Benchmark calculations of nuclear mass tables

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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 eigenvalue 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 equilibrium deformations and excitation energies for odd-nuclei:
  e.g., improving upon Nazarewicz, Riley, Garret, NPA 512 (1990) 61

- Preliminary mass tables 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

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

Surface pairing:

\[ g_n = g_p = 1000 \text{ MeV fm}^3, \alpha = 0.16 \text{ fm}^{-3} \]
Goal: reduce rms by refitting interactions

SLy4

rms = 3.3 MeV

N=4 Refit

rms = 1.7 MeV

579 even-even nuclei

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

Sn isotopes

$S_n$ [MeV]

N
**Odd-even staggering and pairing strength**

3-point filter: \[ \Delta = \frac{1}{2} \cdot (-1)^N \left[ S(N,Z) - S(N-1,Z) \right] \equiv \frac{1}{2} \cdot (-1)^N \frac{\partial^2 B}{\partial^2 N} \]

N = odd(o), even(e)

<table>
<thead>
<tr>
<th>Mechanism</th>
<th>( \Delta_{o}^{(3)} )</th>
<th>( \Delta_{e}^{(3)} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Single-particle</td>
<td>0</td>
<td>( (e_i - e_{i-1})/2 )</td>
</tr>
<tr>
<td>BCS correlation</td>
<td>( \Delta_{BCS} )</td>
<td>( \Delta_{BCS} )</td>
</tr>
<tr>
<td>T-odd pp</td>
<td>( -v_{\nu,\nu}/2 )</td>
<td>( v - v_{\nu,\nu}/2 )</td>
</tr>
<tr>
<td>T-odd DFT</td>
<td>( -e_{cp} )</td>
<td>0</td>
</tr>
<tr>
<td>T-even polarization</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>


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

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

\[ E_{sp} = \sum_{k} e_k \]

\( \Delta_{sp}^{(o)} \approx 0, \quad \Delta_{sp}^{(e)} \approx \frac{e_n - e_{n-1}}{2} \]

\[ \frac{\partial^2 B_{\tilde{E}_{sp}}}{\partial N^2} \approx \frac{\partial^2 B_{macro}}{\partial N^2} \]
Odd-even staggering from ev8-odd

\[ \Delta = \frac{1}{2} \cdot (-1)^N \left[ S(N,Z) - S(N-1, Z) \right] \]
Odd-even staggering with 967 masses!

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

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

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

Skyrme = SLy4

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

\( \alpha = 0.16 \text{ fm}^{-3} \)

search for \( g_n = g_p \)

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

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

LDM: 0.3 MeV
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.