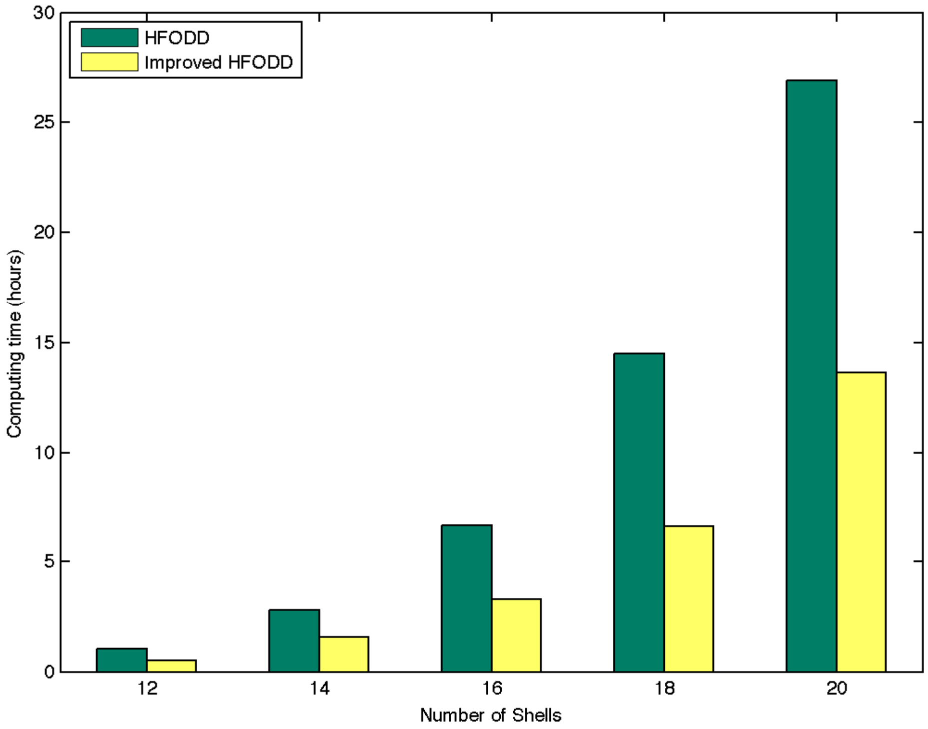
Warming up with HFODD

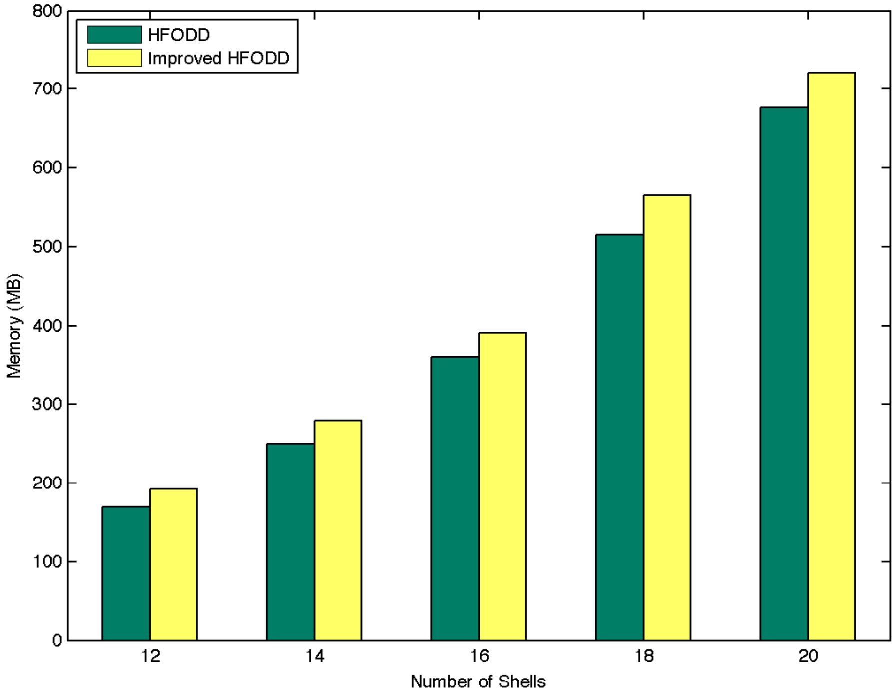
1 - Benchmarking Jan-March/2007 version, HFODD vs. 2.24 - 2.27
2 - ~ 55 cases (nuclei, different parameters)
3 – Tests done at INT/Washington workstations and Jaguar/ORNL (on one single processor). Both ~ 3 GHz clock speed.
4 – On Jaguar (5 GFlops/s): HFODD = 1.25 GFlops/s = 25% capacity



Improvements by **Jason Sarich**, incorporated in code by **Jacek Dobaczewski**

1 – Loops of matrix multiplications replaced by BLAS and LAPACK routines
2 – Similarly for eingevalue problem
3 – Presently: routines incorporated in a standalone code (portable), or links to BLAS and LAPACK (faster, platform optimized)





