

DFT infrastructure

M. Stoitsov

Department of Physics and Astronomy, UT, Knoxville, TN 37996, USA

Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA

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

INRNE, Bulgarian Academy of Sciences, Sofia, Bulgaria

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

- DFT solvers
- Benchmark Results
- Broyden's Method
- Large-Scale Calculations
- Mass Table Explorer

Large-Scale Mass Table Calculations

Papers

- *Particle-number projection and the density functional theory*, J. Dobaczewski, M.V. Stoitsov, W. Nazarewicz, and P.-G. Reinhard, Phys. Rev. C **76**, 054315 (2007).
- *Shell structure beyond the proton drip line studied via proton emission from deformed ^{141}Ho* , M. Karny, K.P. Rykaczewski, R.K. Grzywacz, J.C. Batchelder, C.R. Bingham, C. Goodin, C.J. Gross, J.H. Hamilton, A. Korgul, W. Krolas, S.N. Liddick, K. Li, K.H. Maier, C. Mazzocchi, A. Piechaczek, K. Rykaczewski, D. Schapira, D. Simpson, M.N. Tantawy, J.A. Winger, C.H. Yu, E.F. Zganjar, N. Nikolov, J. Dobaczewski, A.T. Kruppa, W. Nazarewicz, and M.V. Stoitsov, Phys. Lett. B **664**, 52 (2008).
- *New efficient method for performing Hartree-Fock-Bogoliubov calculations for weakly bound nuclei*, M. Stoitsov, N. Michel, K. Matsuyanagi, Phys. Rev. C **77**, 054301 (2008).

Talks

- *Proton-Neutron Correlation Energies From Self-Consistent Large-Scale Mass Calculations*, **M.V. Stoitsov** and W. Nazarewicz, Proceedings Sixth International Conference of the Balkan Physical Union, ed. by S.A. Cetin and I. Hikmet, AIP Conf. Proc. **899**, 26 (2007).
- *Nuclear DFT: questions and challenges*, **W. Nazarewicz**, First FIDIPRO-JSPS Workshop On Energy Density Functionals In Nuclei, Keurusselka, Finland, October 25-27, 2007.
- *Nuclear Structure '07: Exciting, Broad, Relevant*, **W. Nazarewicz**, Fourth International Conference on Fission and Properties of Neutron-Rich Nuclei, Sanibel Island, Florida, Nov 11-17, 2007.
- *Computing Atomic Nuclei*, **W. Nazarewicz**, IOP Annual Nuclear Physics Group Conference, Liverpool, UK, April 1, 2008.
- *Science of rare isotopes: connecting nuclei with the universe*, **W. Nazarewicz**, plenary talk, 2008 APS April Meeting St. Louis, Missouri, April 12, 2008.
- *Large-scale mass table calculations with DFT*, **M. Stoitsov**, The 2nd LACM-EFES-JUSTIPEN Workshop, Joint Institute for Heavy Ion Research, Oak Ridge, Tennessee, USA, January 23-25, 2008
- *Large-scale mass table calculations with the UNEDF project*, **M. Stoitsov**, Mass Olympics, ECT* Workshop, May 26-30, 2008
- *Broyden Mixing for Nuclear Density Functional Calculations*, **M.V. Stoitsov**, Proc. 26th Int. Workshop on Nuclear Theory, Rila Mountains, Bulgaria, June 2007, p. 13.

DFT solvers

- DFT solvers in coordinate space for control against exact numerical integration
 - HFBRAD – box, coordinate space, spherical symmetry
 - HFBAX – rectangular box, B-splines, axial/parity symmetry
 - Ev8 – HF+BCS, 3D-Cartesian mesh

- DFT solvers in configurational (HO) space
 - HFODD – 3D in HO basis, symmetry unrestricted, time-odd components, cranking, projections ...
 - Fast alternative for ground-state calculations
 - HFBTHO – 2D in HO/THO basis, axial/parity symmetry

- New generation HFB solvers
 - highly precise multi-resolution wavelets method
(see the talk of G. Fann)

HFODD/HFBTHO Benchmark

- HFBODD: Approximately 6 h 39 min CPU per nucleus (^{120}Sn)
- HFBTHO: Approximately 3 min CPU per nucleus (^{120}Sn)

