TOWARDS A UNIVERSAL NUCLEAR ENERGY DENSITY FUNCTIONAL

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

1. Mass Table Calculations
2. Optimal parameters of the functional
3. Improving the functional
4. Visualization and development tools

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.

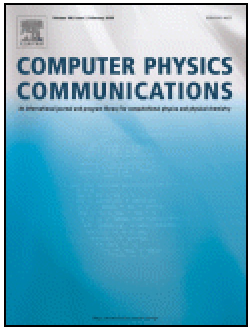
Third, to apply the validated theory to properties of interest that cannot be measured, in particular the transition properties needed for reaction theory.

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

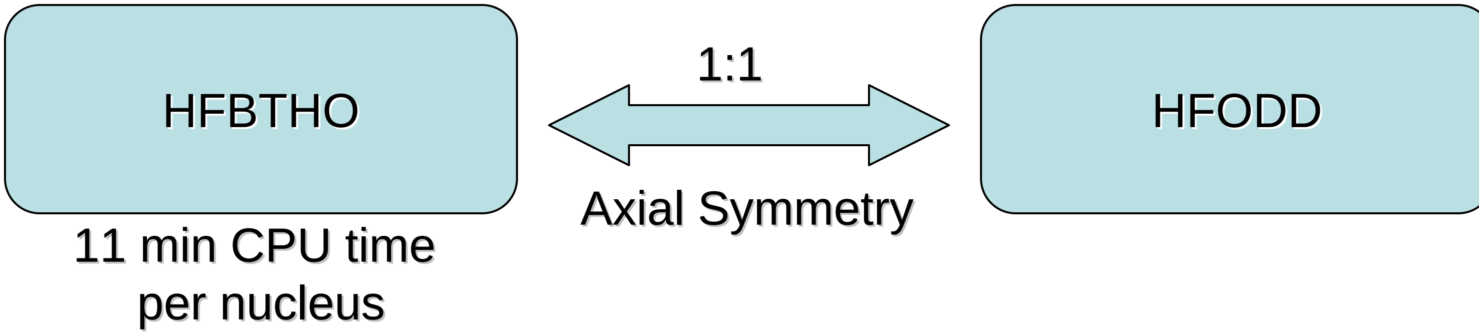


HFBTHO

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

http://massexplorer.org/svn/HFBTHO/trunk

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



HFBTHO/HFODD (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	−8.114078	−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