Figures from **Jorge More's** presentation at SciDAC meeting, June/2007

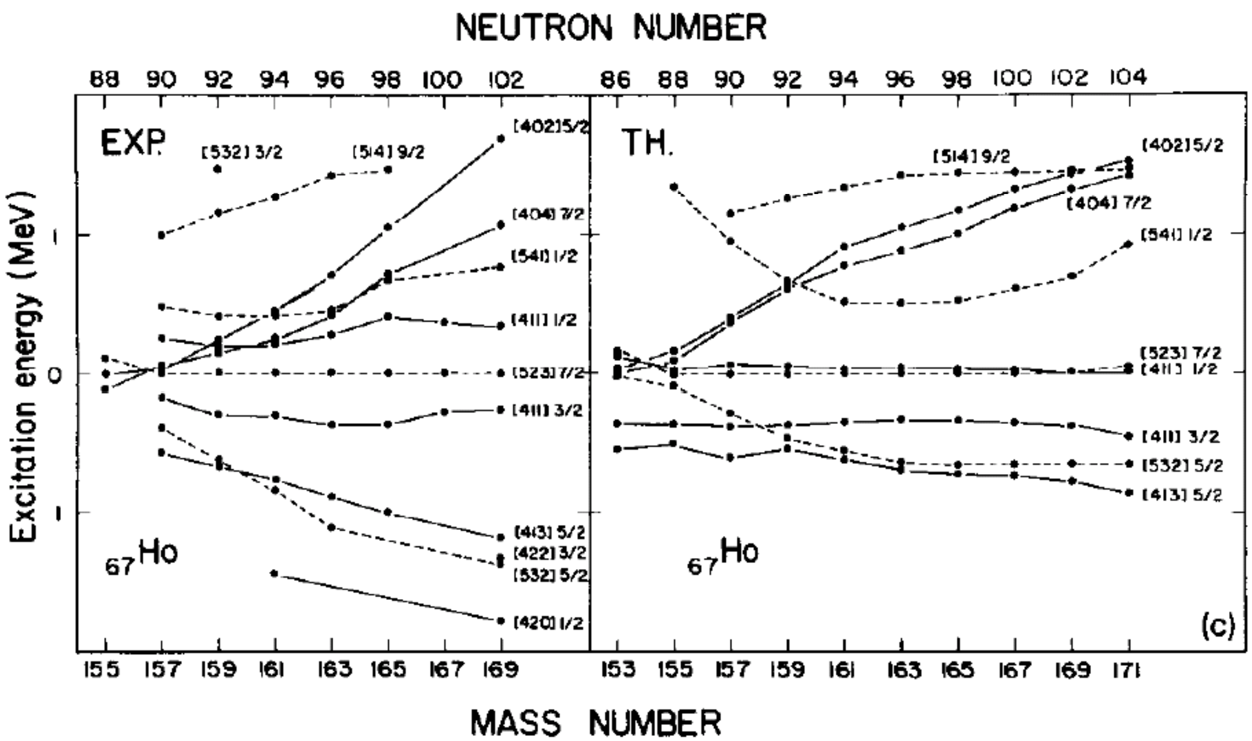
Numerous benchmarks done for the SciDAC project

Goals for HFODD

1 - Present version 2.31 (08/2007) include optimizations (**Sarich+Dobaczewski**), blocking and LN treatment of pairing (**Dobaczewski+Stoitsov**)
2 – Benchmarks with version 2.31 show similar improvements in speed.
3 – **Schunck + Sarich + Stoitsov**: N-Z walk on Jaguar
4 – UT/ORNL DFT-group + Texas (Bertulani): data analysis (chi-square's) and graphics interface.

5 – Goals for 2008, using 3+4:

• Analysis of <u>equilibrium deformations</u> and <u>excitation energies</u> for odd-nuclei:
e.g., improving upon Nazarewicz, Riley, Garret, NPA 512 (1990) 61



• Preliminary <u>mass tables</u> for odd-nuclei:
e.g., improving upon Dobaczewski, Stoitsov, Nazarewicz, nucl-th/0404077

Mass tables with EV8-ODD

EV8 (**P. Bonche, H. Flocard and P.H. Heenen**, CPC 171 (2005) 49)

1 – code has only 6,500 lines

2 - HF+BCS, 3-d coordinate mesh, axial symmetry, small continuum space

EV8 ODD:

3 – Blocking implemented recently by Bertsch.

4 - N-Z walker by Bertulani.

