Large-Scale Mass Table Calculations

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- HFBTHO solver
- Benchmarking the solver
- Accelerating iterations - Broyden’s Method
- Large-Scale Calculations
- Mass Table Explorer

SciDAC UNEDF project

Building a Universal Nuclear Energy Density Functional

A Low-Energy Nuclear Physics National HPC Initiative

George F. Bertsch , University of Washington

The mission of the project is three-fold:

First, to find an optimal functional using all our knowledge of the nucleonic Hamiltonian and basic nuclear properties.

Second, to apply the EDF theory and its extensions to validate the functional using all the available relevant nuclear structure data.

Third, to apply the validated theory to properties of interest that cannot be measured, in particular the transition properties needed for reaction theory.

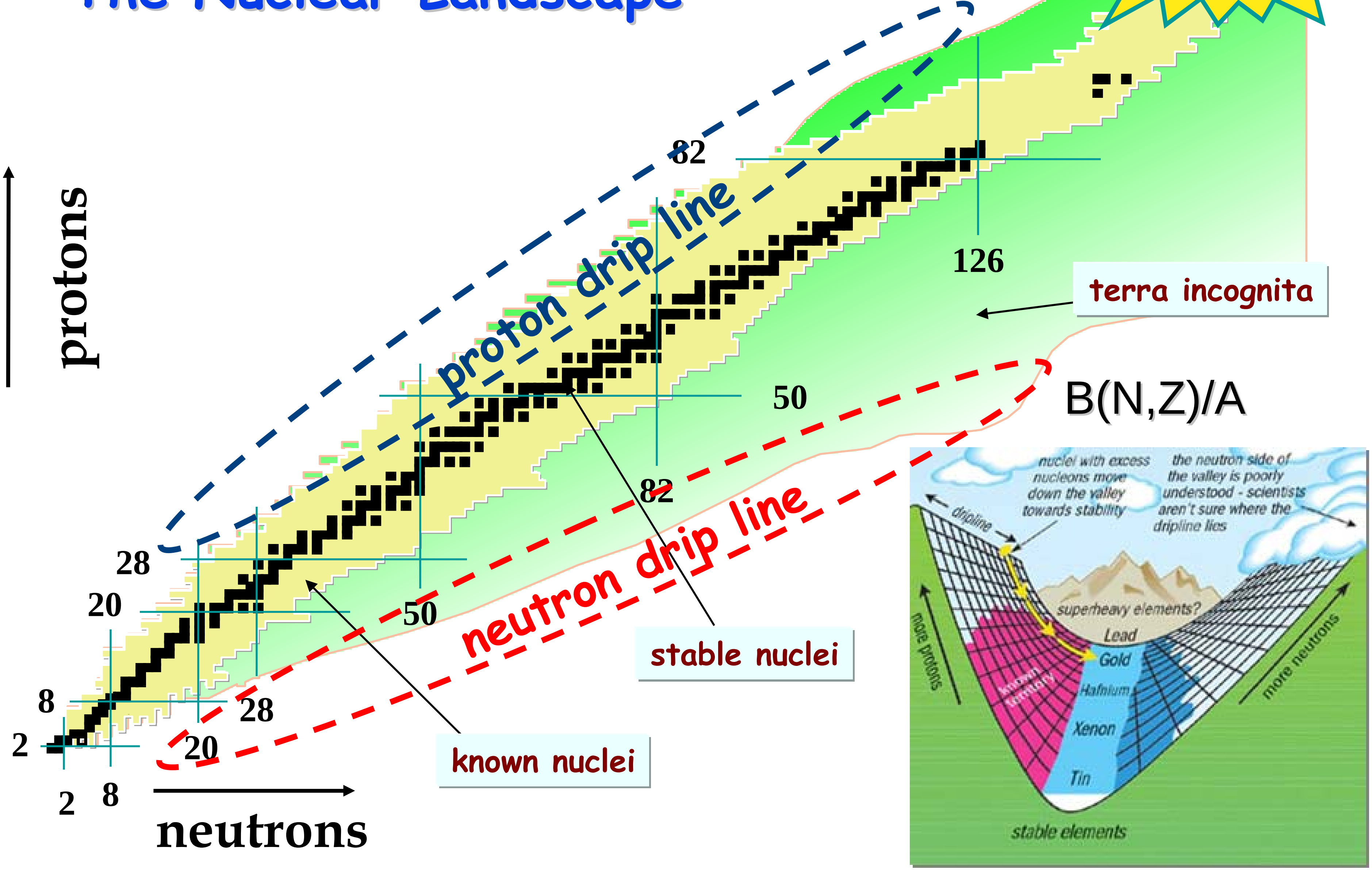
The activities to be supported fall into different areas of nuclear theory and computer science, but the goal can only be achieved by working at the interfaces among these areas. They are: ab initio theory of nuclear wave functions, Effective Field Theory (EFT) and its extensions, self-consistent mean-field description of ground and excited states, large amplitude collective motion, low-energy reaction theory and computer science.

Science Application: Nuclear Physics
Project Title: Building a Universal Nuclear Energy Density Functional
Principal Investigator: George F. Bertsch
Affiliation: University of Washington
Funding Partners: Office of Science, Advanced Scientific Computing Research, and National Nuclear Security Agency
Budget and Duration: Approximately $3 Million per year for five years

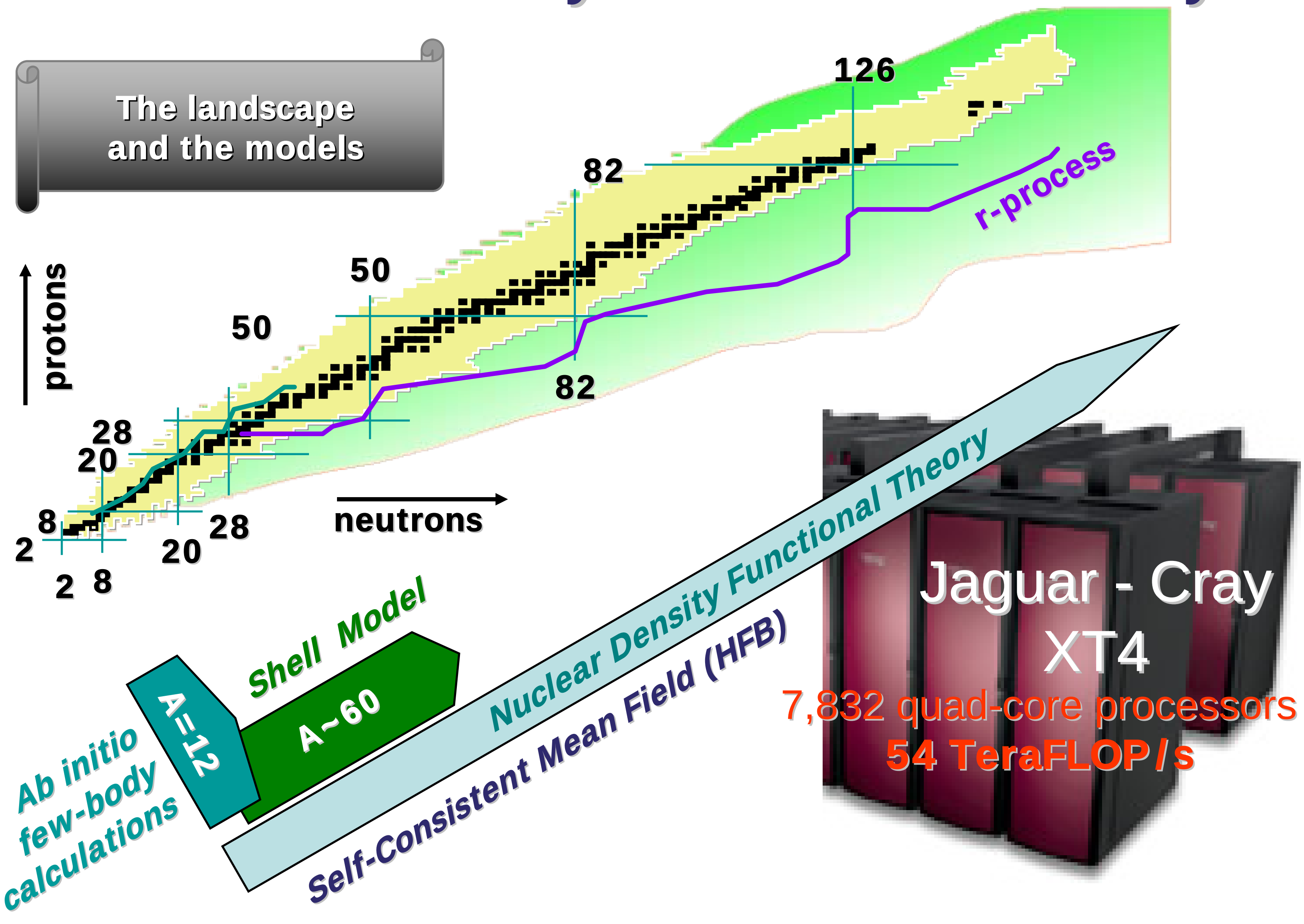
SciDAC
Scientific Discovery through Advanced Computing