HFBTHO/HFODD (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}	1.007644	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^{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^{kin}	1360.437867	1360.442751	1362.407077	1362.409601	1358.912567	1358.886614
E_p^{kin}	827.317590	827.317961	827.123364	827.123676	827.195176	827.191207
E_{SO}	−50.483676	−50.485916	−50.922860	−50.923940	−49.607742	−49.592026
E_{dir}	365.743676	365.743774	365.621013	365.621031	365.736277	365.735680
E_{tot}	−1024.707275	−1024.707272	−1024.301233	−1024.301252	−1024.415866	−1024.416901

^{120}Sn: HFBODD: 6 h 39 min CPU / HFBTHO: 3 min CPU

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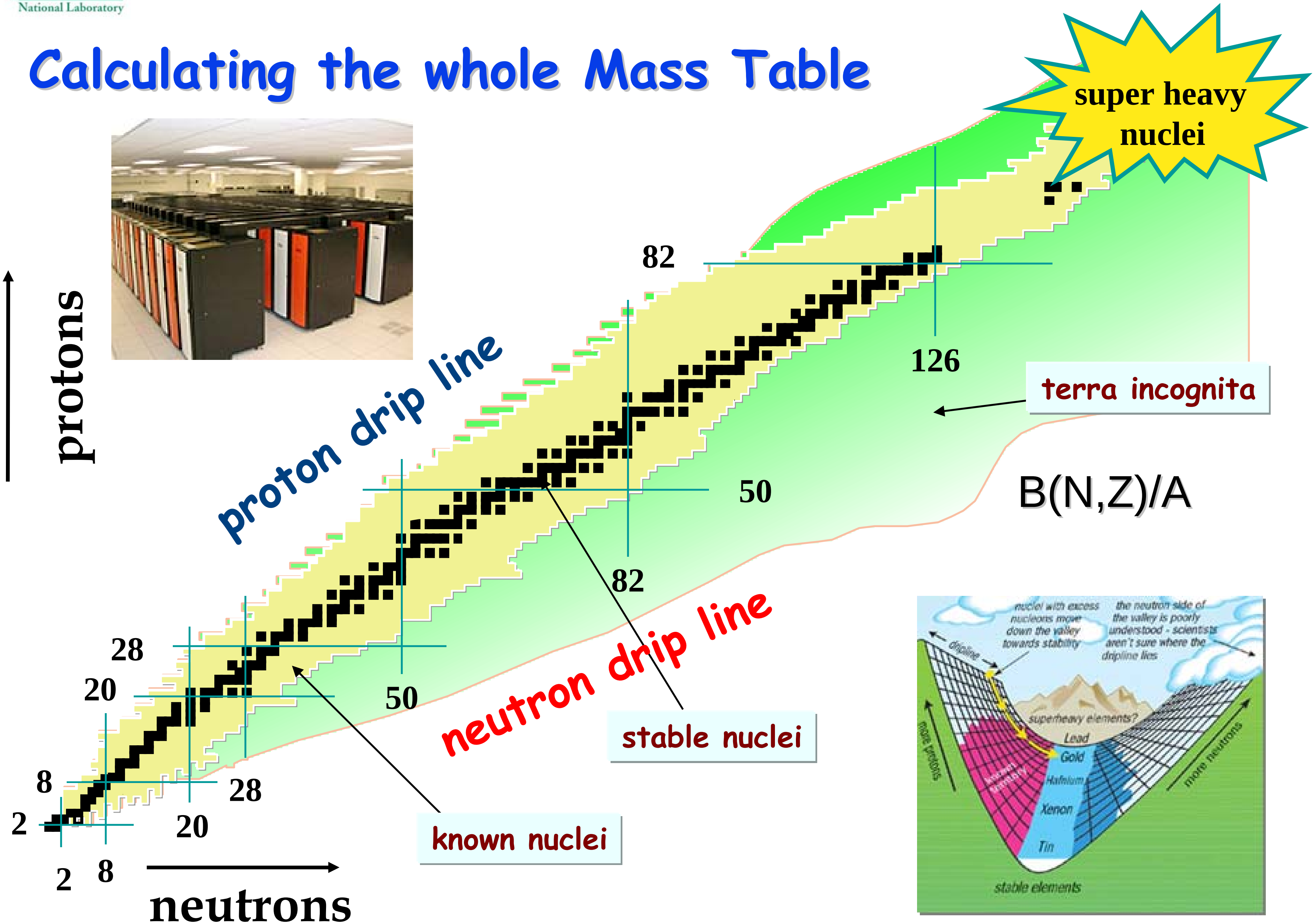
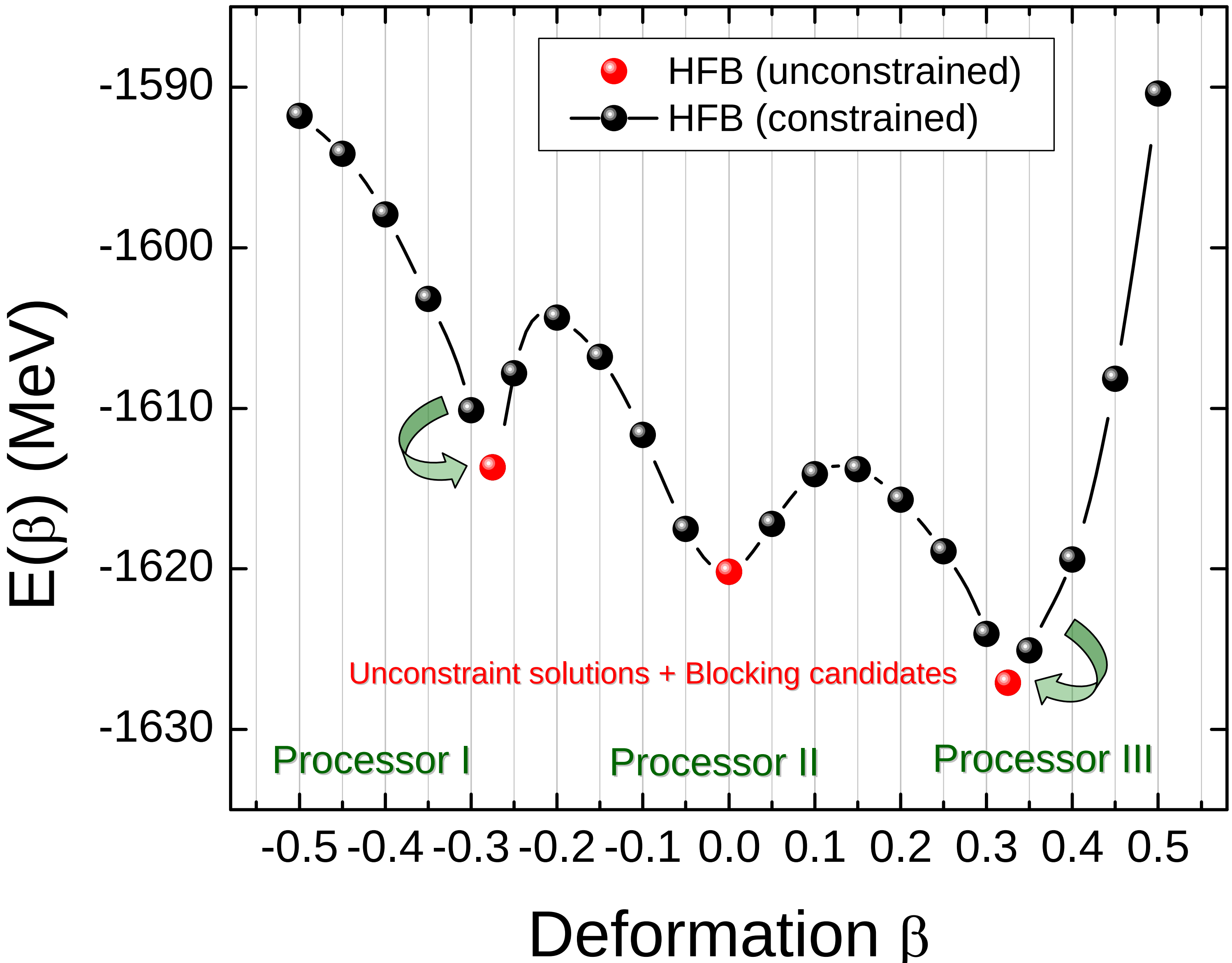
Calculating the whole Mass Table