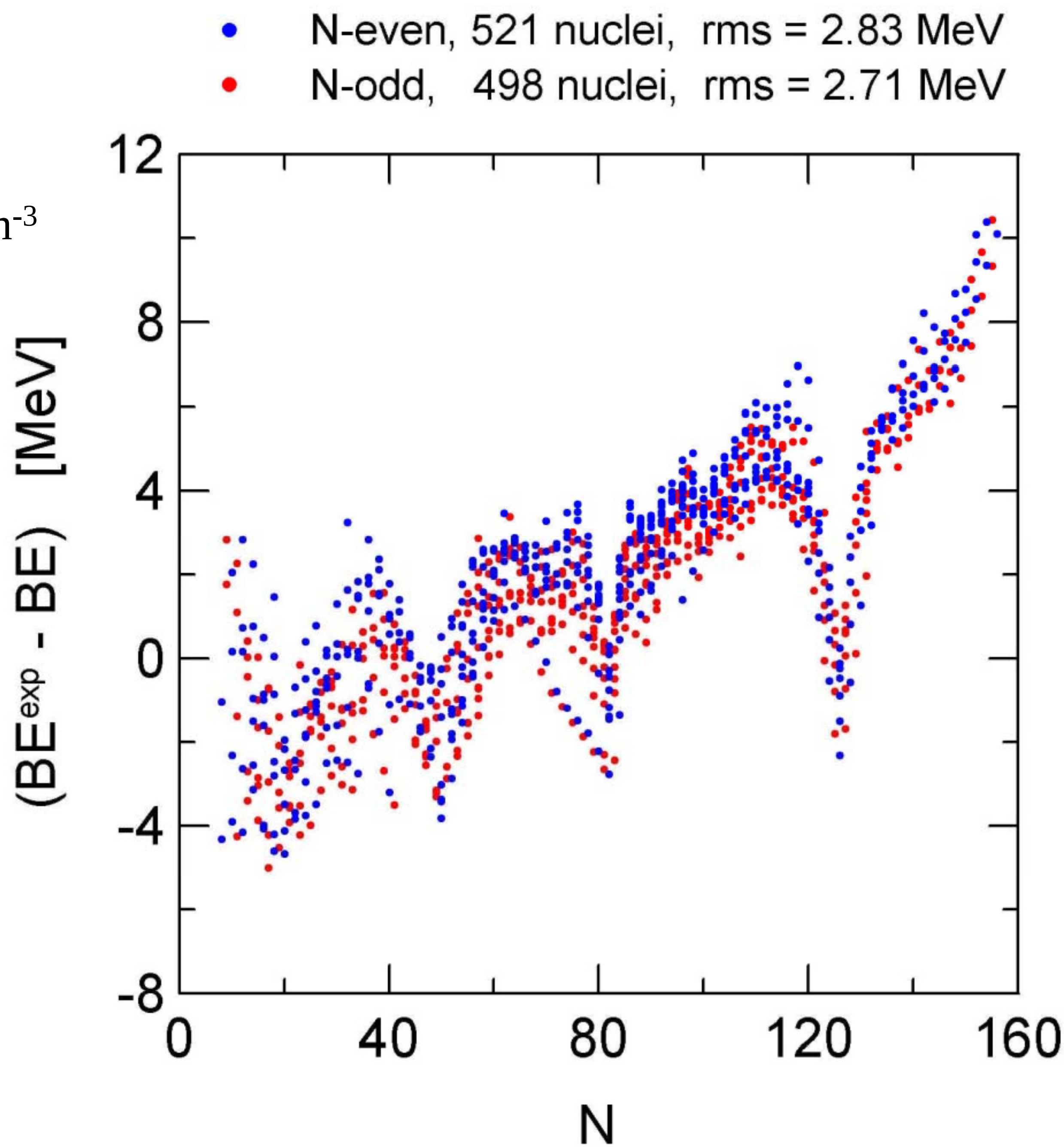
Binding energy residuals

Example: Skyrme = SLy4

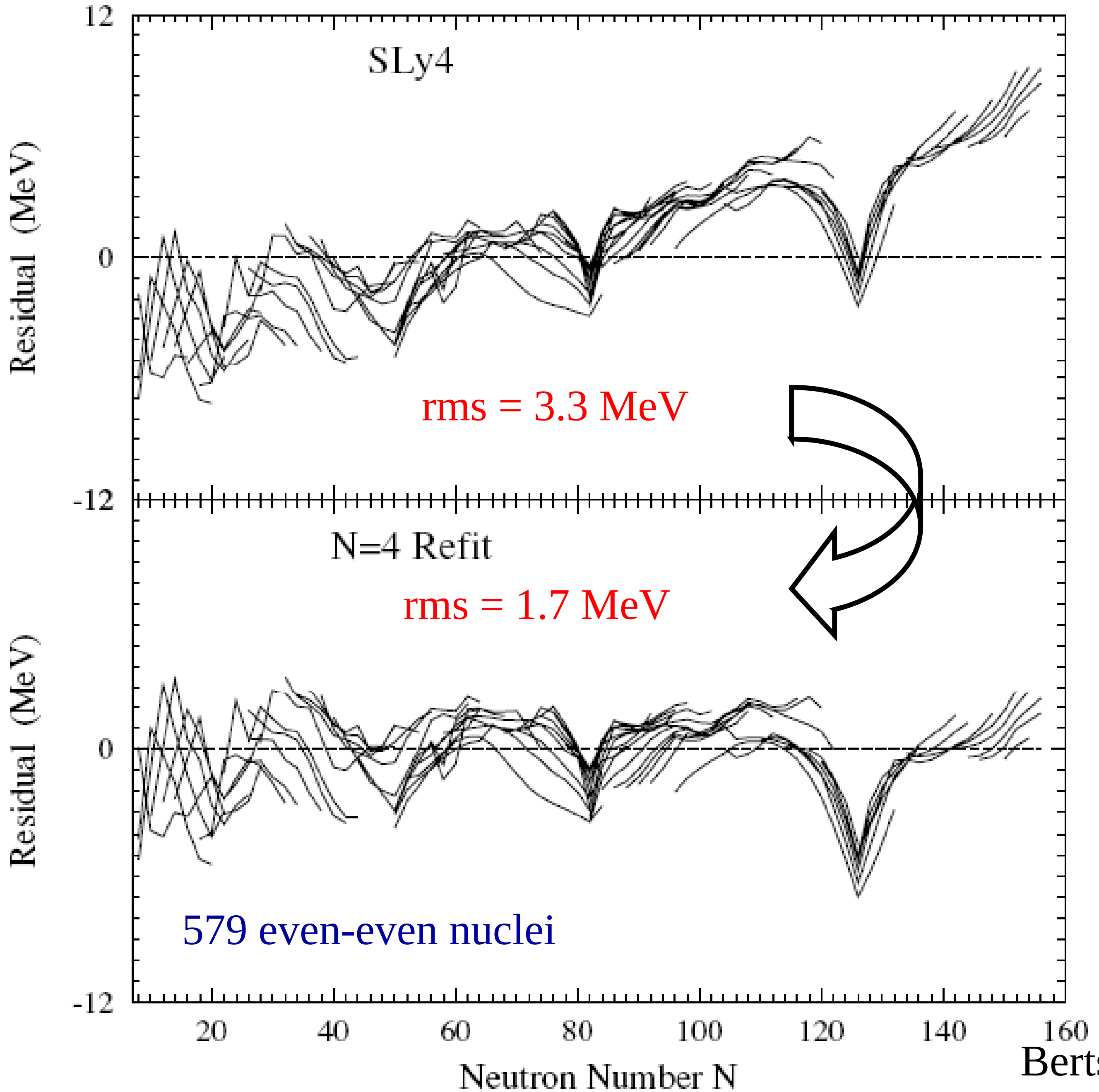
$V_{pairing} = g \cdot \delta(r_{12}) \cdot [1 - \rho(r)/\alpha]$