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_{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	-8.114 078	-8.114 02	-6.9360 59	-6.9360 58	-8.015208	-8.015208
λ_p	-8.8104 77	-8.8104 45	-7.1564 86	-7.1564 77	-8.25 1999	-8.24 5192
Δ_n	0	0	0.3945 72	0.3945 78	1.2446 44	1.2446 45
Δ_p	0	0	0.3906 02	0.3906 05	0	0
E_n^{pair}	0	0	-1.716 979	-1.717 024	-12.4263 88	-12.4263 97
E_p^{pair}	0	0	-1.5286 16	-1.5286 43	0	0
R_n	5.61975 6	5.61975 7	5.357578	5.357578	4.7330 88	4.7331
R_p	5.4600 78	5.4600 90	5.2255 38	5.2255 39	4.5962 94	4.5963
Q_n	-0.00000 1	6.6E-11	11.4739 18	11.4739 20	-0.000000 1	6.6E-11
Q_p	-0.00000 1	4.7E-11	7.8802 21	7.8802 24	-0.000000 1	6.6E-11
E_n^{kin}	2525.99 2765	2525.99 1925	1974.614 008	1974.613 824	1338.2104 78	1338.2105 01
E_p^{kin}	1334.85 5572	1334.85 4465	1118.31 3683	1118.31 3442	829.438 221	829.438 221
E_{SO}	-96.375 045	-96.375 003	-80.1868 09	-80.1868 26	-49.0023 07	-49.0023 16
E_{dir}	827.60 7375	827.60 7885	602.810 248	602.810 352	366.326 962	366.326 917
E_{exc}	-31.2484 79	-31.2484 62	-25.9359 10	-25.9359 05	-19.08958	-19.08958
E_{tot}	-1634.14 8867	-1634.14 8120	-1357.658 500	-1357.658 322	-1018.141 626	-1018.141 673

HFODD/HFBTHO Benchmark

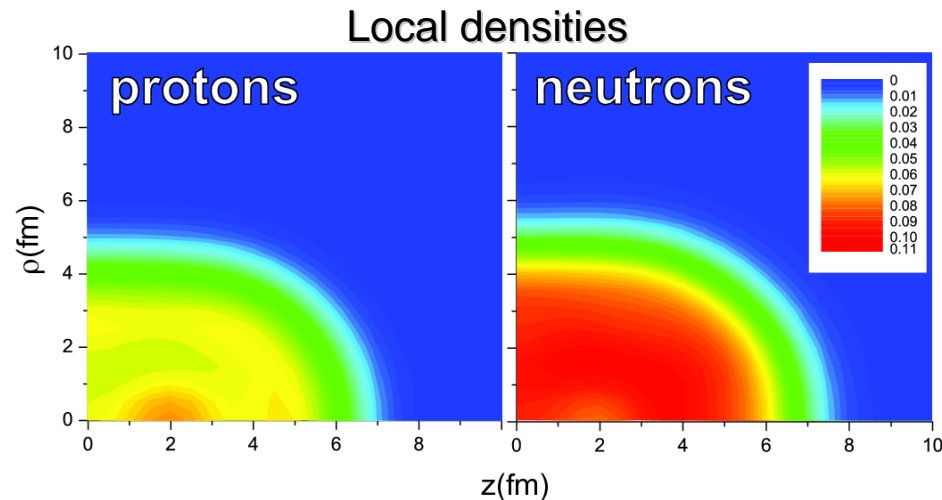
odd nuclei

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_{st}	680	680	680	680	680	680
$b_{\perp} = b_z$	2.0418697	2.0418697	2.0418697	2.0418697	2.0418697	2.0418697
E_{qp}	1.007 644	1.008	1.611 961	1.612	1.38 8951	1.387
λ_n	-7.74 9566	-7.74 94	-7.6961 79	-7.6962	-7.97 2801	-7.97 42
E_n^{pair}	-9.29 4443	-9.29 64	-10.397 019	-10.398 3	-8.703 141	-8.703 5
Δ_n	1.057 516	1.057 6	1.120 611	1.120 7	1.037 402	1.037 3
r_t	4.6895 35	4.6895	4.6904 59	4.6905	4.6895 10	4.6895
β	-0.025 699	-0.0256	0.000 000	0.000 1	0.0 15789	0.0 147
Q_t	-0.86 2706	-0.86 04	0.00 0000	0.00 36	0. 530038	0. 4921
E_n^{kin}	1360.43 7867	1360.442 751	1362.40 7077	1362.40 9601	1358.9 12567	1358.8 86614
E_p^{kin}	827.317 590	827.317 961	827.12 3364	827.12 3676	827.19 5176	827.19 1207
E_{SO}	-50.4 83676	-50.4 85916	-50.92 2860	-50.92 3940	-49.6 07742	-49.5 92026
E_{dir}	365.7436 76	365.7437 74	365.6210 13	365.6210 31	365.736 277	365.735 680
E_{tot}	-1024.7072 75	-1024.7072 72	-1024.301 233	-1024.301 252	-1024.41 5866	-1024.41 6901