http://unedf.org

The Nuclear Landscape



Nuclear Density Functional Theory



HFBTHO solver

M.V. Stoitsov, J. Dobaczewski, W. Nazarewicz, P. Ring
Axially Deformed Solution of the Skyrme-Hartree-Fock-Bogolyubov Equations Using The Transformed Harmonic Oscillator Basis. The program HFBTHO

Computer Physics Communications Volume 167, Issue 1, 1 April 2005, Pages 43-63

- 2D HFB in HO/THO basis (cylindrical coordinates)
- Time-reversal, axial and parity symmetries
- Skyrme type functional and contact delta pairing
- Handling even-even, odd-even and odd-odd nuclei
- Easily extendable to arbitrary functional
- Fast alternative for ground-state calculations
- Continuum discretization as coming from the diagonalization

- DFT solvers in coordinate space
  - HFBRAD – box, coordinate space, spherical symmetry
  - HFB-AX – rectangular box, B-splines, axial/parity symmetry
- DFT solvers in configurational (HO) space
  - HFODD – 3D in HO basis, symmetry unrestricted, time-odd components, cranking, projections …
  - HFBTHO – 2D in HO/THO basis, axial/parity symmetry
- New generation HFB solvers (the talk of G. Fann)

HFBTHO/HFODD Benchmark

even-even nuclei

	^{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	−8.114078	−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^{pair}	0	0	−1.716979	−1.717024	−12.426388	−12.426397
E_p^{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^{kin}	2525.992765	2525.991925	1974.614008	1974.613824	1338.210478	1338.210501
E_p^{kin}	1334.855572	1334.854465	1118.313683	1118.313442	829.438221	829.438221
E_{SO}	−96.375045	−96.375003	−80.186809	−80.186826	−49.002307	−49.002316
E_{dir}	827.607375	827.607885	602.810248	602.810352	366.326962	366.326917
E_{exc}	−31.248479	−31.248462	−25.935910	−25.935905	−19.08958	−19.08958
E_{tot}	−1634.148867	−1634.148120	−1357.658500	−1357.658322	−1018.141626	−1018.141673

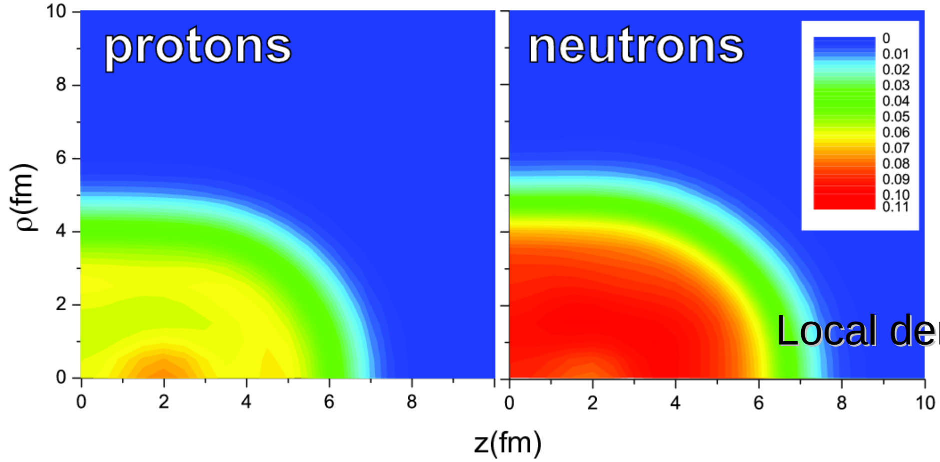
HFODD/HFBTHO Benchmark

odd nuclei	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

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

HFBTHO/HFBAX Benchmark

^{110}Zr	HFB-AX	HFBTHO
	M=13, R_{box}=19.2 fm, Δr=0.6 fm	N_{sh}=20
E_t	-893.983	-893.840
E_C	226.758	226.712
$E^p_{K.}$	632.115	631.882
E^n_K	1368.206	1368.201
E^n_P	-3.200	-3.326
Δ_n	0.636	0.652
λ_n	-3.552	-3.543
Q^n_2	444.02	443.90



Local densities

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]

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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

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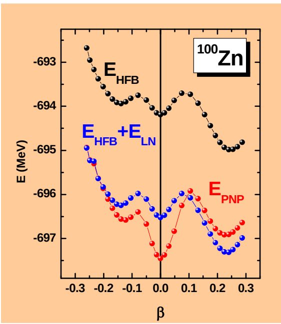
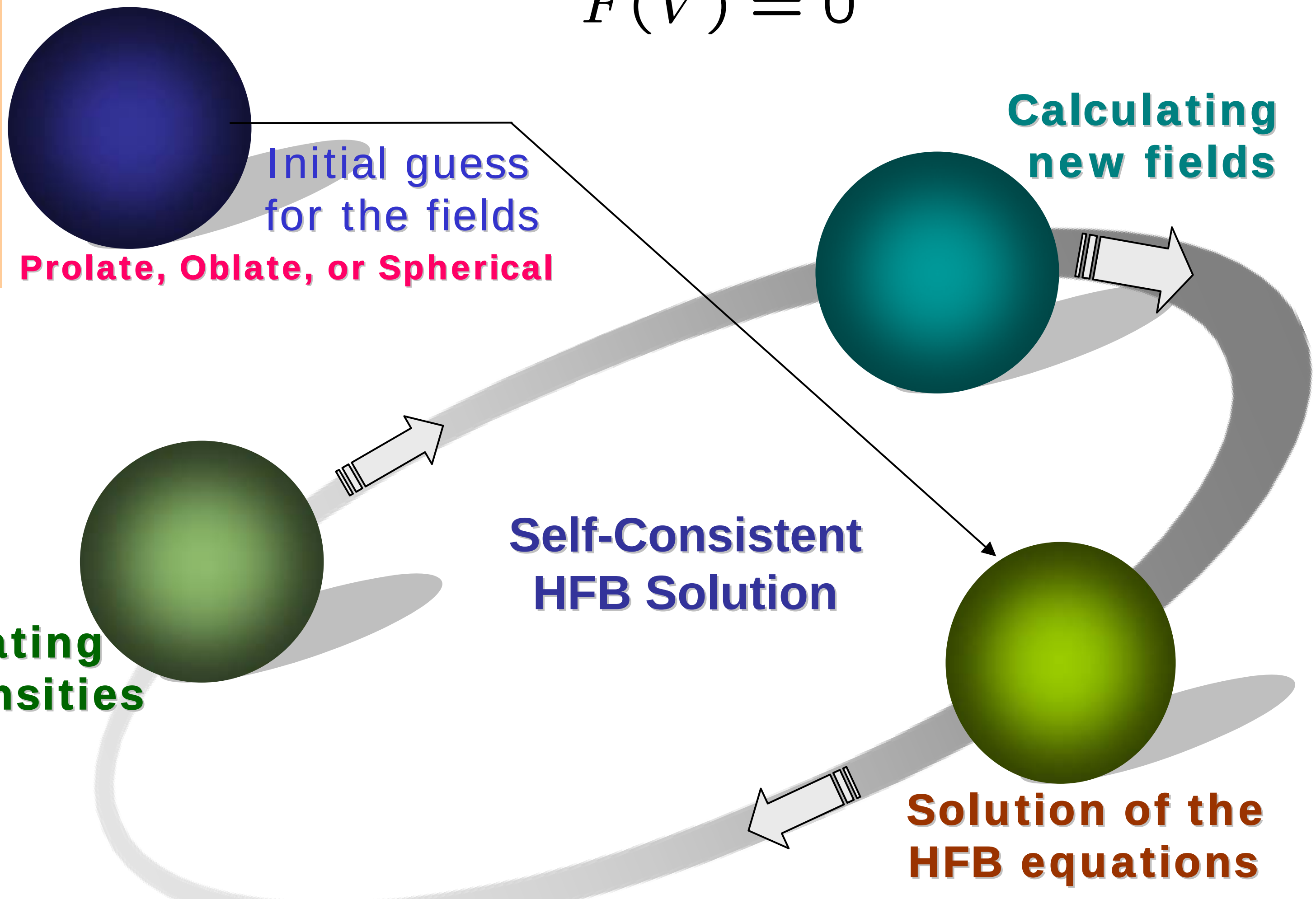
Broyden Mixing

