Large-Scale Mass Table Calculations

M. Stoitsov

J. Dobaczewski, W. Nazarewicz, J. Pei, N. Schunck

Department of Physics and Astronomy, University of Tennessee, Knoxville, TN 37996, USA
Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA

Joint Institute for Heavy-Ion Research, Oak Ridge, Tennessee, 37831, USA

Institute of Nuclear Research and Nuclear Energy, Bulgarian Academy of Sciences, Sofia, Bulgaria

Institute of Theoretical Physics, Warsaw University, ul. Hoża 69, 00-681 Warsaw, Poland

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Large-Scale Mass Table Calculations

- Calculations with existing energy density functionals
  - Comparison with experimental data (filters etc.) to understand what is missing
- Testing new terms/functionals to improve the agreement
  - Experimental data
  - Bench mark results
- Producing new fit for existing parameters
  - Nuclear matter
  - Experimental data
  - Bench mark results
- New physics when analyzing the global trends (drip lines, odd nuclei, …)

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Codes

- Fortran codes for control against exact integration
  - HFBRAD – box, coordinate space, spherical symmetry
  - 2Dspline – rectangular box, splines, axial/parity symmetry
- Official code for UNEDF calculations
  - HFODD – 3D in HO basis, symmetry unrestricted, time-odd components, cranking, projections …
  - Approximately 4 h 39 min CPU per nucleus (^{120}Sn)
- Fast alternative for ground-state calculations
  - HFBTHO – 2D in HO/THO basis, axial/parity symmetry
  - Approximately 3 min CPU per nucleus (^{120}Sn)

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HFODD/HFBTHO even-even nuclei

Nucleus:	^{208}Pb		^{168}Er		^{120}Sn	
Code:	HFBTHO	HFODD	HFBTHO	HFODD	HFBTHO	HFODD
Basis:	2D-HO	3D-HO	2D-HO	3D-HO	2D-HO	3D-HO
N_0	14	14	14	14	14	14
$N_{\rm st}$	680	680	680	680	680	680
$b_\perp = b_z$	2.2348121	2.2348121	2.1566616	2.1566616	2.039048	2.039048
λ_n	−8.114078	−8.11402	−6.936059	−6.936058	−8.015208	−8.015208
λ_p	−8.810477	−8.810445	−7.156486	−7.156477	−8.251999	−8.245192
Δ_n	0	0	0.394572	0.394578	1.244644	1.244645
Δ_p	0	0	0.390602	0.390605	0	0
$E_n^{\rm pair}$	0	0	−1.716979	−1.717024	−12.426388	−12.426397
$E_p^{\rm pair}$	0	0	−1.528616	−1.528643	0	0
R_n	5.619756	5.619757	5.357578	5.357578	4.733088	4.7331
R_p	5.460078	5.460090	5.225538	5.225539	4.596294	4.5963
Q_n	−0.000001	6.6E-11	11.473918	11.473920	−0.0000001	6.6E-11
Q_p	−0.000001	4.7E-11	7.880221	7.880224	−0.0000001	6.6E-11
$E_n^{\rm kin}$	2525.992765	2525.991925	1974.614008	1974.613824	1338.210478	1338.210501
$E_p^{\rm kin}$	1334.855572	1334.854465	1118.313683	1118.313442	829.438221	829.438221
$E_{\rm SO}$	−96.375045	−96.375003	−80.186809	−80.186826	−49.002307	−49.002316
$E_{\rm dir}$	827.607375	827.607885	602.810248	602.810352	366.326962	366.326917
$E_{\rm exc}$	−31.248479	−31.248462	−25.935910	−25.935905	−19.08958	−19.08958
$E_{\rm tot}$	−1634.148867	−1634.148120	−1357.658500	−1357.658322	−1018.141626	−1018.141673

HFODD/HFBTHO odd nuclei

state:	1/2+[4,4,0]		1/2+[4,0,0]		3/2−[5,2,1]	
code:	HFBTHO	HFODD	HFBTHO	HFODD	HFBTHO	HFODD
N_0	14	14	14	14	14	14
$N_{\rm st}$	680	680	680	680	680	680
$b_\perp = b_z$	2.0418697	2.0418697	2.0418697	2.0418697	2.0418697	2.0418697
$E_{\rm qp}$	1.007644	1.008	1.611961	1.612	1.388951	1.387
λ_n	−7.749566	−7.7494	−7.696179	−7.6962	−7.972801	−7.9742
$E_n^{\rm pair}$	−9.294443	−9.2964	−10.397019	−10.3983	−8.703141	−8.7035
Δ_n	1.057516	1.0576	1.120611	1.1207	1.037402	1.0373
r_t	4.689535	4.6895	4.690459	4.6905	4.689510	4.6895
β	−0.025699	−0.0256	0.000000	0.0001	0.015789	0.0147
Q_t	−0.862706	−0.8604	0.000000	0.0036	0.530038	0.4921
$E_n^{\rm kin}$	1360.437867	1360.442751	1362.407077	1362.409601	1358.912567	1358.886614
$E_p^{\rm kin}$	827.317590	827.317961	827.123364	827.123676	827.195176	827.191207
$E_{\rm SO}$	−50.483676	−50.485916	−50.922860	−50.923940	−49.607742	−49.592026
$E_{\rm dir}$	365.743676	365.743774	365.621013	365.621031	365.736277	365.735680
$E_{\rm tot}$	−1024.707275	−1024.707272	−1024.301233	−1024.301252	−1024.415866	−1024.416901