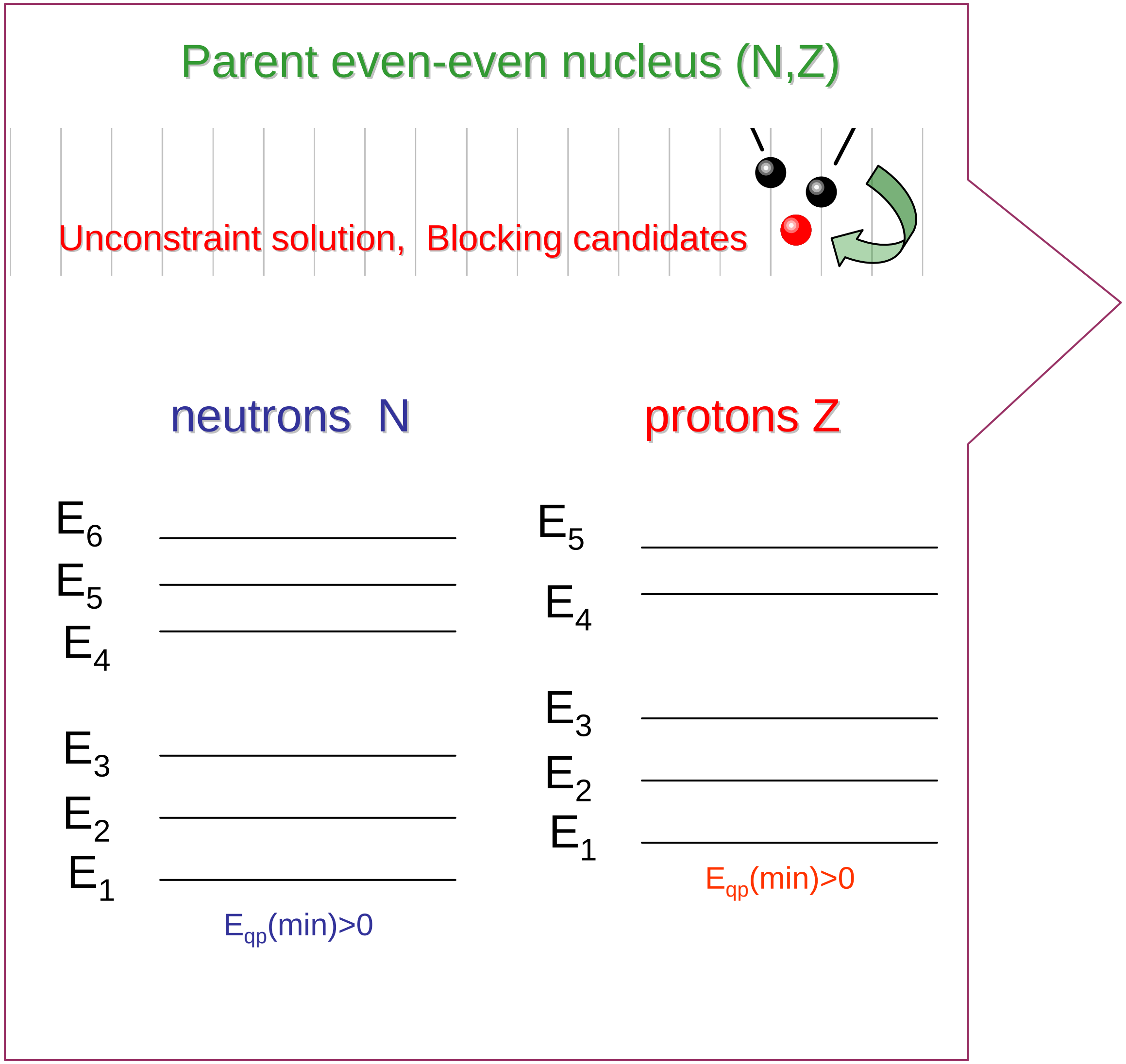
Large-Scale Calculations

Constrained calculations for about 9059 even-even nuclei



Large-Scale Calculations

Blocking calculations for about 837 220 configurations odd nuclei



Self-consitent calculations for odd nuclei with blocking

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

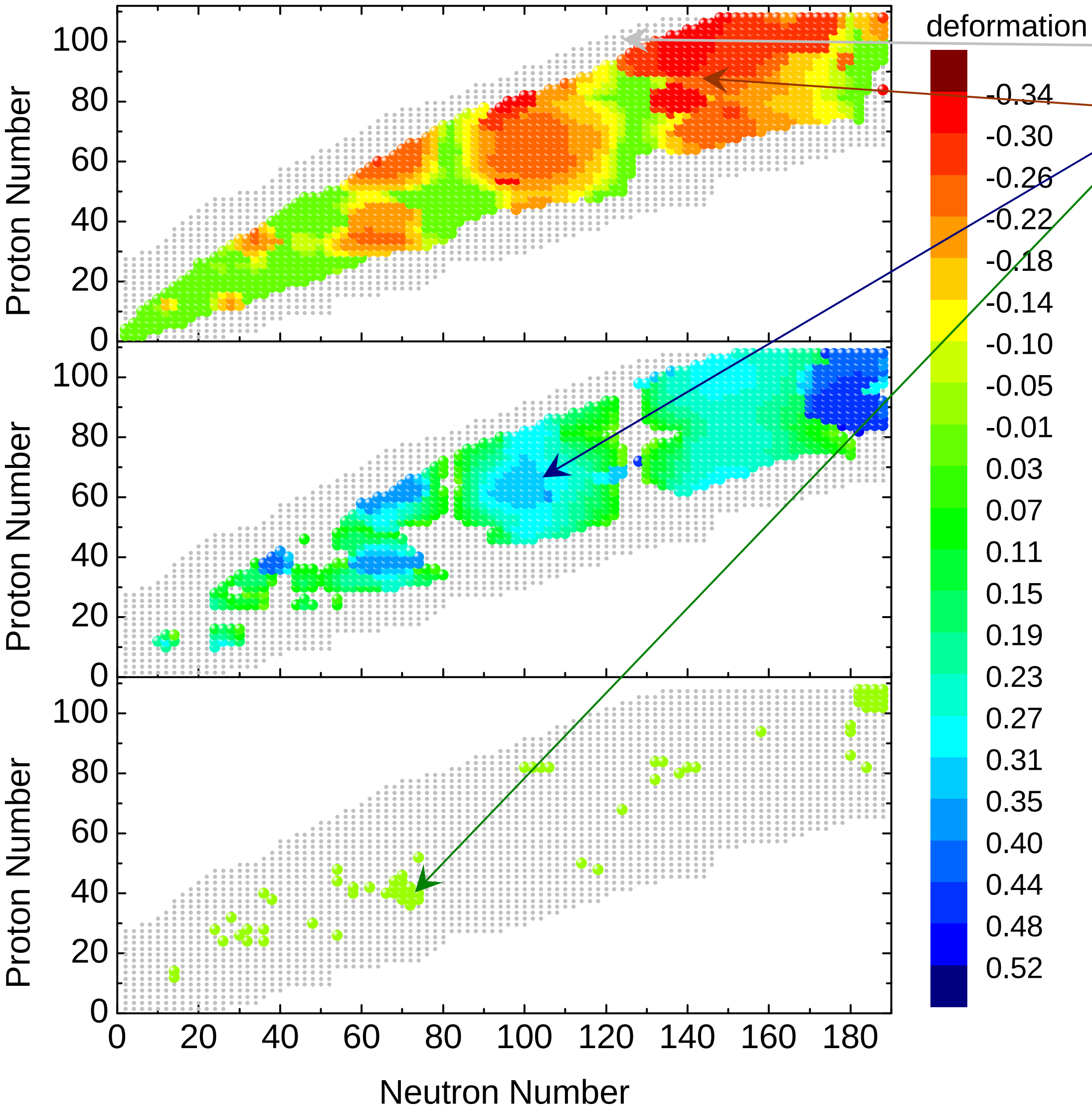
odd-even nucleus (N,Z+1)
5 configurations

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

41 processors

Large-Scale Mass Table Calculations

Calculating the whole Mass Table including even-even, odd-even, odd-odd nuclei



Constrained calculations for 9059 even-even nuclei

2971 even-even bound states

2 CPU hours using 9060 processors

837 220 blocking candidates for odd-even and odd-odd nuclei

12 CPU hours using 9060 processors

After implementing Broyden method

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

A single 14 CPU hours run

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Towards an Optimal Set of Parameters for a Given Functional

Standard Skyrme functional - 13 parameters in ph-part

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

t-parameters

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

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

C-parameters

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

$$C^\rho_t = C^\rho_{t0} + C^\rho_{tD}\ \rho_0^\gamma,\ \ (t=0,1).$$

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

Optimization in Terms of Infinite Nuclear Matter Properties

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Skyrme functional fitting at 13% of the computational expense

Jorge Moré, Jason Sarich, and **Stefan Wild**

Mathematics and

Computer Science Division

Argonne National Laboratory

3rd LACM-EFES-JUSTIPEN Workshop
February 25, 2009

Our Optimization/NLS/NLR Problem

2 measurement types: binding energy (E), radius (R)
$\mathcal{N}_E = 63$ nuclei (27 spherical, 36 deformed)
$\mathcal{N}_R =$ the spherical nuclei from $\mathcal{N}_E$