Surface pairing:

$g_n = g_p = 1000$ MeV fm^3, $\alpha = 0.16$ fm^{-3}



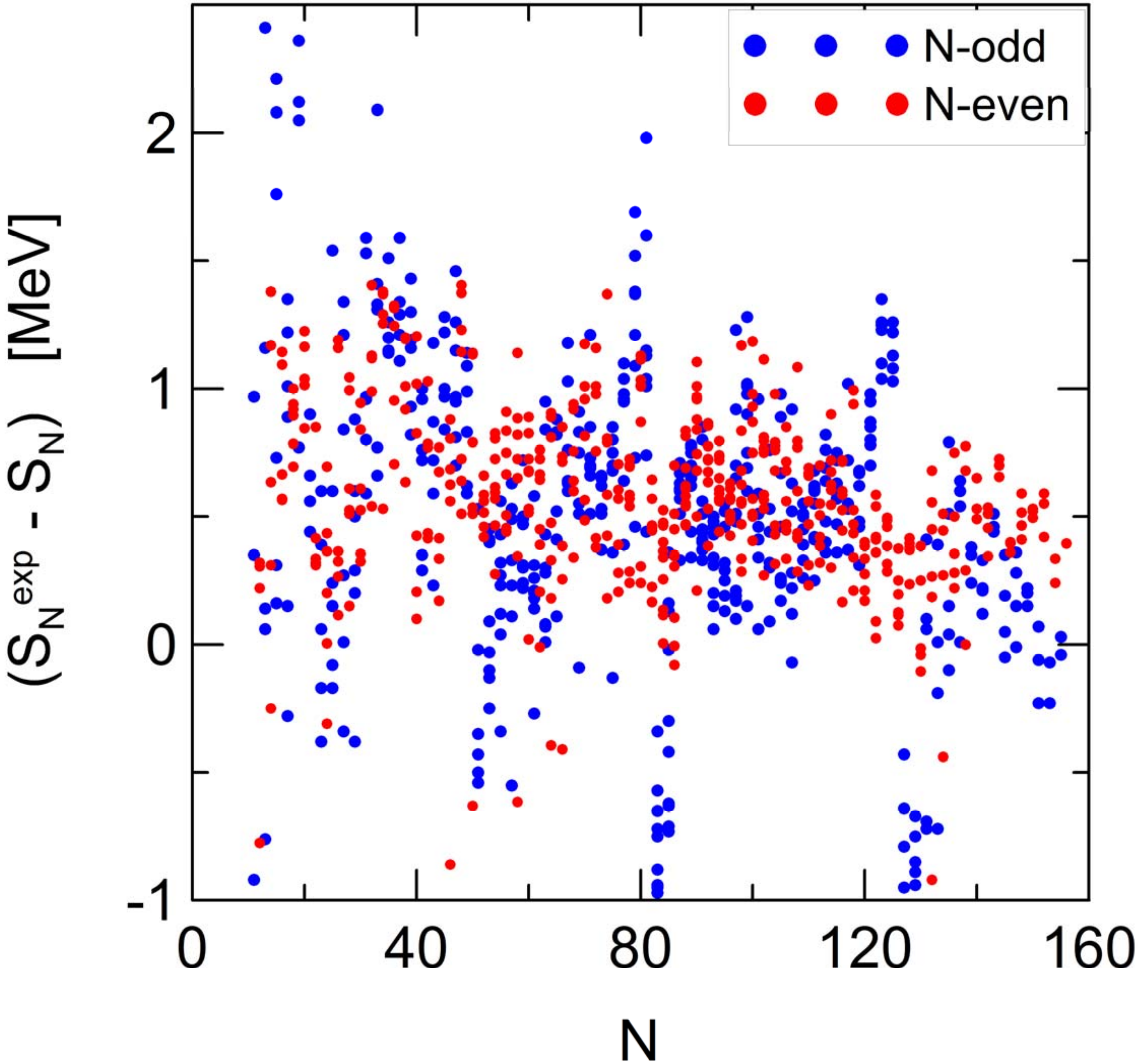
Goal: reduce rms by refitting interactions