$$F^{(m)}(V) = V^{(m)} - V^{(m-1)}$$
$$F(V) = 0$$

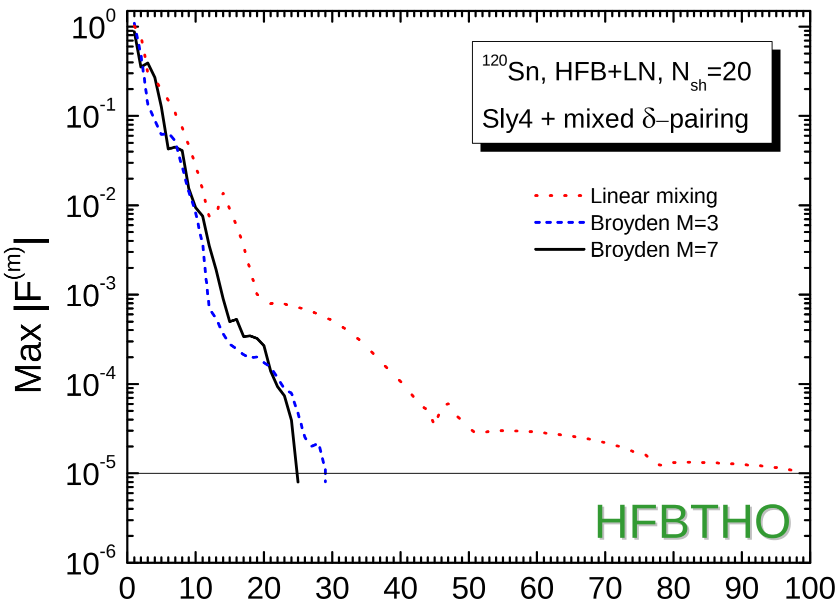


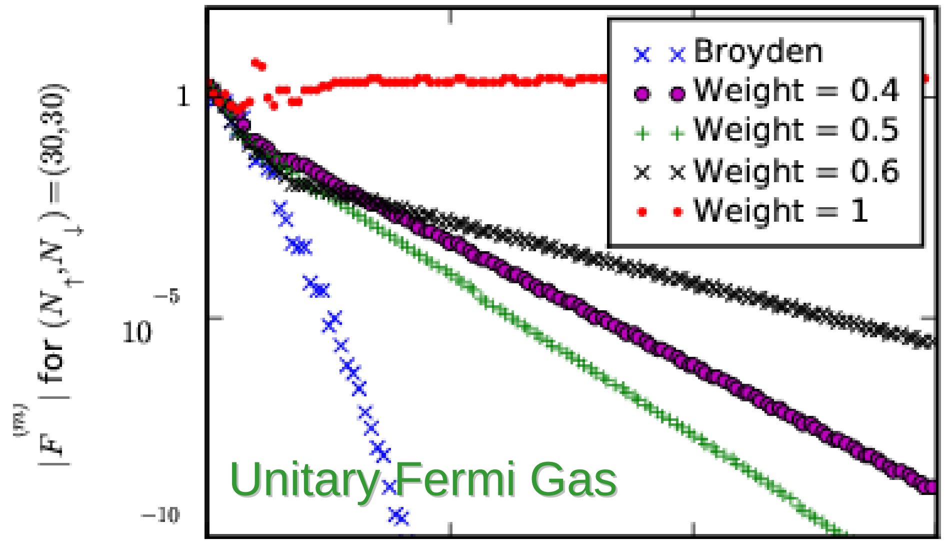


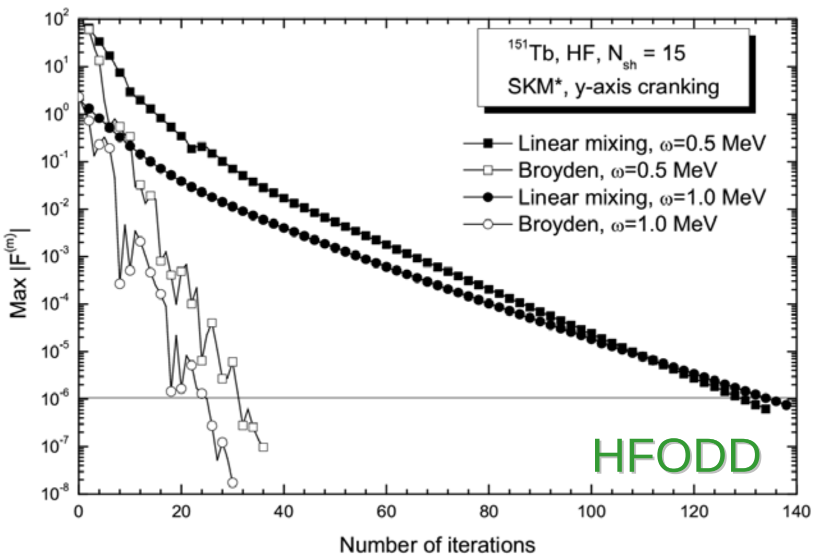
Linear mixing: $V^{(m+1)} = V^{(m)} + \alpha F^{(m)}$

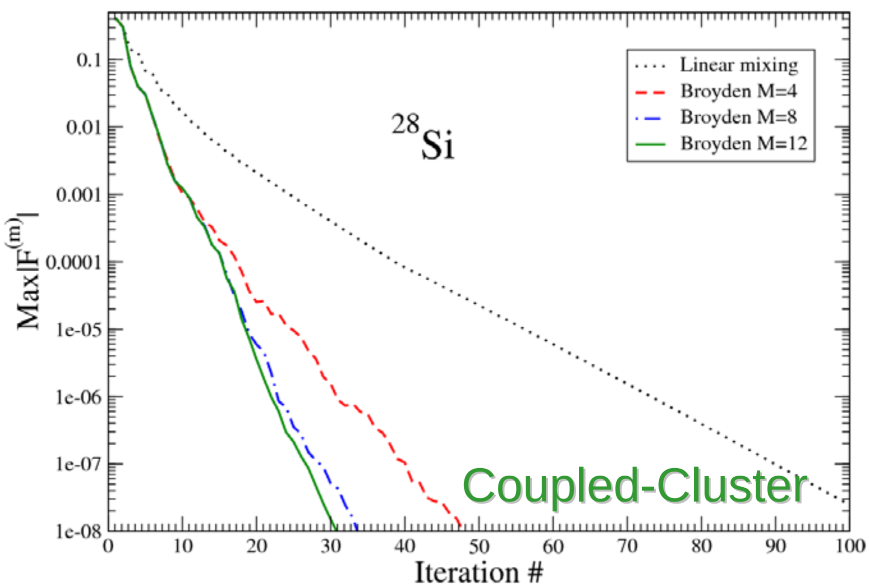
Broyden mixing: $V^{(m+1)} = V^{(m)} - (J^{(m)})^{-1} F^{(m)}$