$d_{t,i}$ experimental data ($t \in \{E, R\}$) for ith nucleus

$s_{t,i}(\theta)$ HFBTHO simulation of type t for ith nucleus

θ 9 simulation parameters from intervals of interest

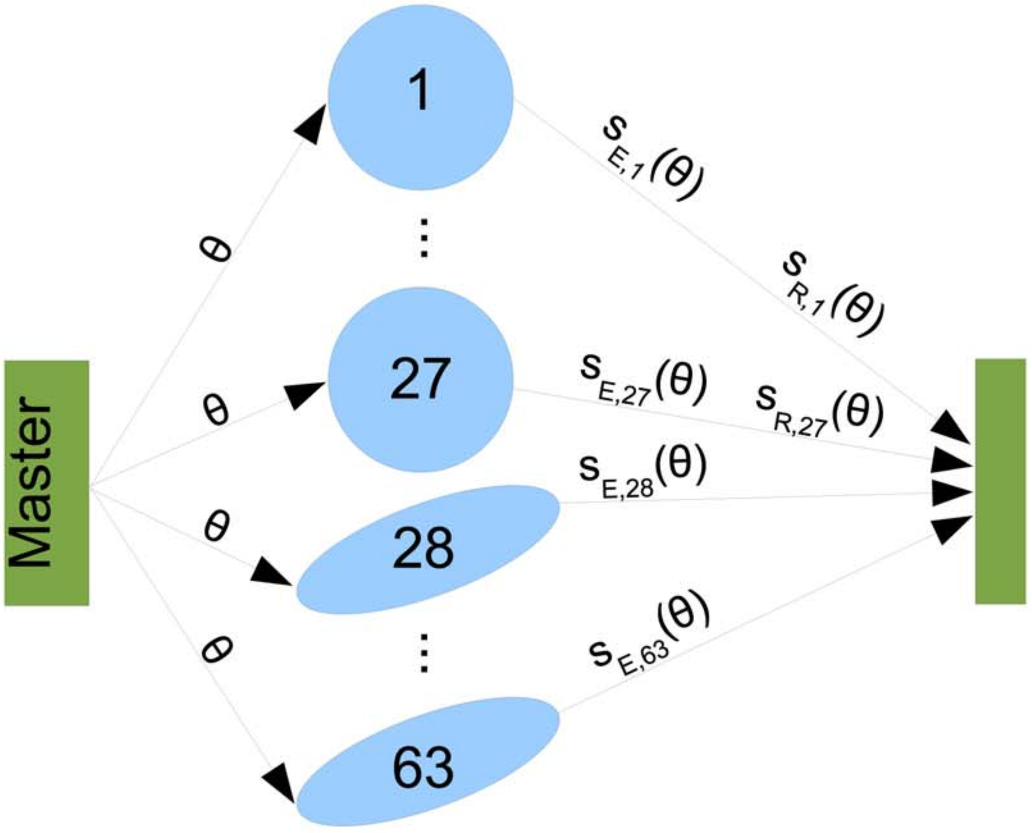
$$f(\theta) = \frac{1}{\sigma_E^2} \sum_{i=1}^{63} \left(d_{E,i} - s_{E,i}(\theta)\right)^2 + \frac{1}{\sigma_R^2} \sum_{i=1}^{27} \left(d_{R,i} - s_{R,i}(\theta)\right)^2,$$

σ_t weights: $\sigma_E = 2$ [MeV], $\sigma_R = .02$ [fm]
Chosen to balance goals of energy and radius fitting

We Cannot Afford 9 Hours per Evaluation!

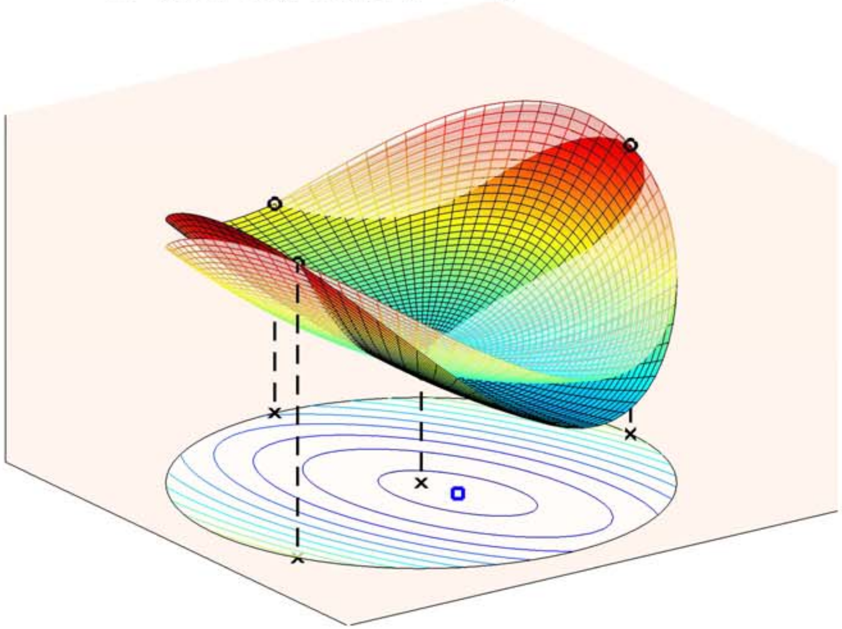
Move to a cluster

- 64 processors for 63 nuclei
- Simulate each nucleus independently
- Will be bound by the longest HFBTHO simulation time



A Sketch of MFQnls

Idea: Build a quadratic model of the objective f in a neighborhood of the current $\theta = \theta^{(k)}$



$$q(\theta^{(k)} + s) = c + g^T s + \frac{1}{2} s^T H s:$$

Find the $\frac{(n+1)(n+2)}{2}$ model coefficients $c, g, H = H^T$ so:

$$q(\hat{\theta}^{(i)}) = f(\hat{\theta}^{(i)}) \quad \forall \hat{\theta}^{(i)} \in \mathcal{Y}$$

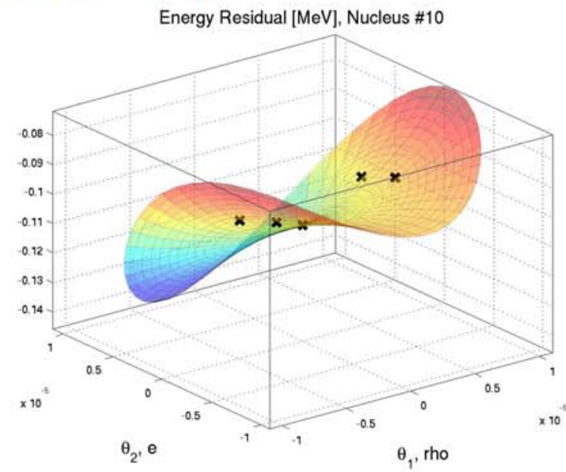
$\mathcal{Y}$ =interpolation set based on the θ at which we've previously evaluated f

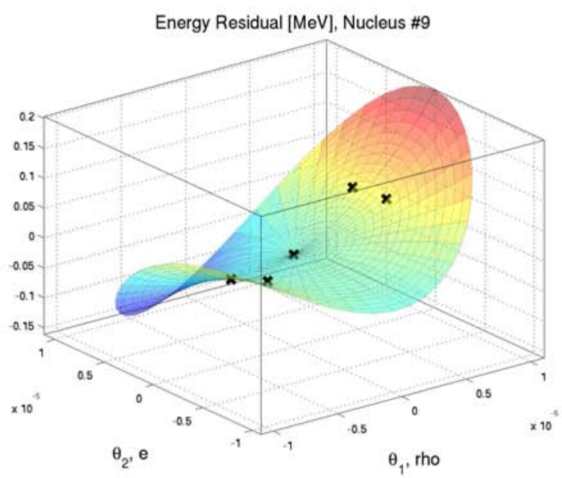
Taking Advantage of the Structure of f

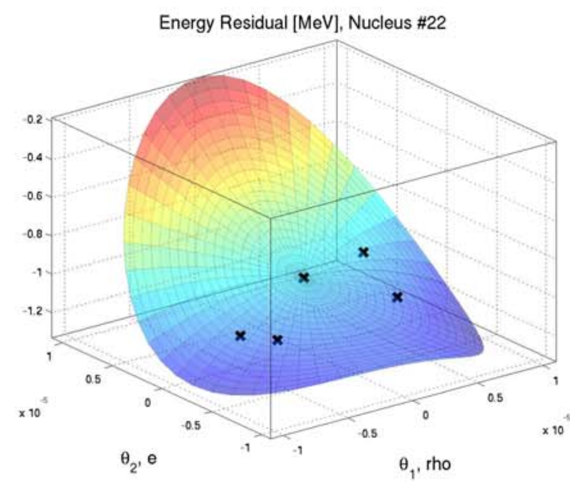
Build an interpolation model for each residual $\frac{d_i - s_{t,i}(\theta)}{\sigma_i}$.