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Scale of the Problem

Science scales with processors

Jaguar@ OAK RIDGE National Laboratory 17064 processors

Even-Even Nuclei

➲ The largest mass table map from SkM* forces enlarged with 10 more nuclei beyond both drip lines contains altogether 2525 even-even nuclei

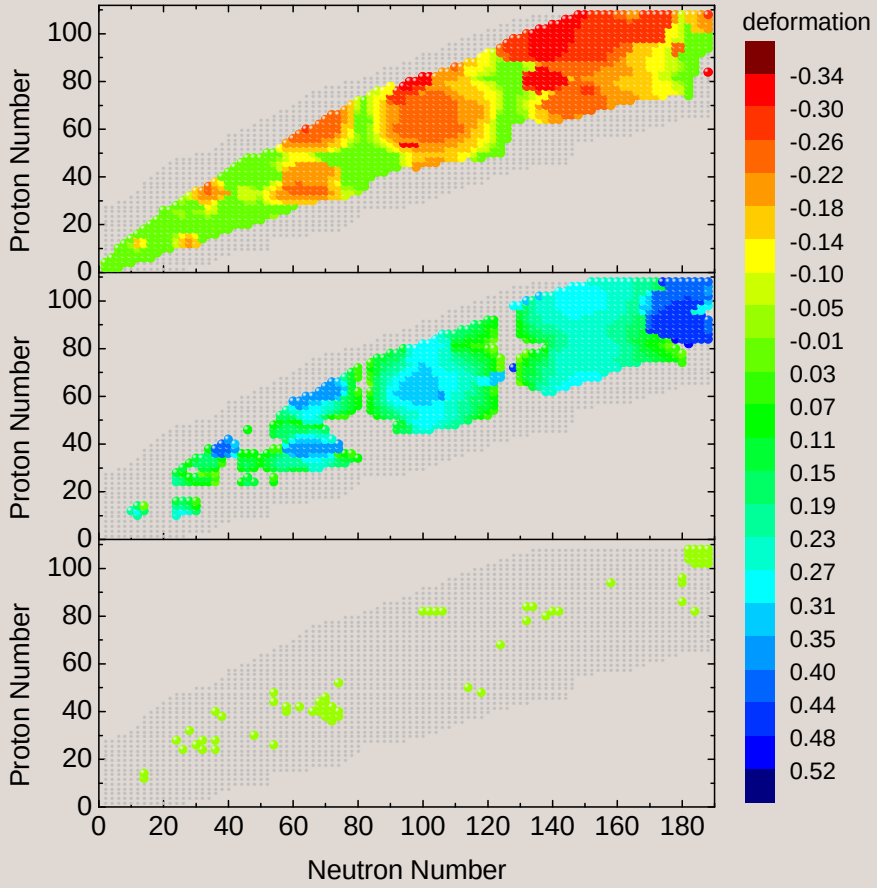
➲ A single processor calculates each nucleus 3 times (prolate, oblate, spherical) and records all nuclear characteristics and blocking candidates

➲ Using 2525 processors - about 4 CPU hours

Odd Nuclei

➲ The resulting even-even mass table contains 2731 nuclei which generate altogether 250754 odd-even and odd-odd states/nuclei at 0.5 MeV threshold for the blocking candidates

➲ Using 10 000 processors - about 24 CPU hours



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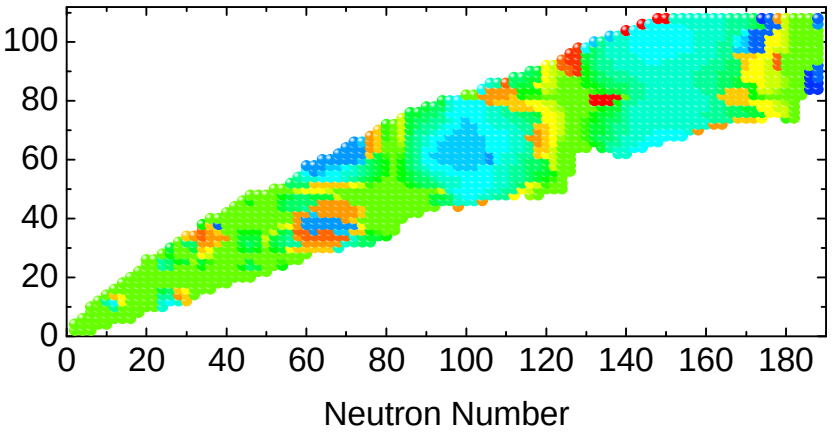
Broyden Mixing

A typical run for the whole even-even mass chart contains about 2731 different bound nuclear states which identify the ground states for all 1527 even-even nuclei entering the mass chart between nuclear drip lines.