Broyden Mixing



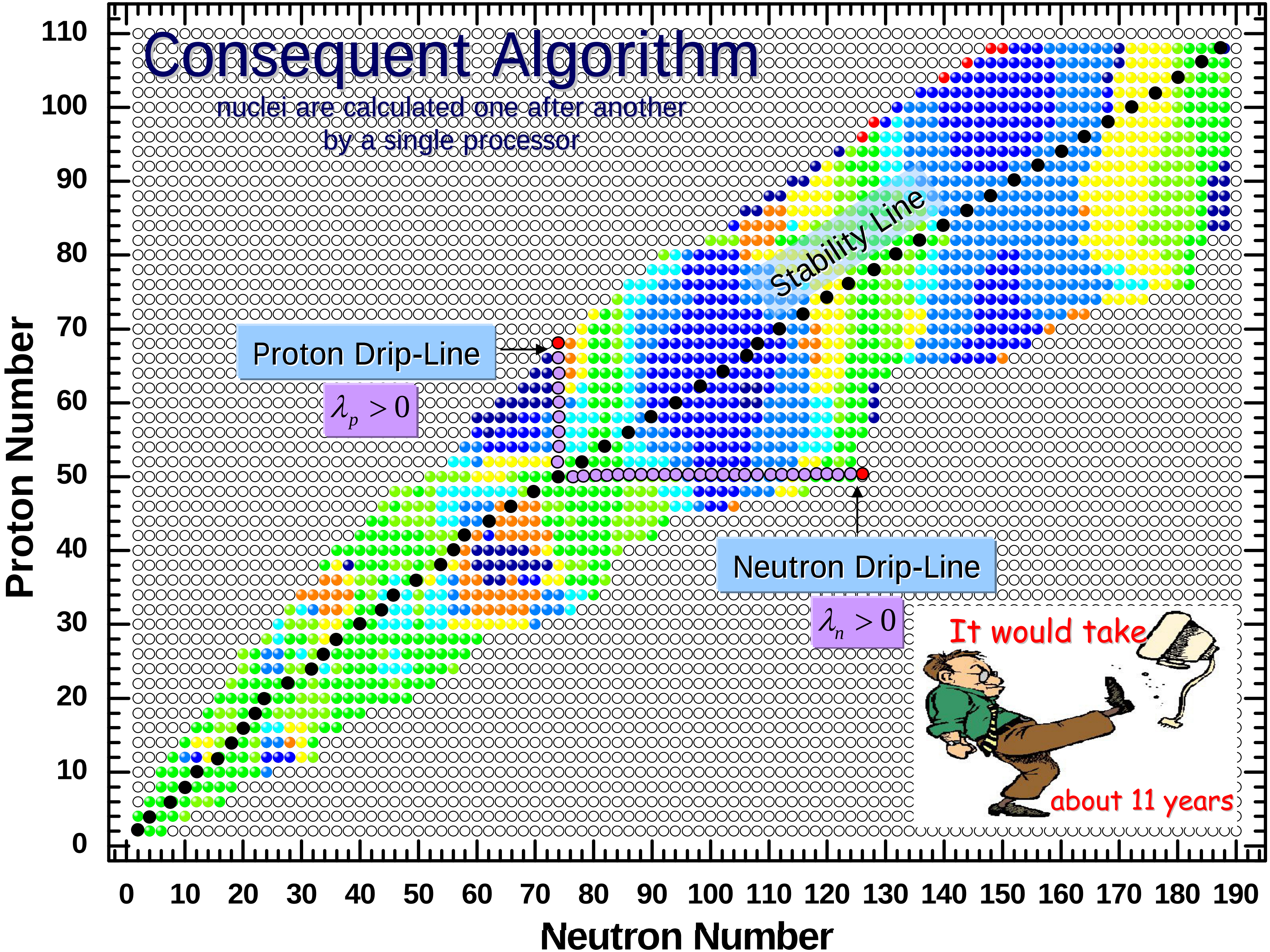






Consequent Algorithm

nuclei are calculated one after another by a single processor



Oak Ridge National Laboratory

November 19-22, 2008

TOP500 SUPERCOMPUTER SITES

PROJECT | LISTS | STATISTICS | RESOURCES | NEWS

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TOP500 List - June 2008 (1-100)

R_{max} and R_{peak} values are in TFlops. For more details about other fields, check the TOP500 description.