HFODD/HFBTHO interface (see the talk of N. Schunck)

HFBAX/HFBTHO Benchmark

^{110}Zr	HFBAX	HFBTHO
	$M=13, R_{box}=19.2 \text{ fm}, \Delta r=0.6 \text{ fm}$	$N_{sh}=20$
E_t	-893.983	-893.840
E_C	226.758	226.712
E_K^p	632.115	631.882
E_K^n	1368.206	1368.201
E_P^n	-3.200	-3.326
Δ_n	0.636	0.652
λ_n	-3.552	-3.543
Q_2^n	444.02	443.90



Broyden's Method in Nuclear Structure Calculations

Andrzej Baran,^{1,2,3} Aurel Bulgac,⁴ Michael McNeil Forbes,⁴ Gaute Hagen,²
Witold Nazarewicz,^{1,2,5,6} Nicolas Schunck,^{1,2} and Mario V. Stoitsov^{1,2,7}

¹*Department of Physics & Astronomy, University of Tennessee, Knoxville, Tennessee 37996, USA*

²*Physics Division, Oak Ridge National Laboratory,
P.O. Box 2008, Oak Ridge, Tennessee 37831, USA*

³*Institute of Physics, University of M. Curie-Sklodowska, ul. Radziszewskiego 10, 20-031 Lublin, Poland*

⁴*Department of Physics, University of Washington, Seattle, WA 98195-1560*

⁵*Institute of Theoretical Physics, Warsaw University, ul. Hoza 69, 00-681 Warsaw, Poland*

⁶*School of Engineering and Science, University of the West of Scotland, Paisley PA1 2BE, UK*

⁷*Institute of Nuclear Research and Nuclear Energy, Bulgarian Academy of Sciences, Sofia, Bulgaria*

Broyden's method, widely used in quantum chemistry electronic-structure calculations for the numerical solution of nonlinear equations in many variables, is applied in the context of the nuclear many-body problem. Examples include the unitary gas problem, the nuclear density functional theory with Skyrme functionals, and the nuclear coupled-cluster theory. The stability of the method, its ease of use, and its rapid convergence rates make Broyden's method a tool of choice for large-scale nuclear structure calculations.

PACS numbers: 21.10.Dr, 21.60.Jz, 21.60.De, 71.15.Mb, 02.60.Cb

submitted to Phys.Rev.C (2008)