Allows us to obtain an approximate

Jacobian, $J \approx \begin{bmatrix} g_1^T \\ \vdots \\ g_m^T \end{bmatrix}$







Sensitivity

Assuming the errors $\frac{d_{t,i} - s_{t,i}(\theta)}{\sigma_t}$ are

- iid Normal with mean zero (← big assumption?)

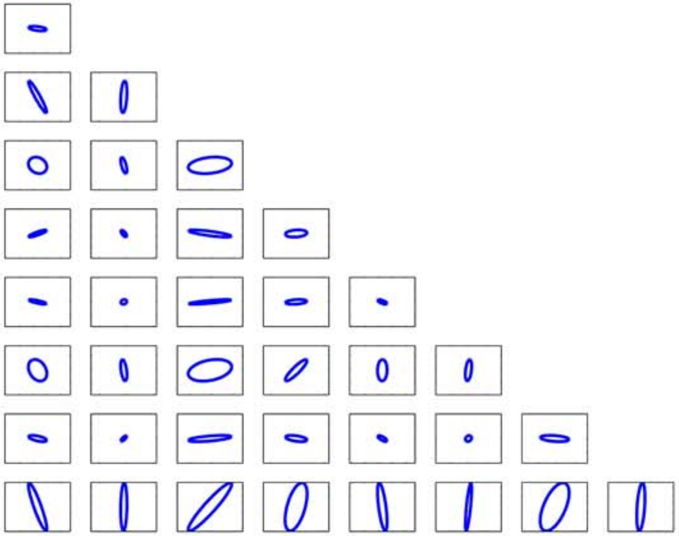
Use Jacobian approximation at $\hat{\theta}$ to estimate the covariance matrix

$$Cov(\hat{\theta}) \approx 2\left(\nabla^2 f(\hat{\theta})\right)^{-1} \approx \left(\hat{J}^T \hat{J}\right)^{-1}$$

Correlations

$$Cor(\theta_i, \theta_j) = \frac{Cov(\theta)_{i,j}}{\sqrt{Cov(\theta)_{i,i} Cov(\theta)_{j,j}}}$$

Reduce the problem by accounting for strong correlations.



Towards the optimal parameters of a given functional

$$\rho_c, \frac{E^{NM}}{A}, K^{NM}, M_s^{*NM}, a_{sym}^{NM}, L^{NM}, M_v^{*NM}, C_t^{\Delta\rho}, C_t^J, C_t^{\nabla J}$$

Correlation Matrix

1	0.0117	0.0168	0.0203	0.0282	0.0164	0.0020
	1	-0.036	-0.035	-0.032	0.026	-0.0004
		1	-0.020	-0.018	0.0168	-0.0009
			1	-0.019	0.0166	-0.0008
				1	0.0125	-0.0012
					1	0.0010
						1

Preliminary estimates

$$\frac{E^{NM}}{A} \approx -16.05 \text{ MeV},$$

$$\rho_c \approx 0.157 \text{ fm}^{-3},$$

$$K^{NM} \approx 218.5 \text{ MeV},$$

$$M_s^{*NM} \approx 0.997,$$

$$a_{sym}^{NM} = 32.36 \text{ MeV},$$

$$L^{NM} \approx 46.3 \text{ MeV},$$

$$M_v^{*NM} \approx 1.37,$$

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Most general form of the functional one can consider by now

$$\mathcal{H}(r) = \frac{\hbar^2}{2m}\tau_0 + \mathcal{H}_0(r) + \mathcal{H}_1(r),$$

$$\begin{aligned}\mathcal{H}_t(r) &= U_t^{\rho\rho}\rho_t^2 + U_t^{\rho\tau}\rho_t\tau_t + U_t^{J^2}J_t^2 \\ &+ U_t^{\rho\Delta\rho}\rho_t\Delta\rho_t + U_t^{\nabla\rho\nabla\rho}(\nabla\rho_t)^2 \\ &+ U_t^{\rho\nabla J}\rho_t\nabla\cdot J_t + U_t^{J\nabla\rho}J_t\cdot\nabla\rho_t,\end{aligned}$$

t=(0,1) , e.g.,

$\rho_0 = \rho_n + \rho_p,$

$\rho_1 = \rho_n - \rho_p$

six densities

$\rho_t,\ \tau_t,\ J_t,$

grouped in fifteen terms proportional to

$\tau_0, \rho_t^2, \rho_t\tau_t, J_t^2, \rho_t\Delta\rho_t, (\nabla\rho_t)^2, \rho_t\nabla\cdot J_t, \nabla\rho_t\cdot J_t$

and multiplied by fifteen amplitudes

$\frac{\hbar^2}{2m}, U_t^{\rho\rho}, U_t^{\rho\tau}, U_t^{J^2}, U_t^{\rho\Delta\rho}, U_t^{\nabla\rho\nabla\rho}, U_t^{\rho\nabla J}, U_t^{J\nabla\rho},$

U ⟶ C : Standard Skyrme functional

U ⟶ D : Functional with density dependent coupling constants

U ⟶ G : DME functional

U ⟶ F : Fayans functional

TOWARDS A UNIVERSAL NUCLEAR ENERGY DENSITY FUNCTIONAL

Standard Skyrme functional

U-functions: C-parameters

$\{C^{\rho}_{t0}, C^{\rho}_{tD}, C^{\Delta\rho}_{t}, C^{\tau}_{t}, C^{J}_{t}, C^{\nabla J}_{t}, \gamma\}$

$$\mathcal{H}(\boldsymbol{r}) = \frac{\hbar^2}{2m}\tau_0 + \mathcal{H}_0(\boldsymbol{r}) + \mathcal{H}_1(\boldsymbol{r}),$$

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

$$C^{\rho}_t = C^{\rho}_{t0} + C^{\rho}_{tD}\,\rho_0^{\gamma}, \quad (t=0,1).$$

$$C^{\rho}_{00} = \tfrac{3}{8}\mathrm{t}_0, \quad C^{\rho}_{10} = -\tfrac{1}{4}\mathrm{t}_0\left(\mathrm{x}_0+\tfrac{1}{2}\right),$$

$$C^{\rho}_{0\mathrm{D}} = \tfrac{1}{16}\mathrm{t}_3, \quad C^{\rho}_{1\mathrm{D}} = -\tfrac{1}{24}\mathrm{t}_3\left(\mathrm{x}_3+\tfrac{1}{2}\right),$$

$$C^{\Delta\rho}_0 = \tfrac{1}{16}\mathrm{t}_2\left(\mathrm{x}_2+\tfrac{5}{4}\right) - \tfrac{9}{64}\mathrm{t}_1,$$

$$C^{\Delta\rho}_1 = \tfrac{3}{32}\mathrm{t}_1\left(\mathrm{x}_1+\tfrac{1}{2}\right) + \tfrac{1}{32}\mathrm{t}_2\left(\mathrm{x}_2+\tfrac{1}{2}\right)$$

$$C^{\tau}_0 = \tfrac{3}{16}\mathrm{t}_1 + \tfrac{1}{4}\mathrm{t}_2\left(\mathrm{x}_2+\tfrac{5}{4}\right),$$