Power data in KW for entire system

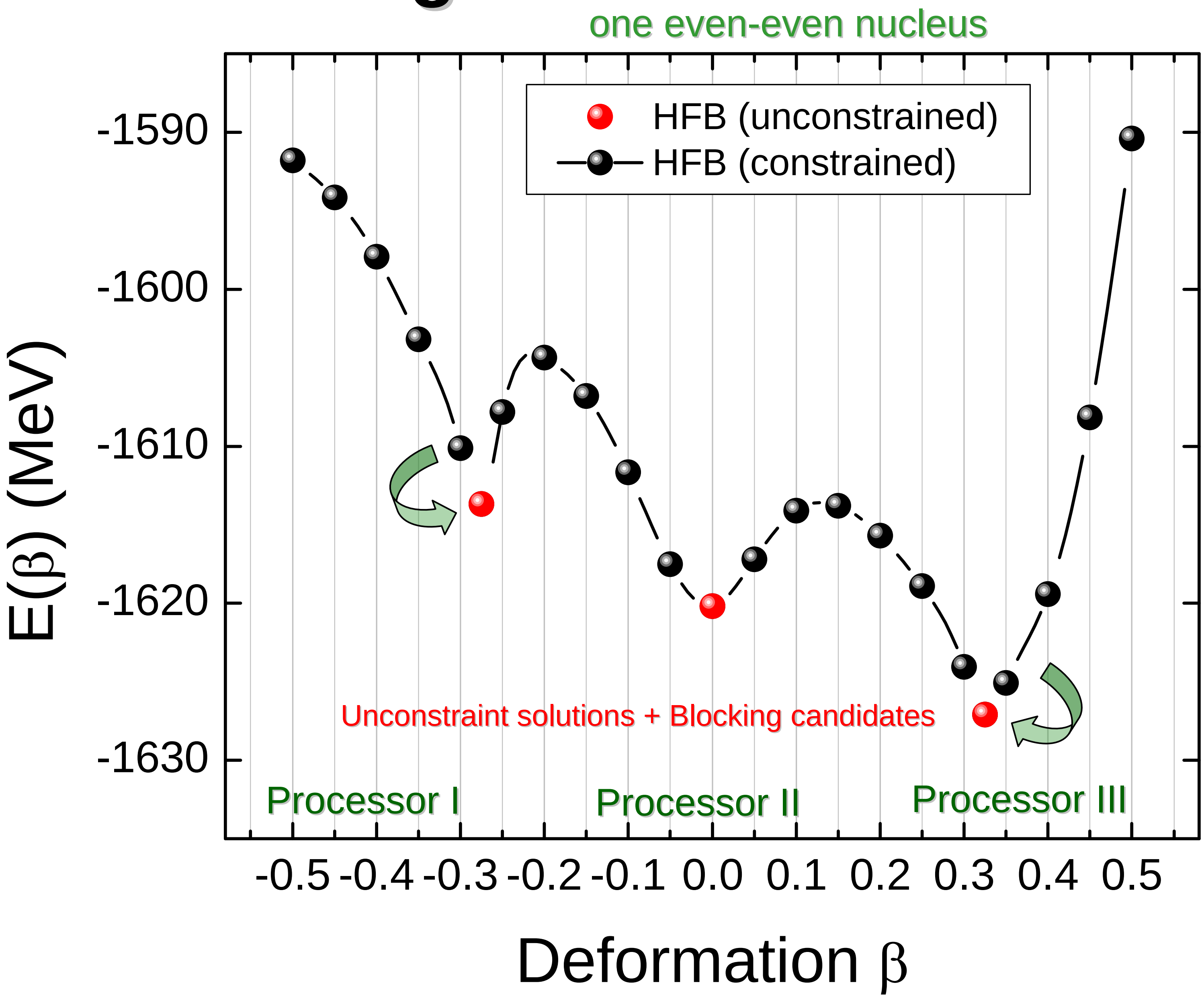
next

Rank	Site	Computer/Year Vendor	Cores	R_{max}	R_{peak}	Power
1	DOE/NNSA/LANL United States	Roadrunner - BladeCenter QS22/LS21 Cluster, PowerXCell 8i 3.2 Ghz / Opteron DC 1.8 GHz , Voltaire Infiniband / 2008 IBM	122400	1026.00	1375.78	2345.50
2	DOE/NNSA/LLNL United States	BlueGene/L - eServer Blue Gene Solution / 2007 IBM	212992	478.20	596.38	2329.60
3	Argonne National Laboratory United States	Blue Gene/P Solution / 2007 IBM	163840	450.30	557.06	1260.00
4	Texas Advanced Computing Center/Univ. of Texas United States	Ranger - SunBlade x6420, Opteron Quad 2Ghz, Infiniband / 2008 Sun Microsystems	62976	326.00	503.81	2000.00
5	DOE/Oak Ridge National Laboratory United States	Jaguar - Cray XT4 QuadCore 2.1 GHz / 2008 Cray Inc.	30976	205.00	260.20	1580.71
6	Forschungszentrum Juelich (FZJ) Germany	JUGENE - Blue Gene/P Solution / 2007 IBM	65536	180.00	222.82	504.00
7	New Mexico Computing Applications Center (NMCAC) United States	Encanto - SGI Altix ICE 8200, Xeon quad core 3.0 GHz / 2007 SGI	14336	133.20	172.03	861.63
8	Computational Research Laboratories, TATA SONS India	EKA - Cluster Platform 3000 BL460c, Xeon 53xx 3GHz, Infiniband / 2008 Hewlett-Packard	14384	132.80	172.61	786.00
9	IDRIS France	Blue Gene/P Solution / 2008 IBM	40960	112.50	139.26	315.00
10	Total Exploration Production France	SGI Altix ICE 8200EX, Xeon quad core 3.0 GHz / 2008 SGI	10240	106.10	122.88	442.00

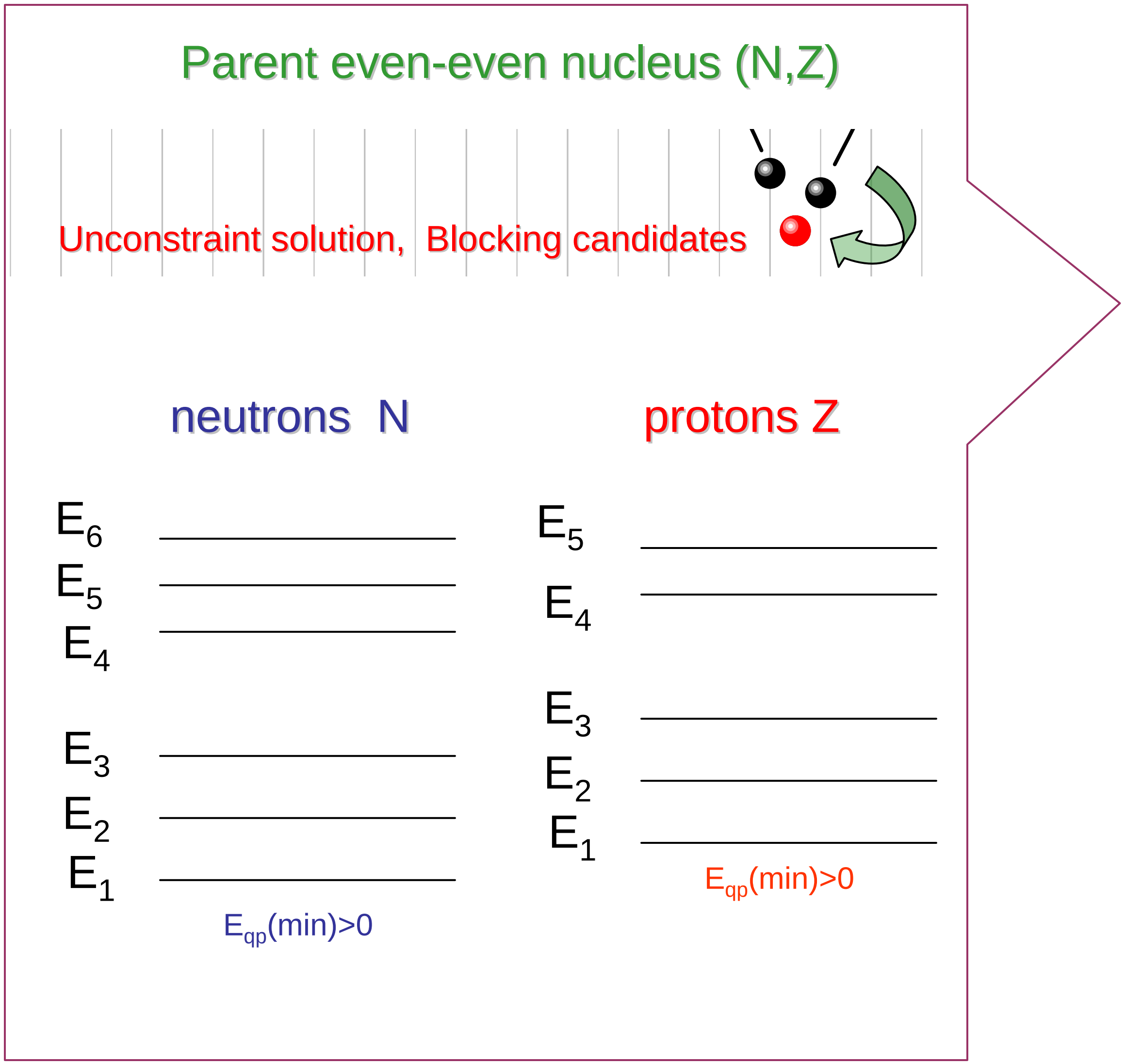
Large-Scale Mass Table Calculations

Jaguar is currently rated the 5th most powerful computer in the world with 54 teraflops and 7,832 AMD Barcelona quad-core Opteron processors.