Broyden Mixing

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

$$F(V) = 0 \quad \text{Calculating new fields}$$



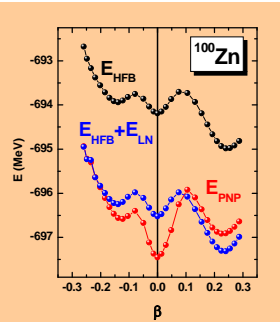
Self-Consistent HFB Solution

Calculating new densities

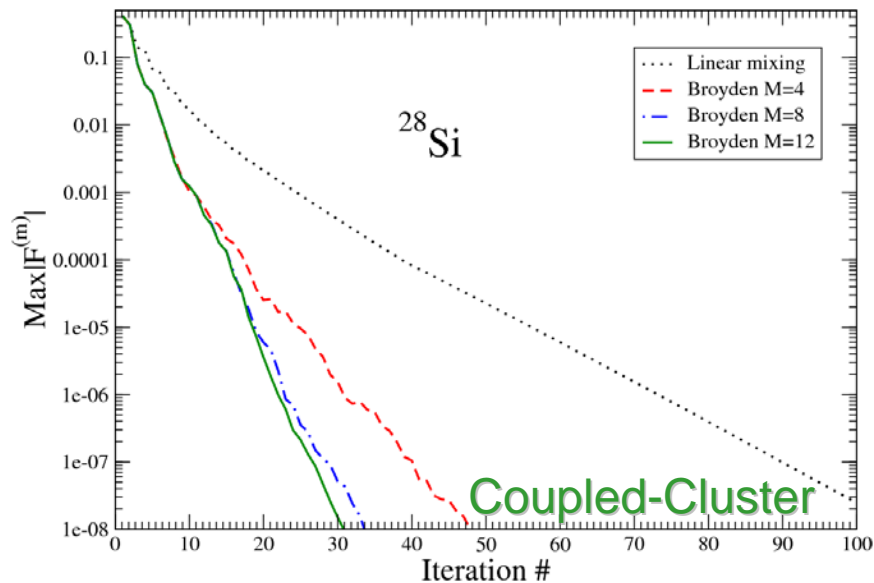
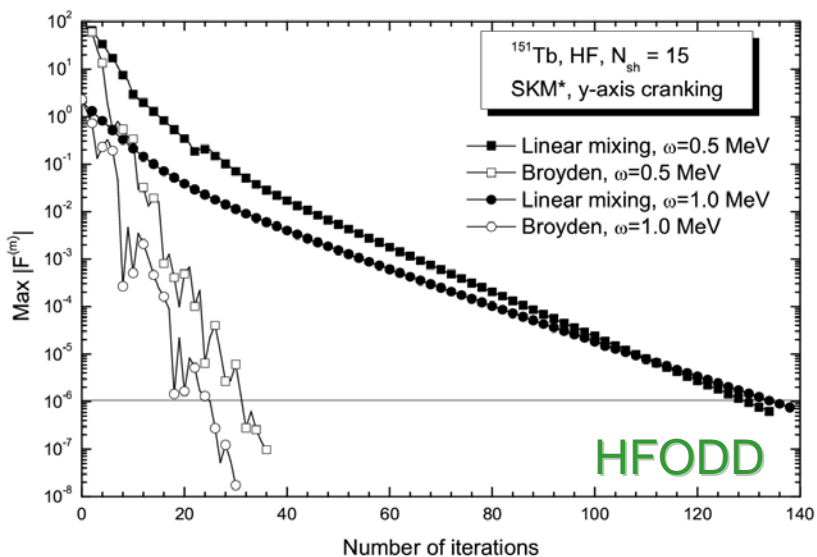
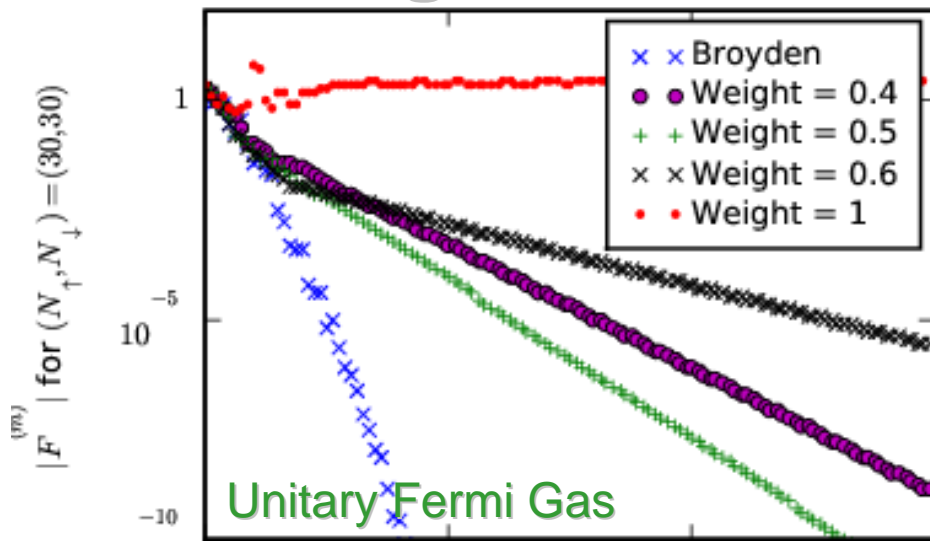
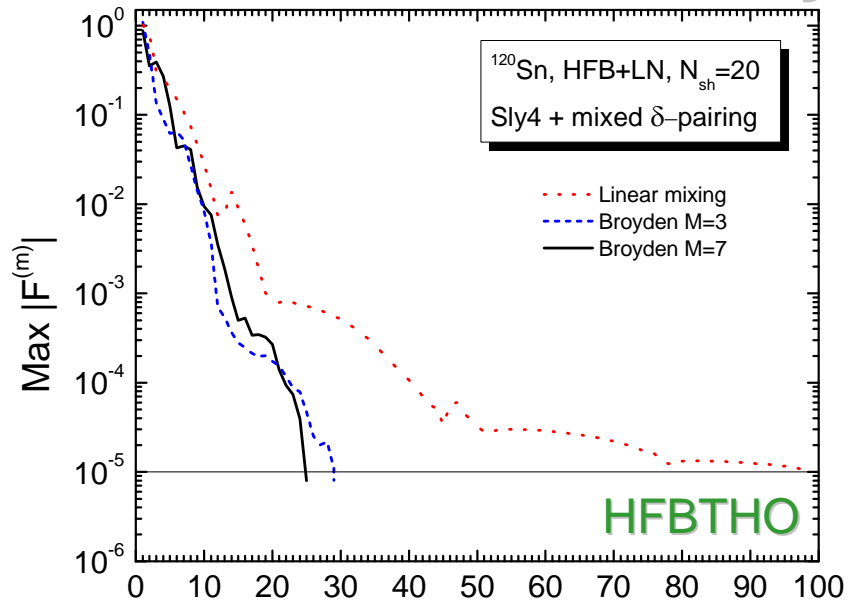
Solution of the HFB equations