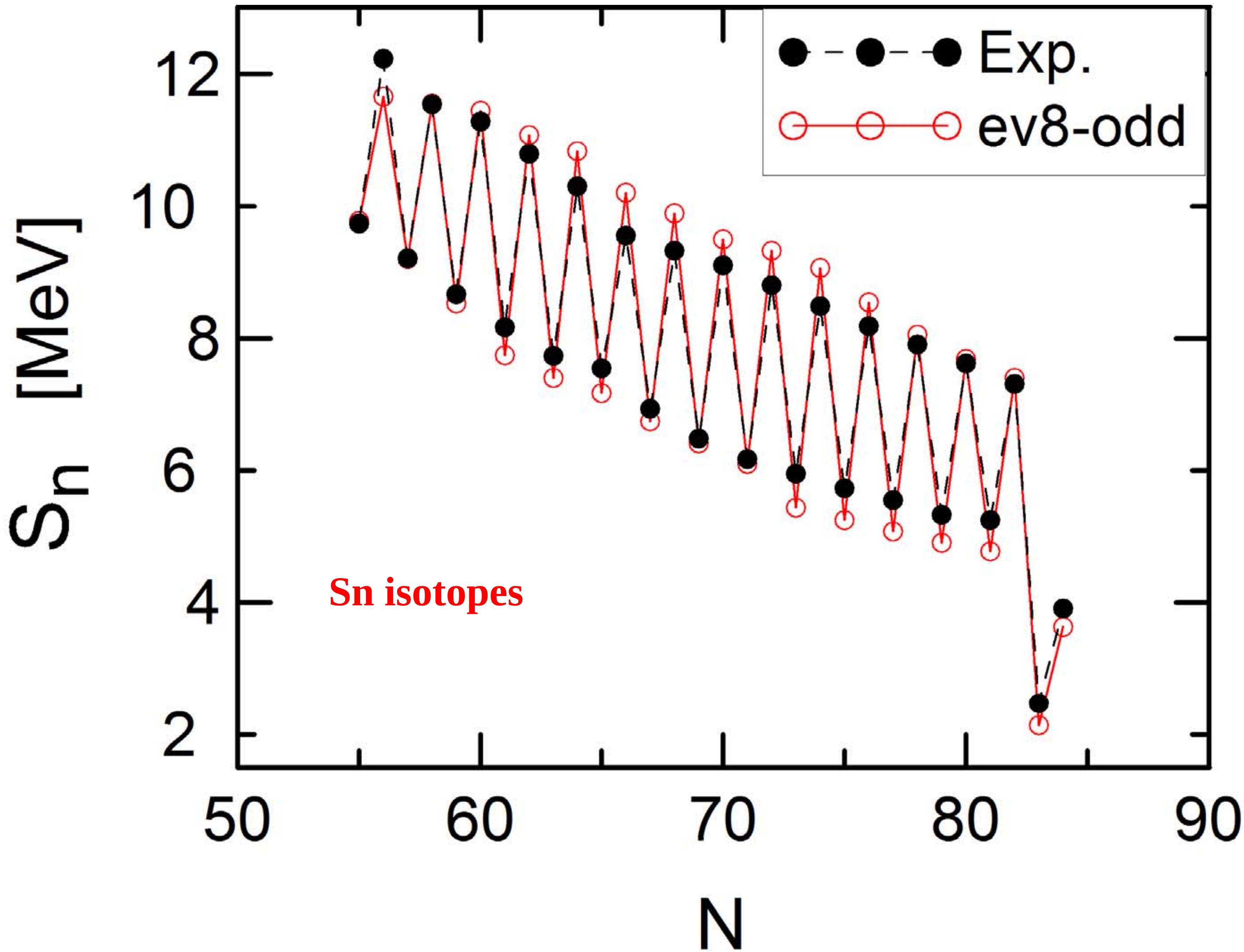
Bertsch, Sabbey, Uusnakki,
PRC **71**, 054311 (2005)