Large-Scale Calculations



Large-Scale Calculations



Self-consitent calculations for odd nuclei with blocking

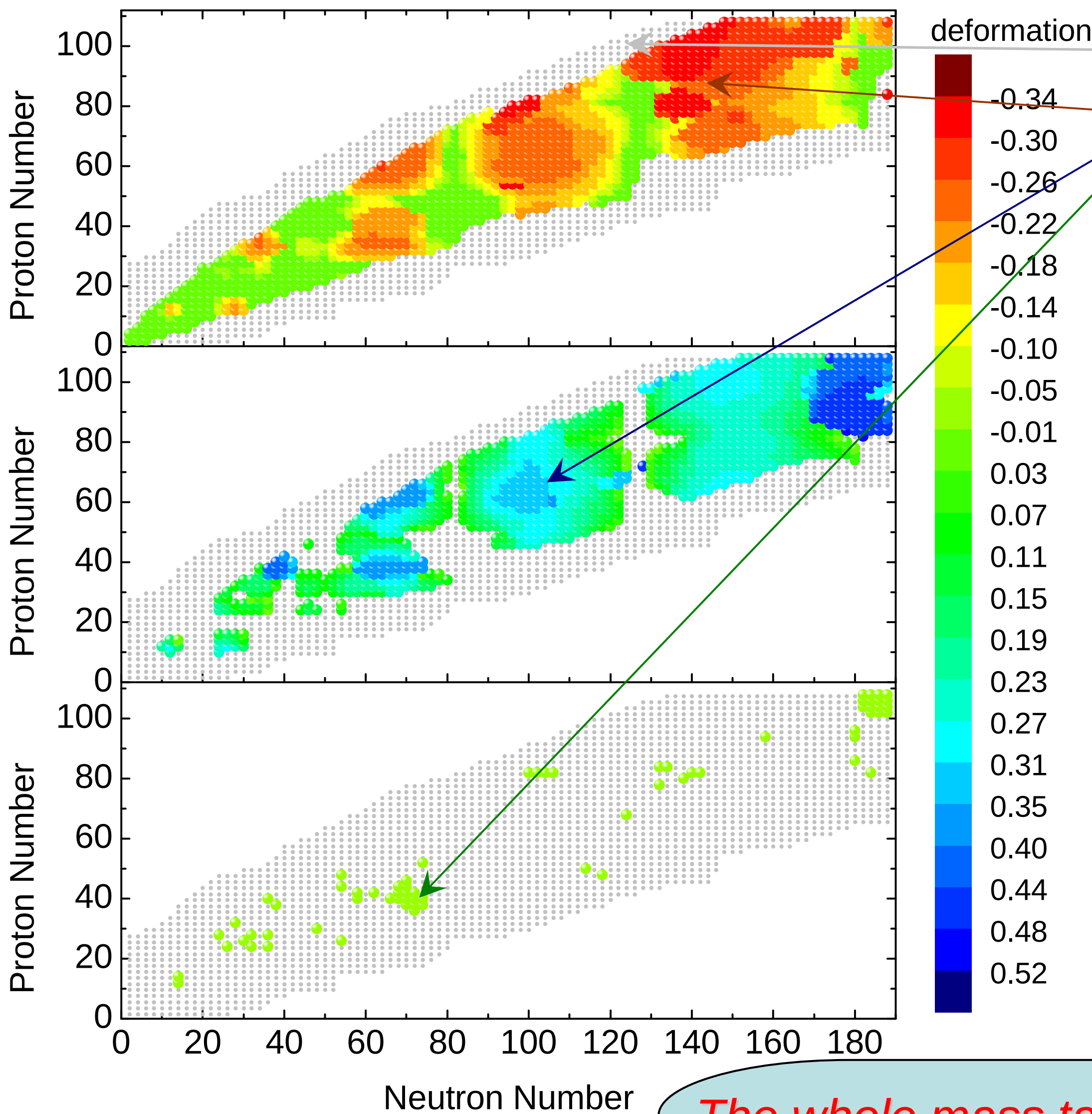
odd-even nucleus (N+1,Z)
6 configurations

odd-even nucleus (N,Z+1)
5 configurations

odd-odd nucleus (N+1,Z+1)
6x5=30 configurations

41 processors

Large-Scale Mass Table Calculations



9525 even-even states

2731 even-even bound states

2 CPU hours using 4000 processors

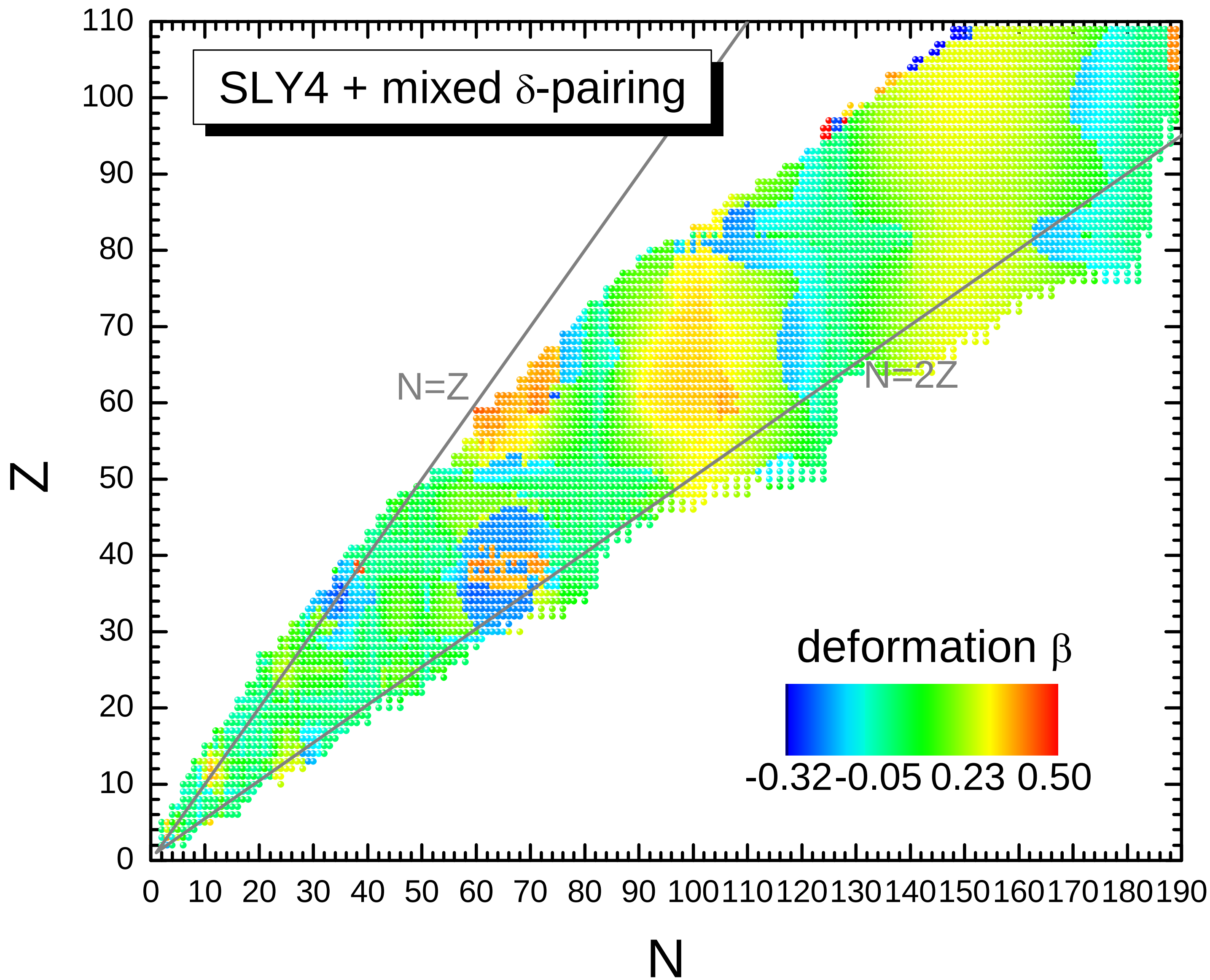
800754 odd-even and odd-odd states within 2 MeV E_{qp} threshold for the blocking candidates