Linear mixing: $V^{(m+1)} = V^{(m-1)} + \alpha F^{(m)}$

Broyden mixing: $V^{(m+1)} = V^{(m-1)} - (J^{(m)})^{-1} F^{(m)}$



Broyden Mixing



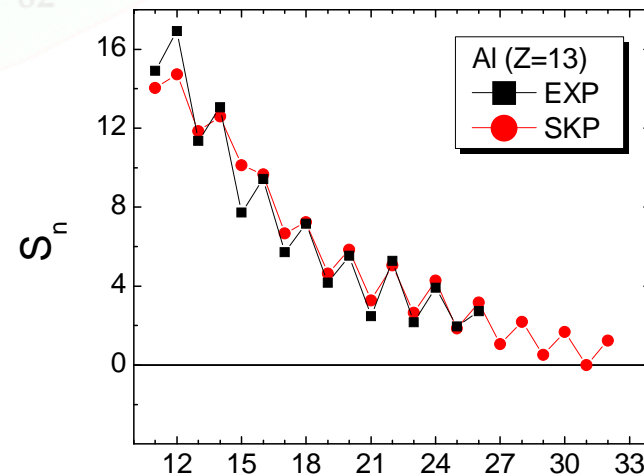
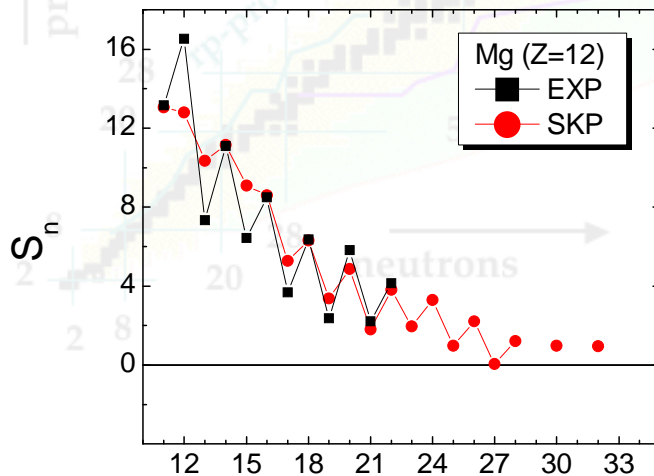
Large-Scale Mass Table Calculations

First Year Achievement

- ✓ Complete mass-table calculations with existing (standard) energy density functionals including all even-even, odd-even and odd-odd nuclei