Separation energy residuals

$$S(N,Z) = M(N-1,Z) + M_n - M(N,Z)$$



Odd-even staggering



Odd-even staggering and pairing strength

3-point filter: **$\Delta = \frac{1}{2} \cdot (-1)^N [S(N,Z) - S(N-1, Z)] \cong \frac{1}{2} \cdot (-1)^N \partial^2 B / \partial^2 N$**

N = odd(o), even(e)

Mechanism	$\Delta_o^{(3)}$	$\Delta_e^{(3)}$
Single-particle	0	$(e_i - e_{i-i})/2$
BCS correlation	Δ_{BCS}	Δ_{BCS}
T-odd pp	$-v_{i\bar{i},i\bar{i}}/2$	$\bar{v} - v_{i\bar{i},i\bar{i}}/2$
T-odd DFT		
T-even polarization	$-e_{cp}$	0

Table by Bertsch

Satula, Dobaczewski, Nazarewicz, PRL.81,3599 (1998).

Rutz, Bender, Reinhard, Maruhn, PL B468, 1 (1999).

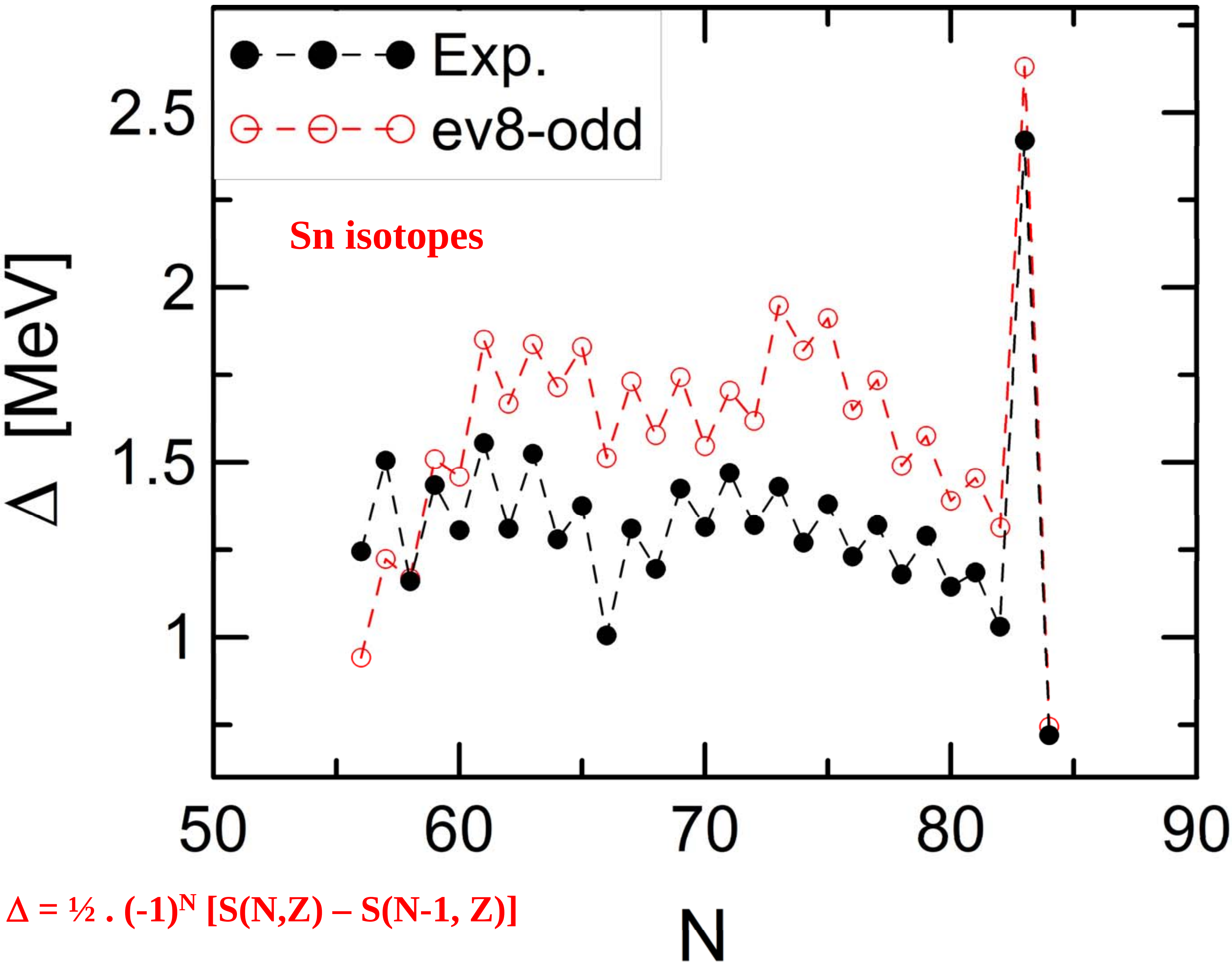
$$B = E_{sp} - \tilde{E}_{sp} + E_{macro}$$