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

Large-Scale Mass Table Calculations

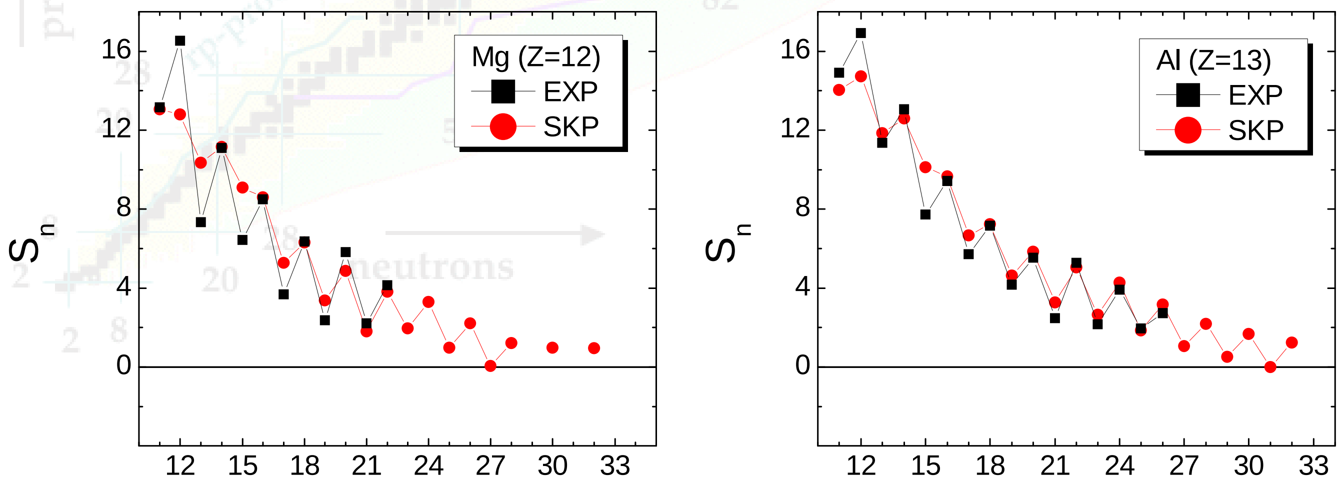


Large-Scale Mass Table Calculations

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

Data already used to compare with experiment

δV_{pn} , $\Delta_0^{(3)}$, ^{141}Ho, ^{40}Mg



MassExplorer.org

Off-line Version

- Written in Java
- Can work on any computer
- Large sets of visualization tools
- One can compare with his own data
- Save data and images in many formats

On-line Version

- Use Python, Gnuplot, PHP, Ajax
- Visualization right from the browser
  - one can apply mass filters
  - plot 2D and 3D charts
  - compare nuclear characteristics
  - rms errors with exp. data

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

❑ Beginning the development of optimization procedure
- Nuclear matter
- Experimental data
- Benchmark results
- Errors and correlations among parameters and observables

❑ Testing new terms and exploring non-standard functionals
- density dependent coupling constants
- higher gradients
- derived trough DME

Optimization Procedure

standard functional with 13 ph-parameters

t-parameters

$\{t_0, t_1, t_2, t_3, x_0, x_1, x_2, x_3, to, te, b_4, b'_4, \gamma\}$

$$
\begin{aligned}
\mathcal{H}(\boldsymbol{r}) &= \frac{\hbar^2}{2m}\tau \\
&+ \frac{1}{2}t_0\left(\left(\frac{x_0}{2}+1\right)\rho^2 - \left(x_0+\frac{1}{2}\right)\sum_q \rho_q^2\right) \\
&+ \frac{1}{4}t_1\left(\left(\frac{x_1}{2}+1\right)\rho\,\tau - \left(x_1+\frac{1}{2}\right)\sum_q \rho_q\tau_q\right) \\
&+ \frac{1}{4}t_2\left(\left(\frac{x_2}{2}+1\right)\rho\,\tau + \left(x_2+\frac{1}{2}\right)\sum_q \rho_q\tau_q\right) \\
&- \frac{3}{16}t_1\left(\left(\frac{x_1}{2}+1\right)\rho\Delta\rho + \left(x_1+\frac{1}{2}\right)\sum_q \rho_q\Delta\rho_q\right) \\
&+ \frac{1}{16}t_2\left(\left(\frac{x_2}{2}+1\right)\rho\Delta\rho + \left(x_2+\frac{1}{2}\right)\sum_q \rho_q\Delta\rho_q\right) \\
&+ \frac{1}{12}t_3\left(\left(\frac{x_3}{2}+1\right)\rho^2 - \left(x_3+\frac{1}{2}\right)\sum_q \rho_q^2\right)\rho^\gamma \\
&- \frac{1}{8}\left(t_1x_1 + t_2x_2 - 5(to+te)\right)\sum_q \boldsymbol{J}_q^2 \\
&- \frac{1}{16}\left(t_1\left(x_1-1\right) + t_2\left(x_2+1\right) - 10to\right)\boldsymbol{J}_n.\boldsymbol{J}_p \\
&- \left(b_4\rho\, \boldsymbol{\nabla}\cdot\boldsymbol{J} + b'_4\sum_q \rho_q\boldsymbol{\nabla}\cdot\boldsymbol{J}_q\right),
\end{aligned}
$$

C-parameters

$\{C^\rho_{t0}, C^\rho_{tD}, C^{\Delta\rho}_t, C^\tau_t, C^J_t, C^{\nabla J}_t, \gamma\}$

$$
\begin{aligned}
\mathcal{H}(\boldsymbol{r}) &= \tfrac{\hbar^2}{2m}\tau_0 + \mathcal{H}_0(\boldsymbol{r}) + \mathcal{H}_1(\boldsymbol{r}), \\
\mathcal{H}_t(\boldsymbol{r}) &= C^\rho_t\rho_t^2 + C^{\Delta\rho}_t\rho_t\Delta\rho_t + C^\tau_t\rho_t\tau_t \\
&+ \tfrac{1}{2}C^J_t\boldsymbol{J}_t^2 + C^{\nabla J}_t\rho_t\boldsymbol{\nabla}\cdot\boldsymbol{J}_t,
\end{aligned}
$$

$$C^\rho_t = C^\rho_{t0} + C^\rho_{tD}\ \rho_0^\gamma.$$

$$
\begin{aligned}
C^\rho_{00} &= \tfrac{3}{8}t_0, \quad C^\rho_{10} = -\tfrac{1}{4}t_0\left(x_0+\tfrac{1}{2}\right), \\
C^\rho_{0D} &= \tfrac{1}{16}t_3, \quad C^\rho_{1D} = -\tfrac{1}{24}t_3\left(x_3+\tfrac{1}{2}\right), \\
C^{\Delta\rho}_0 &= \tfrac{1}{16}t_2\left(x_2+\tfrac{5}{4}\right) - \tfrac{9}{64}t_1, \\
C^{\Delta\rho}_1 &= \tfrac{3}{32}t_1\left(x_1+\tfrac{1}{2}\right) + \tfrac{1}{32}t_2\left(x_2+\tfrac{1}{2}\right) \\
C^\tau_0 &= \tfrac{3}{16}t_1 + \tfrac{1}{4}t_2\left(x_2+\tfrac{5}{4}\right), \\
C^\tau_1 &= -\tfrac{1}{8}t_1\left(x_1+\tfrac{1}{2}\right) + \tfrac{1}{8}t_2\left(x_2+\tfrac{1}{2}\right), \\
C^J_0 &= -\tfrac{1}{8}(t_1(x_1-\tfrac{1}{2}) + t_2(x_2+\tfrac{1}{2})) + \tfrac{5}{16}(3\ to + te), \\
C^J_1 &= \tfrac{1}{16}(t_1 - t_2) + \tfrac{5}{16}(to - te), \\
C^{\nabla J}_0 &= -b_4 - \tfrac{1}{2}b'_4, \quad C^{\nabla J}_1 = -\tfrac{1}{2}b'_4,
\end{aligned}
$$

Optimization Procedure

t*x problem

$$t_0 = \frac{8}{3}C^\rho_{00}, \quad t_0x_0 = -\frac{3}{4}\left(C^\rho_{00} + 3C^\rho_{10}\right),$$

$$t_1 = -\frac{4}{3}(4C_0^{\Delta\rho} - C_0^\tau),$$

$$x_1 = -\frac{2}{3\,t_1}\left(-4C_0^{\Delta\rho} - 12C_1^{\Delta\rho} + C_0^\tau + 3C_1^\tau\right.$$

$$t_2 = \frac{4}{3}(4C_0^{\Delta\rho} - 8C_1^{\Delta\rho} + 3C_0^\tau - 6C_1^\tau),$$

$$x_2 = \frac{2}{3\,t_2}\left(-4C_0^{\Delta\rho} + 20C_1^{\Delta\rho} - 3C_0^\tau + 15C\right.$$

$$t_3 = 16C^\rho_{0d}, \quad x_3 = -\frac{8}{t_3}\left(C^\rho_{0d} + 3C^\rho_{1d}\right),$$

$$to = \frac{4}{15}(3C_0^J + 3C_1^J + 4C_0^{\Delta\rho} + 4C_1^{\Delta\rho}),$$

$$te = \frac{4}{15}(3C_0^J - 9C_1^J - 4C_0^{\Delta\rho} + 12C_1^{\Delta\rho} - 2$$

$$b_4 = -C_0^{\nabla J} + C_1^{\nabla J}, \quad b_4' = -2C_1^{\nabla J},$$

TABLE I: The lower ($\mathbf{v}_0$) and upper ($\mathbf{v}_1$) limits, maximum displacement ($\mathbf{d}$) and initial values ($\mathbf{v}_{in}$) for the Skyrme parameters used to minimize the χ^2 value within the SAM.