$$C^{\tau}_1 = -\tfrac{1}{8}\mathrm{t}_1\left(\mathrm{x}_1+\tfrac{1}{2}\right) + \tfrac{1}{8}\mathrm{t}_2\left(\mathrm{x}_2+\tfrac{1}{2}\right),$$

$$C^{J}_0 = -\tfrac{1}{8}(\mathrm{t}_1(\mathrm{x}_1-\tfrac{1}{2}) + \mathrm{t}_2(\mathrm{x}_2+\tfrac{1}{2})) + \tfrac{5}{16}(3\,to + te),$$

$$C^{J}_1 = \tfrac{1}{16}(\mathrm{t}_1-\mathrm{t}_2) + \tfrac{5}{16}(to - te),$$

$$C^{\nabla J}_0 = -b_4 - \tfrac{1}{2}b_4', \quad C^{\nabla J}_1 = -\tfrac{1}{2}b_4',$$

$$\begin{aligned}
\mathcal{H}(\boldsymbol{r}) = {} & \frac{\hbar^2}{2m}\tau \\
& + \frac{1}{2}\mathrm{t}_0\left(\left(\frac{\mathrm{x}_0}{2}+1\right)\rho^2 - \left(\mathrm{x}_0+\frac{1}{2}\right)\sum_q \rho_q^2\right) \\
& + \frac{1}{4}\mathrm{t}_1\left(\left(\frac{\mathrm{x}_1}{2}+1\right)\rho\,\tau - \left(\mathrm{x}_1+\frac{1}{2}\right)\sum_q \rho_q\tau_q\right) \\
& + \frac{1}{4}\mathrm{t}_2\left(\left(\frac{\mathrm{x}_2}{2}+1\right)\rho\,\tau + \left(\mathrm{x}_2+\frac{1}{2}\right)\sum_q \rho_q\tau_q\right) \\
& - \frac{3}{16}\mathrm{t}_1\left(\left(\frac{\mathrm{x}_1}{2}+1\right)\rho\Delta\rho + \left(\mathrm{x}_1+\frac{1}{2}\right)\sum_q \rho_q\Delta\rho_q\right) \\
& + \frac{1}{16}\mathrm{t}_2\left(\left(\frac{\mathrm{x}_2}{2}+1\right)\rho\Delta\rho + \left(\mathrm{x}_2+\frac{1}{2}\right)\sum_q \rho_q\Delta\rho_q\right) \\
& + \frac{1}{12}\mathrm{t}_3\left(\left(\frac{\mathrm{x}_3}{2}+1\right)\rho^2 - \left(\mathrm{x}_3+\frac{1}{2}\right)\sum_q \rho_q^2\right)\rho^{\gamma} \\
& - \frac{1}{8}\left(\mathrm{t}_1\mathrm{x}_1 + \mathrm{t}_2\mathrm{x}_2 - 5(\mathrm{to}+\mathrm{te})\right)\sum_q \boldsymbol{J}_q^2 \\
& - \frac{1}{16}\left(\mathrm{t}_1\left(\mathrm{x}_1-1\right) + \mathrm{t}_2\left(\mathrm{x}_2+1\right) - 10\mathrm{to}\right)\boldsymbol{J}_n.\boldsymbol{J}_p \\
& - \left(\mathrm{b}_4\rho\,\boldsymbol{\nabla}\cdot\boldsymbol{J} + \mathrm{b}_4'\sum_q \rho_q\boldsymbol{\nabla}\cdot\boldsymbol{J}_q\right),
\end{aligned}$$

TOWARDS A UNIVERSAL NUCLEAR ENERGY DENSITY FUNCTIONAL

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.

M. Kortelainen *et al.*, to be published

TOWARDS A UNIVERSAL NUCLEAR ENERGY DENSITY FUNCTIONAL

Density Dependent Coupling Constants

U ⟶

$$D_t^m = C_t^m \left(1 + \tilde{\alpha}_t^m \left(1 - \mathrm{y}_0^{\gamma_t^m}\right) + \tilde{\beta}_t^m \, \mathrm{y}_1^{\eta_t^m}\right)$$

$$= C_t^m + \alpha_t^m \left(1 - \mathrm{y}_0^{\gamma_t^m}\right) + \beta_t^m \, \mathrm{y}_1^{\eta_t^m},$$

$$\mathrm{y}_0 = \left(\frac{\rho_0}{\rho_c}\right), \quad \mathrm{y}_1 = \left(\frac{\rho_1}{\rho_c}\right)^2.$$

$$m = \{\rho\rho, \rho\tau, J^2, \rho\Delta\rho, \nabla\rho\nabla\rho, \rho\nabla J, J\nabla\rho\}$$

A set of 66 independent parameters
38 coupling constants $\{C, \alpha, \beta\}$, and 28 powers $\{\gamma, \eta\}$

$$\{C_t^{\rho\rho}, C_t^{\rho\Delta\rho}, C_t^{\rho\tau}, C_t^{J^2}, C_t^{\rho\nabla J}\}$$

$$\{\alpha_t^m, \beta_t^m, \gamma_t^m, \eta_t^m\}.$$

Microscopically Based Nuclear Energy Functionals

S. K. Bogner

National Superconducting Cyclotron Laboratory and Department of Physics and Astronomy, Michigan State University, East Lansing, MI 48824

Abstract. A major goal of the SciDAC project "Building a Universal Nuclear Energy Density Functional" is to develop next-generation nuclear energy density functionals that give controlled extrapolations away from stability with improved performance across the mass table. One strategy is to identify missing physics in phenomenological Skyrme functionals based on our understanding of the underlying internucleon interactions and microscopic many-body theory. In this contribution, I describe ongoing efforts to use the density matrix expansion of Negele and Vautherin to incorporate missing finite-range effects from the underlying two- and three-nucleon interactions into phenomenological Skyrme functionals.

DENSITY MATRIX EXPANSION

The dominant many-body perturbation theory (MBPT) contributions to bulk nuclear properties like ground state energies take the generic form

$$\langle V \rangle = \frac{1}{2}\sum_{\{\sigma\tau\}} \int d\mathbf{r}_1 \cdots \int d\mathbf{r}_4 \, \langle \mathbf{r}_1\sigma_1\tau_1\mathbf{r}_2\sigma_2\tau_2|\widehat{\mathscr{V}}|\mathbf{r}_3\sigma_3\tau_3\mathbf{r}_4\sigma_4\tau_4\rangle \times \rho(\mathbf{r}_3\sigma_3\tau_3,\mathbf{r}_1\sigma_1\tau_1)\rho(\mathbf{r}_4\sigma_4\tau_4,\mathbf{r}_2\sigma_2\tau_4)$$

but any truncation will give results depending on the particular choice for $k_{\rm F}$. The standard LDA choice of Negele and Vautherin corresponds to:

$$k_{\rm F}(\mathbf{R}) = (3\pi^2\rho(\mathbf{R})/2)^{1/3}\,, \tag{10}$$

though alternative choices such as the one introduced by Campi and Bouyssy [33]

$$k_F(\mathbf{R}) = \sqrt{\frac{5}{3}\frac{\tau(\mathbf{R}) - \frac{1}{4}\nabla^2\rho(\mathbf{R})}{\rho(\mathbf{R})}}\,, \tag{11}$$

may be useful to optimize the convergence of truncated expansions of Eq. (9), and to introduce novel τ and $\nabla^2\rho$ dependencies analogous to those found in Coulomb Meta-GGA functionals [19]. Truncating Eq. (9) to terms with $n \leqslant 1$ yields the fundamental equation of the DME,

$$\hat{\rho}(\mathbf{R}+\frac{\mathbf{r}}{2},\mathbf{R}-\frac{\mathbf{r}}{2}) \approx \rho_{\rm SL}(k_{\rm F}(\mathbf{R})r)\rho(\mathbf{R}) + r^2 g(k_{\rm F}(\mathbf{R})r)\left[\frac{1}{4}\nabla^2\rho(\mathbf{R}) - \tau(\mathbf{R}) + \frac{3}{5}k_{\rm F}(\mathbf{R})^2\rho(\mathbf{R})\right], \tag{12}$$

where

$$\rho_{\rm SL}(x) \equiv 3j_1(x)/x\,, \qquad g(x) \equiv 35j_3(x)/2x^3\,, \tag{13}$$