At the end of the run:
2032 converge for up to 500 iterations
404 converge up to 1000 iterations
123 converge up to 2000 iterations
152 converge up to 6000 iterations
26 which still do not converge

$$V^{(m+1)} = (1-\alpha)V^{(m-1)} + \alpha V^{(m)}$$

$$= V^{(m)} + \alpha F^{(m)}(V)$$

$$F^{(m)}(V) = V^{(m-1)} - V^{(m)}$$

$$F(V) = 0$$

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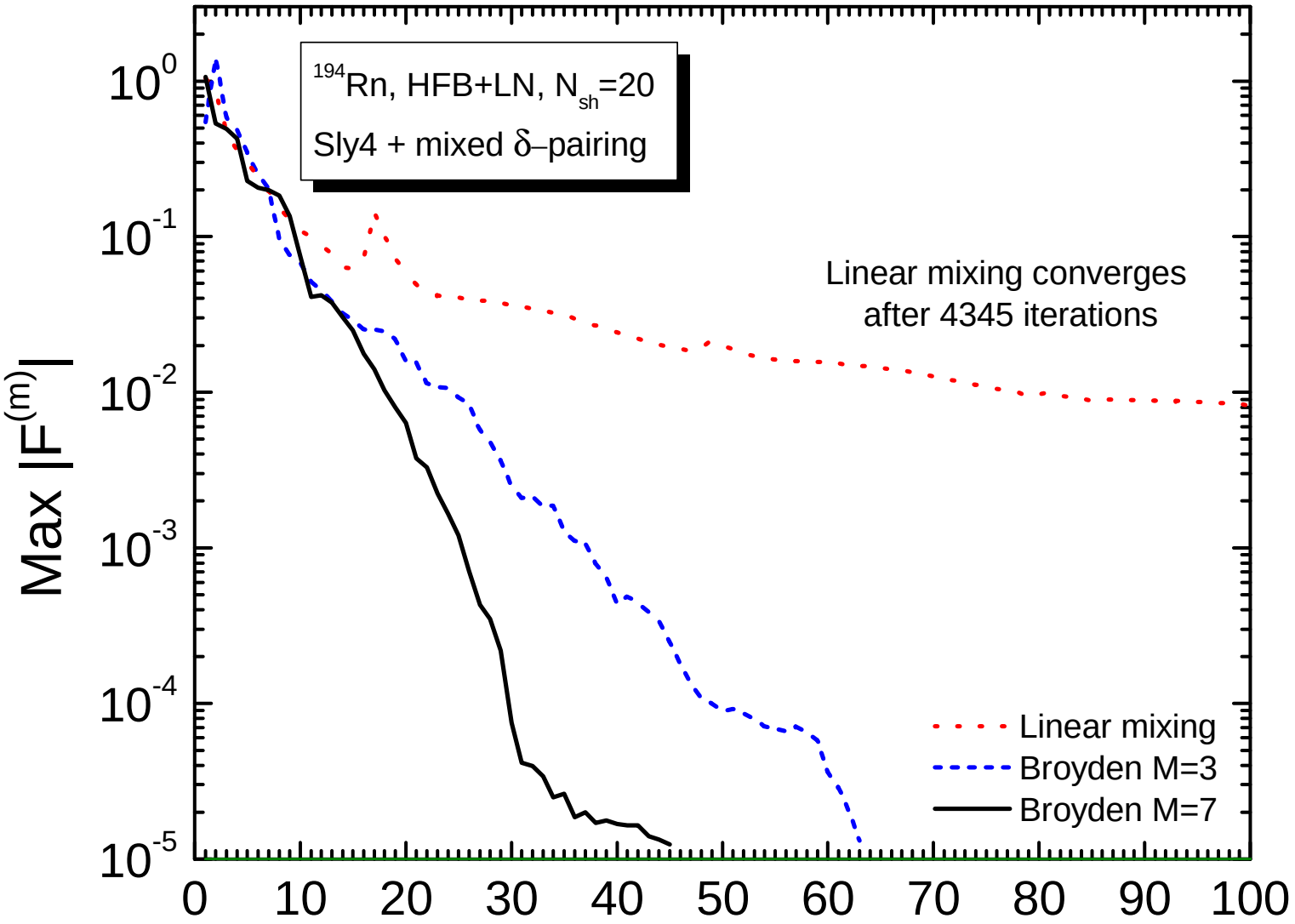
Broyden Mixing



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To do list

- Complete mass tables with all major Skyrme functionals
- Interface HFODD/HFBTHO
- Analysis of the global trends
- New terms/functionals
- Work on the fitting strategy