	$\mathbf{v}_0$	$\mathbf{v}_1$	$\mathbf{d}$	$\mathbf{v}_{in}$
t_0(MeV·fm^3)	−3000.0	−1500.0	50.0	−1603.0
t_1(MeV·fm^5)	−500.0	500.0	20.0	515.9
t_2(MeV·fm^5)	−500.0	500.0	20.0	84.5
t_{31}(MeV·fm$^{3(\alpha_1+1)}$)	1000.0	3000.0	50.0	1333.3
t_{32} (MeV·fm$^{3(\alpha_2+1)}$)	−1000	0.0	50.0	0.0
t_{33} (MeV·fm$^{3(\alpha_3+1)}$)	−500.0	500.0	20.0	0.0
x_0	−4.0	4.0	0.1	−0.02
x_1	−4.0	4.0	0.1	−0.5
x_2	−4.0	4.0	0.1	−1.713

TABLE III: The values of the Skyrme parameters for GSkI, GSkII and SSk interactions obtained by minimizing the χ^2.

	GSkI	GSkII	SSk
t_0(MeV·fm^3)	−1855.45	−1855.99	−2523.52
t_1(MeV·fm^5)	397.23	393.08	435.00
t_2(MeV·fm^5)	264.63	266.08	−382.04
t_{31}(MeV·fm$^{3(\alpha_1+1)}$)	2309.67	2307.15	2372.49
t_{32} (MeV·fm$^{3(\alpha_2+1)}$)	−449.01	−448.28	−−
t_{33} (MeV·fm$^{3(\alpha_3+1)}$)	−53.31	−−	−−
x_0	0.1180	0.0909	0.6835
x_1	−1.7586	−0.7203	−0.4519
x_2	−1.8068	−1.8369	−0.9214

Optimization Procedure

nuclear matter hints

$$\frac{E^{NM}}{A} \equiv W(\rho_c) \approx -16 \text{ MeV},$$

$$P^{NM} \equiv \rho^2 \frac{dW(\rho)}{d\rho}\bigg|_{\rho=\rho_c} = 0, \;\; \rho_c \approx 0.16 \text{ fm}$$

$$K^{NM} = 9\rho^2 \frac{d^2W(\rho)}{d\rho^2}\bigg|_{\rho=\rho_c} \approx 220 \text{ MeV},$$

$$M_s^{*NM} = \frac{2m}{\hbar^2}\frac{dW}{d\tau}\bigg|_{\rho=\rho_c} \approx 1,$$

$$a_{sym}^{NM} \equiv \frac{1}{2}\frac{d^2W(I,\rho)}{dI^2}\bigg|_{\substack{\rho=\rho_c\\ I=0}} = 32.5 \text{ MeV},$$

$$L^{NM} \equiv 3\rho_c \frac{da_{sym}^{NM}}{d\rho_c} \approx 50 \text{ MeV},$$

$$M_v^{*NM} \approx 1,$$

Nuclear matter
(7 parameters)

$$\gamma = \frac{-K^{NM} + \frac{\hbar^2}{2m}\left(4M_s^{*NM} - 3\right)\tau_c - 9\frac{E^{NM}}{A}}{\frac{\hbar^2}{2m}\left(6M_s^{*NM} - 9\right)\tau_c + 9\frac{E^{NM}}{A}},$$

$$C_{00}^{\rho} = \frac{\frac{\hbar^2}{2m}\left(\left(2-3\gamma\right)M_s^{*NM} - 3\right)\tau_c + 3\left(1+\gamma\right)\frac{E^{NM}}{A}}{3\gamma\rho_c},$$

$$C_{0D}^{\rho} = \frac{\frac{\hbar^2}{2m}\left(3 - 2M_s^{*NM}\right)\tau_c - 3\frac{E^{NM}}{A}}{3\gamma\rho_c^{1+\gamma}},$$

$$C_0^{\tau} = \frac{\hbar^2}{2m}\left(M_s^{*NM} - 1\right)\frac{1}{\rho_c}.$$

$$\begin{aligned} C_1^{\tau} &= C_0^{\tau} - \frac{\hbar^2}{2m}\left(M_v^{*NM} - 1\right)\frac{1}{\rho_c} \\ &= \frac{\hbar^2}{2m}\left(M_s^{*NM} - M_v^{*NM}\right)\frac{1}{\rho_c}, \end{aligned}$$

$$\begin{aligned} C_{10}^{\rho} &= \frac{1}{27\gamma\rho_c}\Big[27\left(1+\gamma\right)a_{sym}^{NM}{}_C - 9L^{NM} \\ &\quad - 5\left(\left(1+3\gamma\right)\frac{\hbar^2}{2m} - \left(2-3\gamma\right)\left(C_0^{\tau} + 3C_1^{\tau}\right)\rho_c\right)\tau_c\Big], \end{aligned}$$

$$\begin{aligned} C_{1D}^{\rho} &= \frac{1}{27\gamma\rho_c^{\gamma+1}}\Big[-27a_{sym}^{NM}{}_C + 9L^{NM} \\ &\quad + 5\left(\frac{\hbar^2}{2m} - 2\rho_c\left(C_0^{\tau} + 3C_1^{\tau}\right)\right)\tau_c\Big], \end{aligned}$$

Non-standard functionals

density dependent coupling constants

I. Density dependence of all the coupling constants

For the time-reversal and spherical symmetries imposed, the extended EDF reads

$$\mathcal{H}_t(r) = C_t^\rho \rho_t^2 + C_t^\tau \rho_t \tau_t + C_t^{\Delta\rho} \rho_t \Delta\rho_t + \tfrac{1}{2} C_t^J J_t^2 + C_t^{\nabla J} \rho_t \nabla \cdot J_t$$
$$+ C_t^{\nabla\rho} (\nabla\rho_t)^2 + C_t^{\nabla\rho'} (\nabla\rho_t) \cdot J_t$$

and depends linearly on 38 coupling constants,

$$C_t^\rho,\quad C_t^\tau,\quad C_t^{\Delta\rho},\quad C_t^{\mathrm{J}},\quad \text{and}\quad C_t^{\nabla \mathrm{J}},$$

$$\alpha_t^\rho,\quad \alpha_t^\tau,\quad \alpha_t^{\Delta\rho},\quad \alpha_t^{\mathrm{J}},\quad \alpha_t^{\nabla \mathrm{J}},\quad \alpha_t^{\nabla\rho},\quad \text{and}\quad \alpha_t^{\nabla\rho'},$$

$$\beta_t^\rho,\quad \beta_t^\tau,\quad \beta_t^{\Delta\rho},\quad \beta_t^{\mathrm{J}},\quad \beta_t^{\nabla \mathrm{J}},\quad \beta_t^{\nabla\rho},\quad \text{and}\quad \beta_t^{\nabla\rho'},$$

for $t = 0$ and 1, i.e.,

$$C_t^m(\rho_0, \rho_1) = C_t^m \left[1 + \alpha_t^m \left(1 - \left(\frac{\rho_0}{\rho_{\mathrm{sat}}} \right)^{\gamma_t^m} \right) + \beta_t^m \left(\left(\frac{\rho_1}{\rho_{\mathrm{sat}}} \right)^2 \right)^{\eta_t^m} \right]$$

and on 28 powers γ_t^m and η_t^m.

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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

❑ Beginning the development of optimization procedure
- Nuclear matter
- Experimental data
- Benchmark results
- Errors and correlations among parameters and observables

❑ Testing new terms and exploring non-standard functionals
- density dependent coupling constants
- higher gradients
- derived trough DME