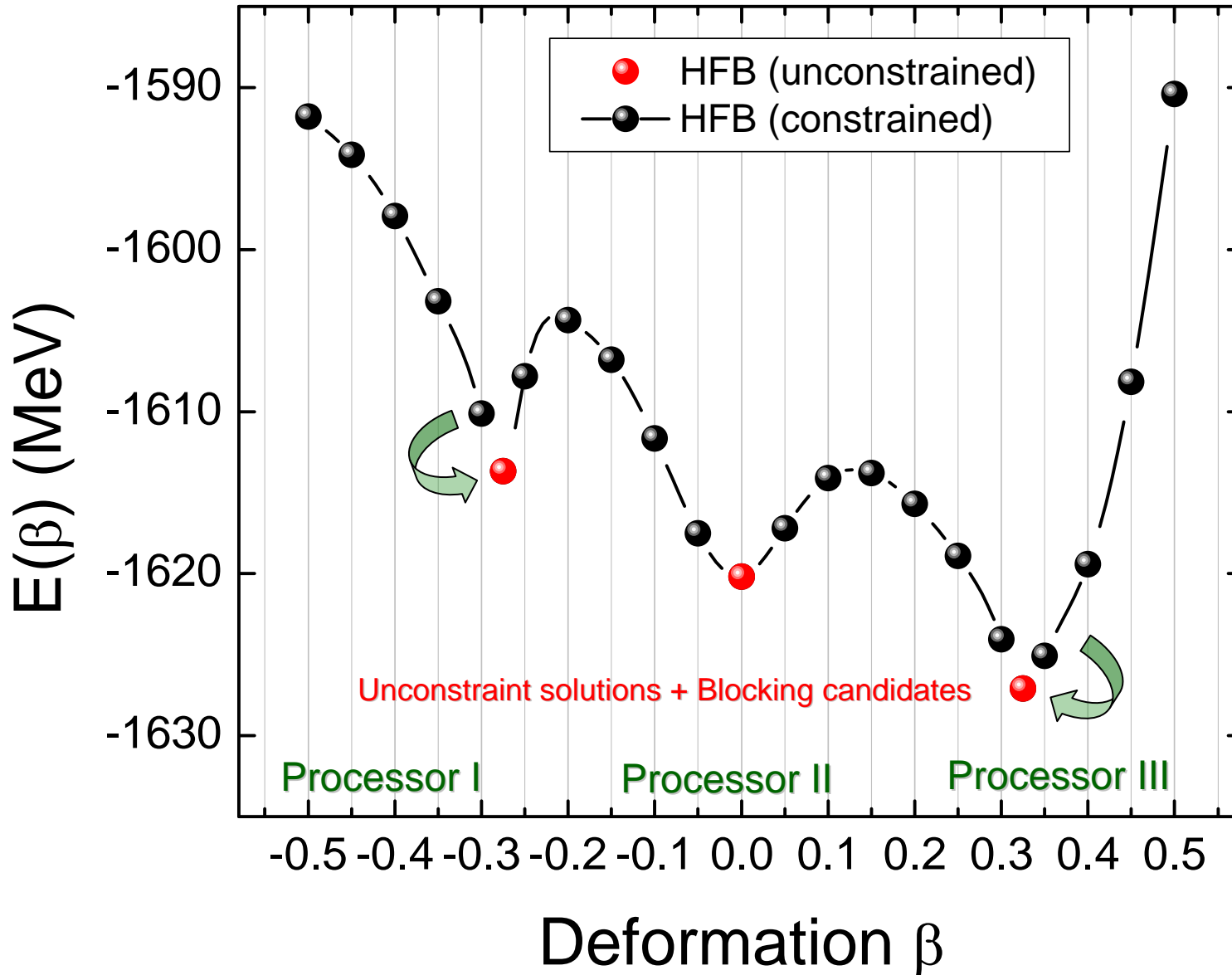
Data already used to compare with experiment