To illustrate some of the non-trivial density dependencies that arise from finite-range effects, we give a sampling of results that are obtained by applying the DME to the Hartree-Fock contributions of the long-range parts of the chiral EFT NN interaction thru N^{2}LO [34]. Thru this order, the finite-range interactions can be decomposed as

$$V_{NN} = V_C + \tau_1 \cdot \tau_2 W_C + \left[V_S + \tau_1 \cdot \tau_2 W_S \right] \vec{\sigma}_1 \cdot \vec{\sigma}_2 + \left[V_T + \tau_1 \cdot \tau_2 W_T \right] \vec{\sigma}_1 \cdot \vec{q}\, \vec{\sigma}_2 \cdot \vec{q} + i \left[V_{LS} + \tau_1 \cdot \tau_2 W_{LS} \right] \left(\vec{\sigma}_1 + \vec{\sigma}_2 \right) \cdot \left(\vec{q} \times \vec{k} \right), \quad (15)$$

Skyrme-like EDF's from the DME

$$\mathcal{E} = \frac{\tau}{2M} + \frac{3}{8} t_0 \rho^2 + \frac{1}{16} t_3 \rho^{2+\alpha} + \frac{1}{16}(3t_1 + 5t_2)\rho\tau + \frac{1}{64}(9t_1 - 5t_2)|\nabla\rho|^2 + \cdots \quad \text{Skyrme}$$

$$\mathcal{E} = \frac{\tau}{2M} + A[\rho] + B[\rho]\tau + C[\rho]|\nabla\rho|^2 + \cdots \quad \text{DME}$$

- coupling *constants* --> coupling *functions*

  - finite range effects encoded as ρ-dependence in ABC
  - microscopic isovector, spin-orbit terms
  - well-suited for existing SkyHF codes

Novel density-dependencies in EDF from 1π and 2π exchanges:

$$\rho^{7/3}, \;\; \rho^{4/3}, \;\; \rho^{2/3}, \;\; \frac{1}{\rho^{2/3}} log(1 + c\rho^{2/3}), \;\; \ldots$$

TOWARDS A UNIVERSAL NUCLEAR ENERGY DENSITY FUNCTIONAL

DME FUNCTIONAL

U ⟶

$$
\begin{aligned}
G_t^{\rho\rho} &= C_t^{\rho\rho} + \mathrm{G}\, g_t^{\rho\rho}(\rho_0),\\
G_t^{\rho\tau} &= C_t^{\rho\tau} + \mathrm{G}\, g_t^{\rho\tau}(\rho_0),\\
G_t^{J^2} &= C_t^{J^2} + \mathrm{G}\, g_t^{J^2}(\rho_0),\\
G_t^{\rho\Delta\rho} &= C_t^{\rho\Delta\rho} + \mathrm{G}\, g_t^{\rho\Delta\rho}(\rho_0),\\
G_t^{\nabla\rho\nabla\rho} &= C_t^{\nabla\rho\nabla\rho} + \mathrm{G}\, g_t^{\nabla\rho\nabla\rho}(\rho_0),\\
G_t^{\rho\nabla J} &= C_t^{\rho\nabla J} + \mathrm{G}\, g_t^{\rho\nabla J}(\rho_0),\\
G_t^{J\nabla\rho} &= C_t^{J\nabla\rho} + \mathrm{G}\, g_t^{J\nabla\rho}(\rho_0).
\end{aligned}
$$

$$
g_t^m(\rho_0) = \frac{1}{2}\left(A^m(\rho_0) + (-1)^t B^m(\rho_0)\right),
$$

$$
m = \{\rho\rho, \rho\tau, J^2, \rho\Delta\rho, \nabla\rho\nabla\rho, \rho\nabla J, J\nabla\rho\}
$$

$$
\begin{aligned}
A^{\rho\rho} &= \frac{1}{256\, u^6}\{12u\left(35+4u^2\right)\tan^{-1}(2u)\\
&- \frac{3}{4u^2}\left(7+16u^2\left(8-9u^2\right)\right)\log\left(4u^2+1\right)\\
&+ \left(21-498u^2-64u^4+16u^6\right)\},\\
A^{\rho\Delta\rho} &= \frac{35}{3072\, m_\pi^2\, u^8}\{3-72u^2-4u^4\\
&- \frac{1}{4u^2}\left(3+54u^2-72u^4\right)\log\left(1+4u^2\right)\\
&+ 60\tan^{-1}(2u)u\}, \quad B^{\rho\Delta\rho} = 2A^{\rho\Delta\rho},\\
A^{J^2} &= \frac{1}{48\, m_\pi^2}\left(\frac{5+12u^2}{(1+4u^2)^2} + \frac{\log\left(4u^2+1\right)}{4u^2}\right),\\
A^{\rho\tau} &= -4A^{\rho\Delta\rho}, \quad B^{\rho\tau} = 2A^{\rho\Delta\rho}, \quad B^{J^2} = 2A^{J^2},\\
A^{\rho\nabla J} &= B^{\rho\nabla J} = 0, \quad A^{J\nabla\rho} = B^{J\nabla\rho} = 0,
\end{aligned}
$$

$$
u = k_F/m_\pi \qquad G = \mathrm{g}_A^2/f_\pi^2
$$

$$
\{C_{t0}^{\rho\rho}, C_{t\mathrm{D}}^{\rho\rho}, C_t^{\rho\Delta\rho}, C_t^{\rho\tau}, C_t^{J^2}, C_t^{\rho\nabla J}, \gamma, G\},
$$

TOWARDS A UNIVERSAL NUCLEAR ENERGY DENSITY FUNCTIONAL

Density Dependent Coupling Constants

$$W(\rho,I) = W(\rho)+S_2(\rho)I^2+S_4(\rho)I^4,$$

$$W(\rho) = = \frac{E^{NM}}{A}+\frac{P^{NM}}{\rho_c^2}(\rho-\rho_c)+\frac{K^{NM}}{18\rho_c^2}(\rho-\rho_c)^2$$

$$S_2(\rho) = a_{sym}^{NM}+\frac{L^{NM}}{3\rho_c}(\rho-\rho_c)+\frac{\Delta K^{NM}}{18\rho_c^2}(\rho-\rho_c)$$