$$E_{sp} = \sum_k e_k$$

$$\Delta^{(o)}{}_{sp} \approx 0, \qquad \Delta^{(e)}{}_{sp} \approx \frac{e_n - e_{n-1}}{2}$$

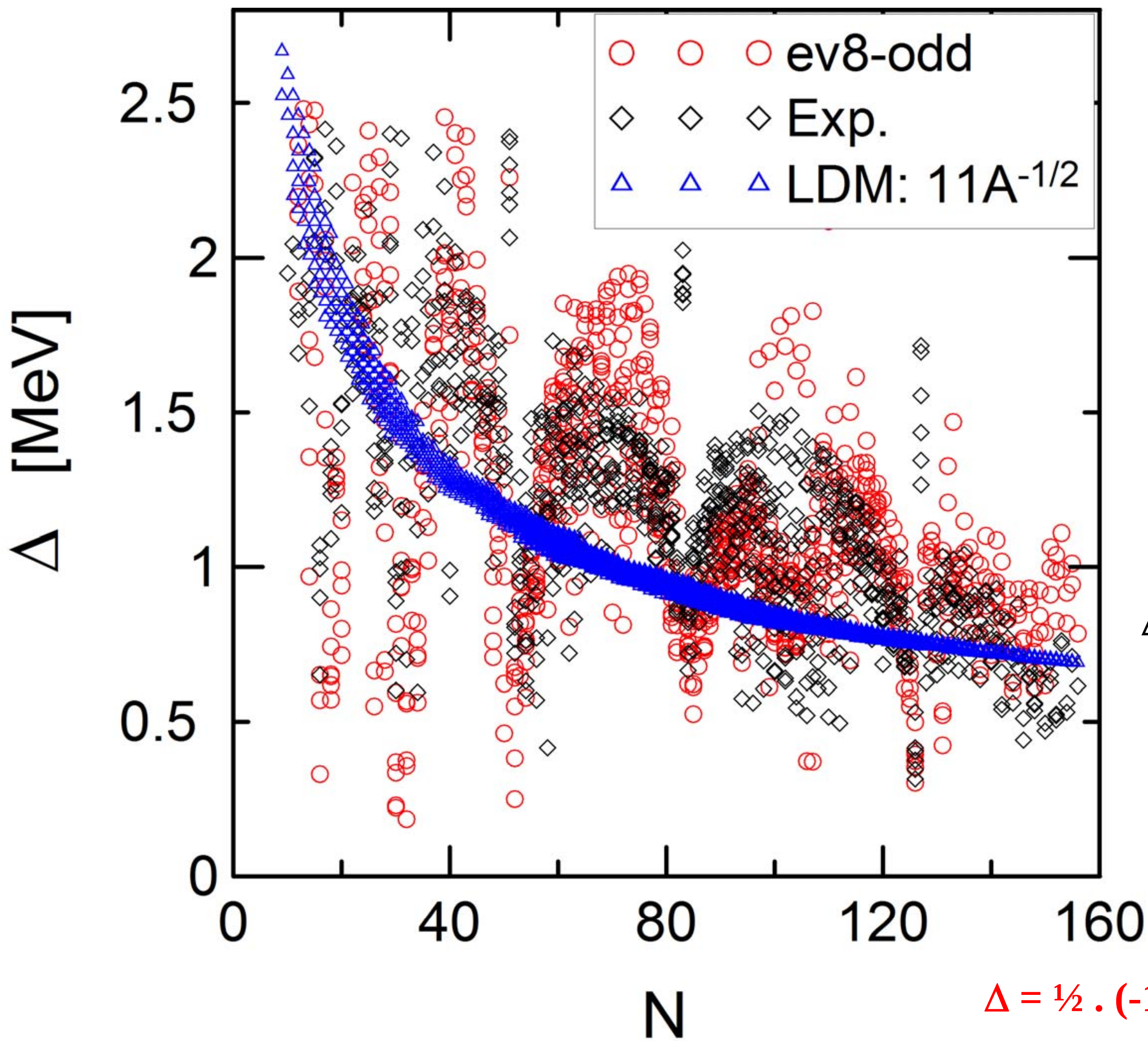
$$\partial^2 B_{\tilde{E}_{sp}} / \partial N^2 \approx \partial^2 B_{macro} / \partial N^2$$

Odd-even staggering from ev8-odd



$\Delta = \frac{1}{2} \cdot (-1)^N [S(N,Z) - S(N-1, Z)]$

Odd-even staggering with 967 masses!