$$\delta V_{pn} , \Delta_0^{(3)}, {}^{141}\text{Ho}, {}^{40}\text{Mg}$$

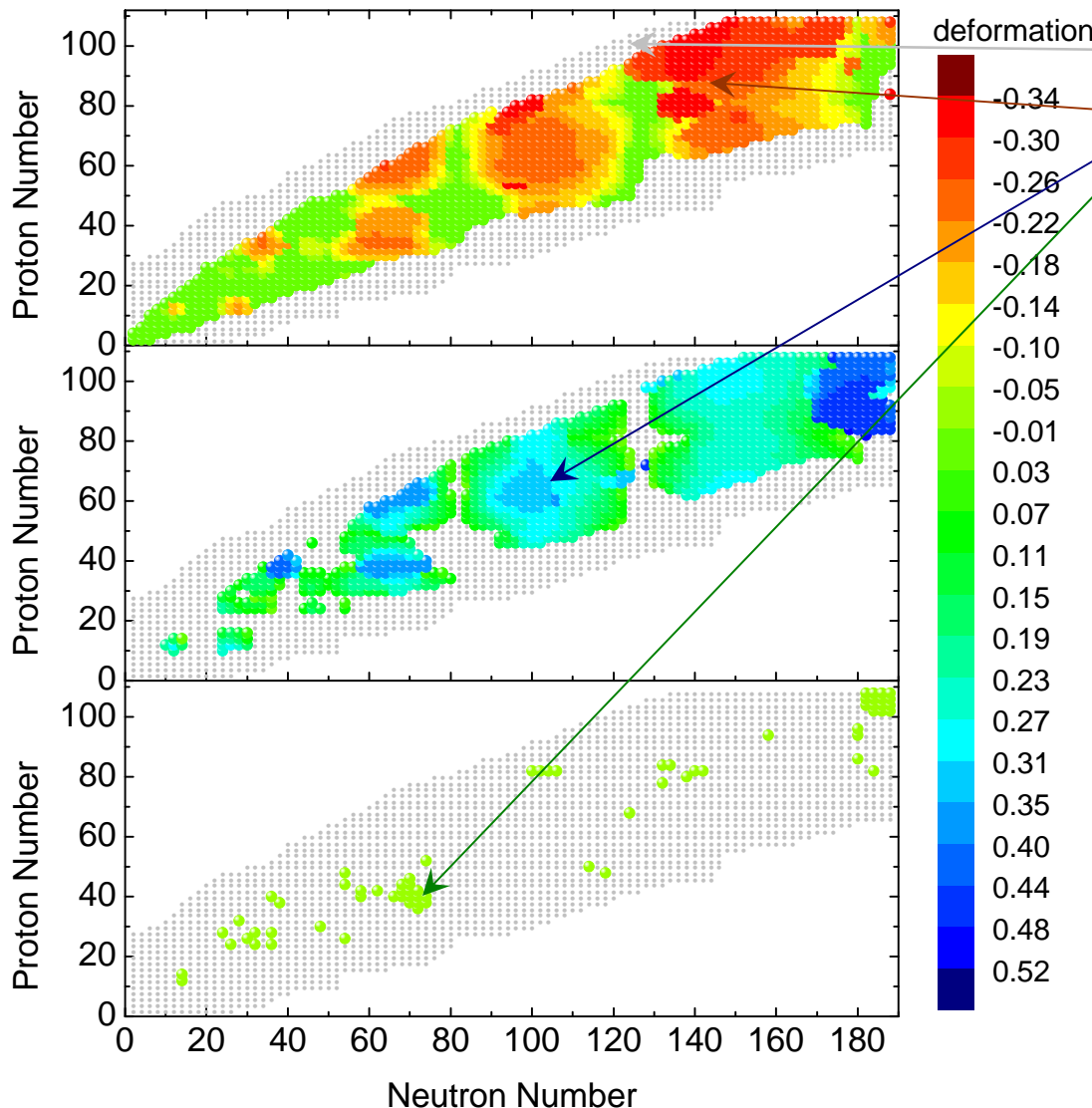


Large-Scale Calculations

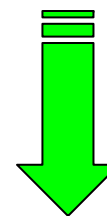
one even-even nucleus



Large-Scale Mass Table Calculations



2525 even-even nuclei
2731 even-even bound states
2 CPU hours
using 4000 processors



800754 odd-even and odd-odd states within 2 MeV E_{qp} threshold for the blocking candidates

21 CPU hours
using 4000 processors

After implementing Broyden's method

- all even-even nuclear states converge
- for odd nuclei: about 0.5%, usually high lying, configurations still diverge

The whole mass table
in a single 24 CPU hours run

MassExplorer.org

MTeX
Mass Table Explorer

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News

Recent MTeX 4.1beta release can be downloaded [here](#)

Additional data files available for Mass Tables calculated with different functionals can be downloaded [here](#)

ScreenShots from MTeX can be seen [here](#)

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[Periodic Table](#)

Mass Table explorer

... science scales with processors ...

Mass Table Explorer is a java application aimed to facilitate the visualization of the huge array of data coming from modern multiprocessors computers helping to understand challenging phenomena seen across the nuclear mass chart.