From even-even to even-odd and odd-odd (absolute value):

$$\Delta_{LDM} = \frac{11}{A^{1/2}} \text{ MeV}$$

$\Delta = ½ . (-1)^N [S(N,Z) – S(N-1, Z)]$

Dependence on pairing strength

Skyrme = SLy4

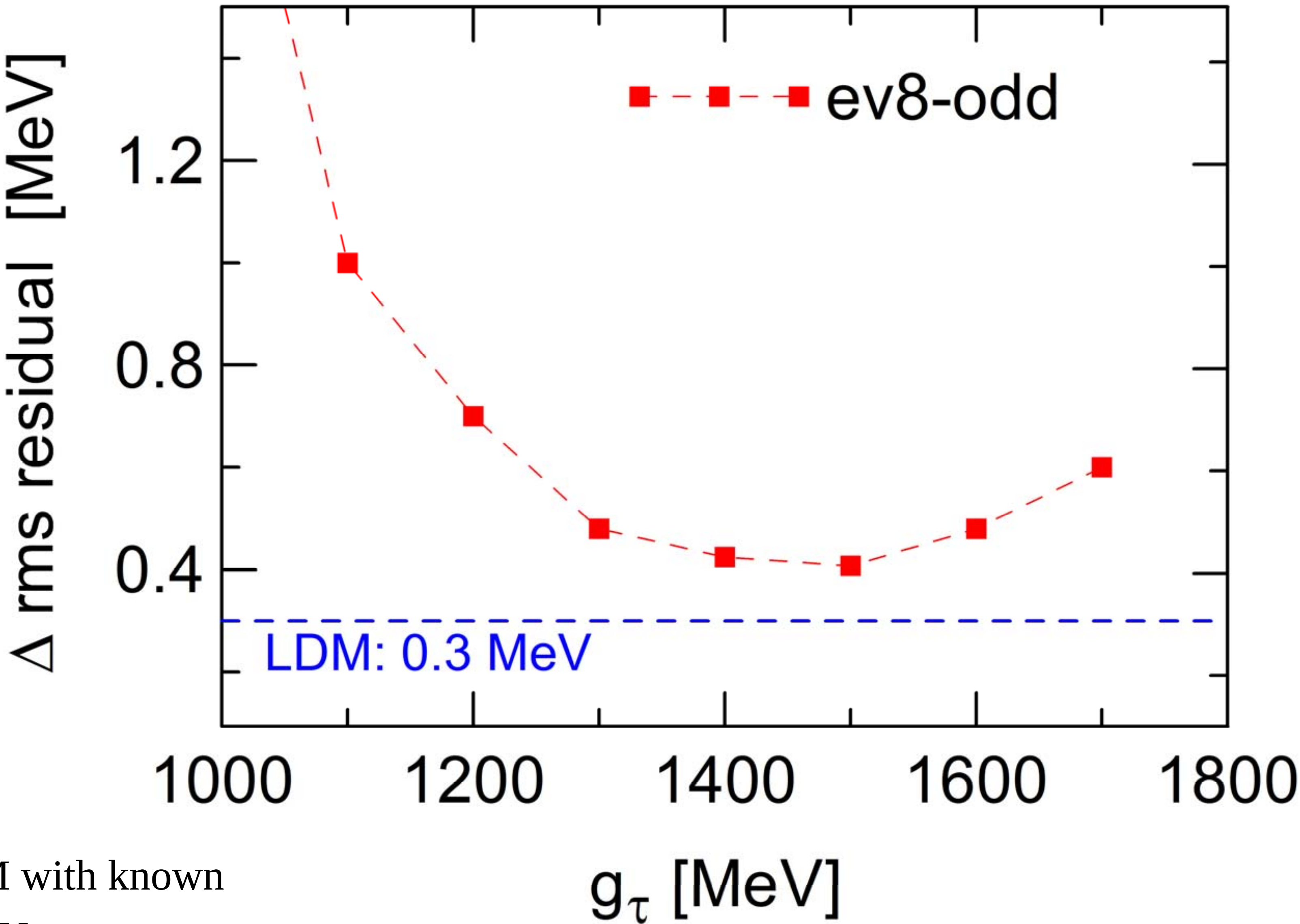
$V_{pairing} = g \, . \, \delta(r_{12}) \, . \, [1- \rho(r)/\alpha]$

$\alpha = 0.16 \text{ fm}^{-3}$

search for $g_n = g_p$

$\Delta = ½ \, . \, (-1)^N \, [S(N,Z) – S(N-1, Z)]$

From even-even to even-odd and odd-odd (absolute value):



$$\Delta_{LDM} = \frac{11}{A^{1/2}} \text{ MeV}$$

rms residual for LDM with known exp. data = 0.299 MeV

In progress

1 – BCS+Lipkin-Nogami mass table.

2 – Functional parameters chi-square including odd isotopes and isotones.

3 – Mass table in one-two weeks on a single processor.

4- Runs on NERSC supercomputers for minima search.