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Mass Tables

- [ADMC-2003](#)
- [Map of the Nuclides](#)
- [D1S Gogny](#)
- [Droplet Model](#)
- [HFB-14 BRUSLIB](#)

Java Tools

- [Janis](#)
- [NucAstroData](#)

HFB (Mixed Pairing)

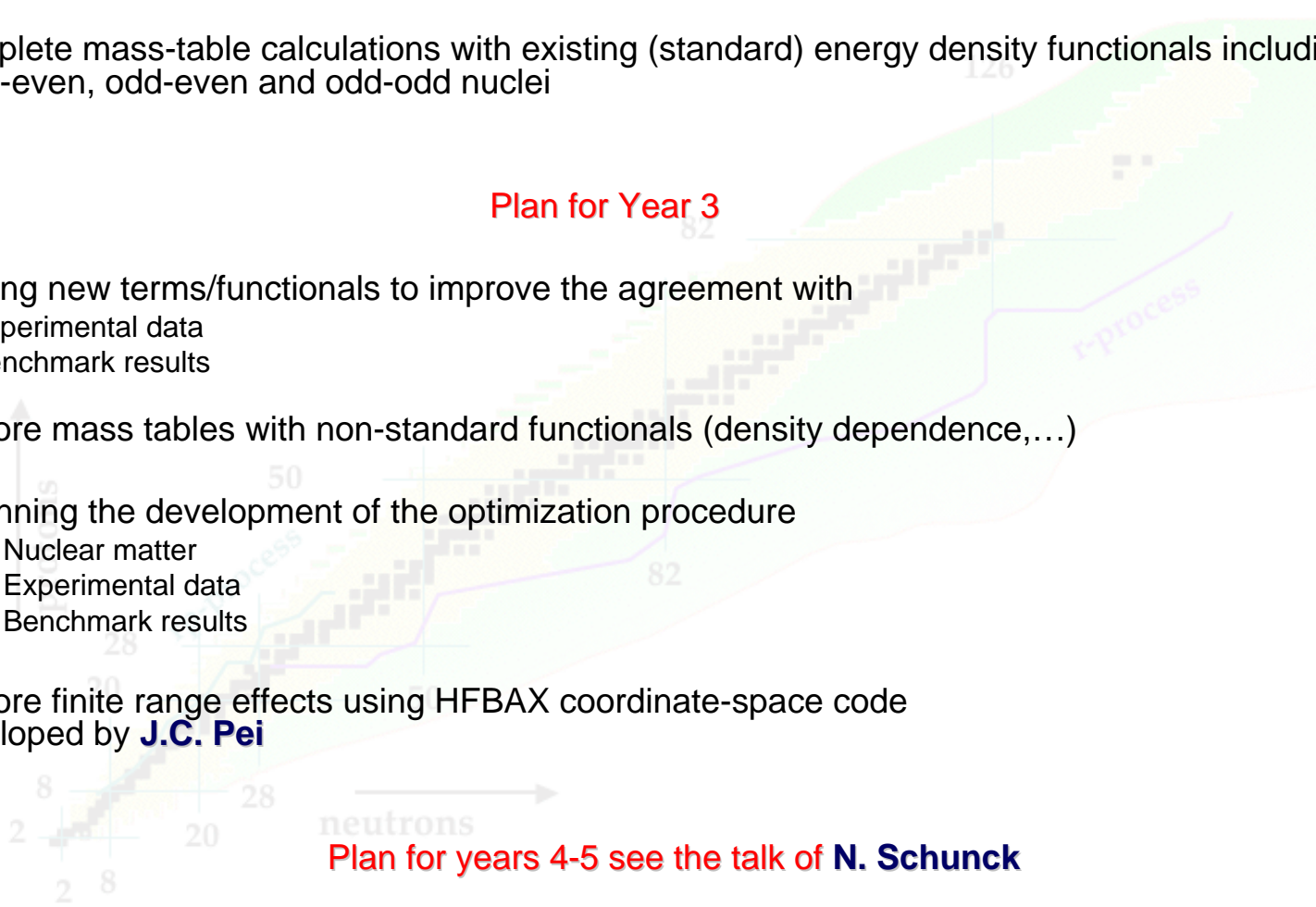
- SLY4 (with & without LN)
- SKP (LN)
- SKM* (LN)

Large-Scale Mass Table Calculations

- ✓ Complete mass-table calculations with existing (standard) energy density functionals including all even-even, odd-even and odd-odd nuclei

Plan for Year 3

- ❑ Testing new terms/functionals to improve the agreement with
 - Experimental data
 - Benchmark results
- ❑ Explore mass tables with non-standard functionals (density dependence,...)
- ❑ Beginning the development of the optimization procedure
 - Nuclear matter
 - Experimental data
 - Benchmark results
- ❑ Explore finite range effects using HFBOX coordinate-space code developed by **J.C. Pei**



Plan for years 4-5 see the talk of **N. Schunck**