SLY4

$$\frac{E^{NM}}{A} = -15.972 \text{ MeV}, \quad a_{sym}^{NM} = 32.0 \text{ MeV},$$

$$\rho_c = 0.15954 \text{ fm}^{-3}, \quad L^{NM} = 45.962 \text{ MeV},$$

$$K^{NM} = 229.9 \text{ MeV}, \quad \Delta K^{NM} = -119.696 \text{ MeV},$$

$$M_s^{*NM} = 1.4396, \quad M_v^{*NM} = 1.24984\ .$$

$$G = \frac{K^{NM}+9(\gamma+1)\frac{E^{NM}}{A}+\frac{\hbar^2}{2m}\left(3(1-3\gamma)\tau_c-2(2-3\gamma)M_s^{*NM}\right)}{\tilde{k}_F^c\rho_c\left((1-3\gamma)g_0^{\rho\rho'}+\tilde{k}_F^c g_0^{\rho\rho''}+\left((5-3\gamma)g_0^{\rho\tau'}+\tilde{k}_F^c g_0^{\rho\tau''}\right)\tau_c\right)}$$

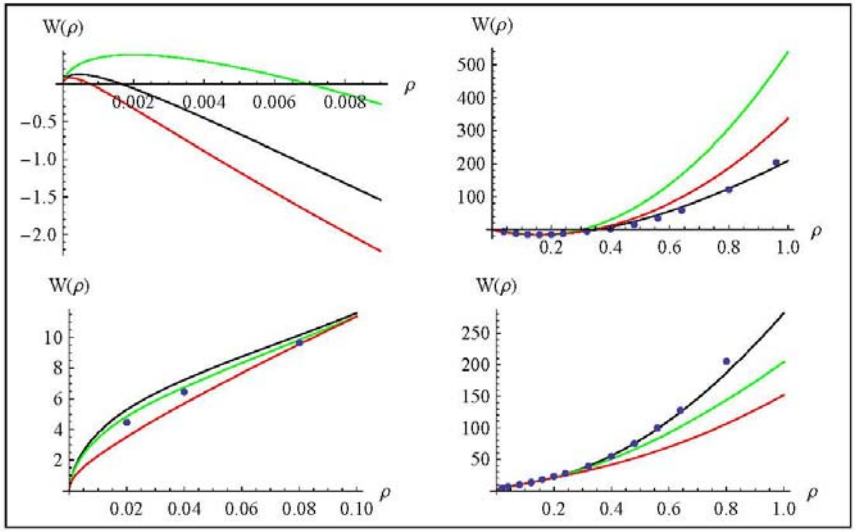
$$C_{00}^{\rho\rho} = \frac{\frac{\hbar^2}{2m}\left((2-3\gamma)M_s^{*NM}-3\right)\tau_c+3(1+\gamma)\frac{E^{NM}}{A}}{3\gamma\rho_c} + G\,\frac{-3g_0^{\rho\rho}+\tilde{k}_F^c\left(g_0^{\rho\rho'}+\tau_c g_0^{\rho\tau'}\right)}{3\gamma},$$

$$C_{0D}^{\rho\rho} = \frac{\frac{\hbar^2}{2m}\left(3-2M_s^{*NM}\right)\tau_c-3\frac{E^{NM}}{A}}{3\gamma\rho_c^{1+\gamma}} - G\frac{\tilde{k}_F^c(g_0^{\rho\rho'}+\tau_c g_0^{\rho\tau'})}{3\gamma\rho_c^{\gamma}},$$

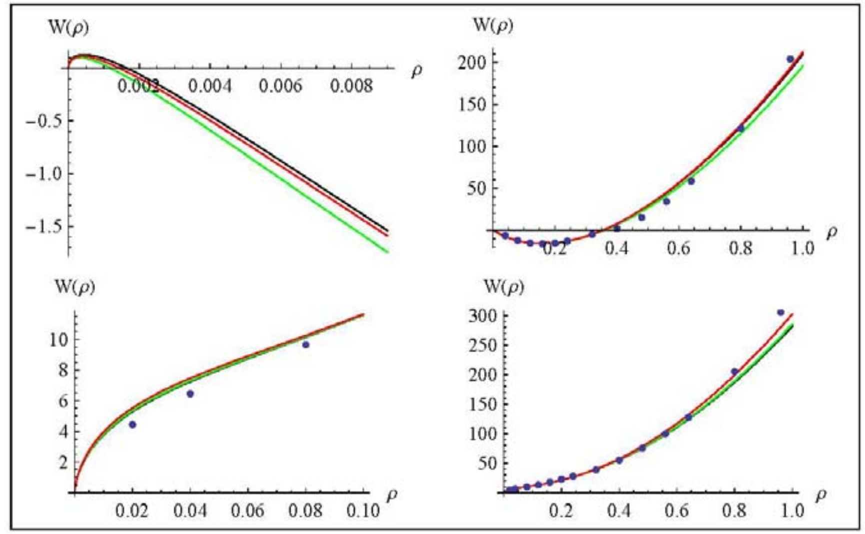
$$C_1^{\rho\tau} = C_0^{\tau}-\frac{\hbar^2}{2m}\left(M_v^{*NM}-1\right)\frac{1}{\rho_c} + G\left(g_0^{\rho\tau}-g_1^{\rho\tau}\right),$$

$$C_{10}^{\rho\rho} = \frac{1}{27\gamma\rho_c}\Bigg[27(1+\gamma)\,a_{sym}^{NM}{}_C-9L^{NM} - 5\left((1+3\gamma)\frac{\hbar^2}{2m}-(2-3\gamma)\left(C_0^{\tau}+3C_1^{\tau}\right)\rho_c\right)\tau_c\Bigg] - G\frac{27\gamma g_1^{\rho\rho}+(60\gamma-40)g_0^{\rho\tau}\tau_c}{27\gamma}$$

gamma=1,G=9454.9

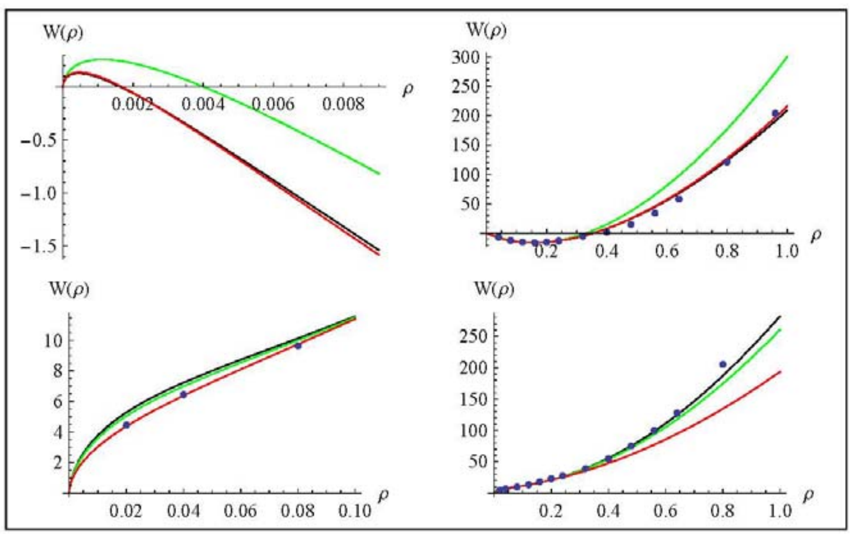


gamma=0.1G=-703.79

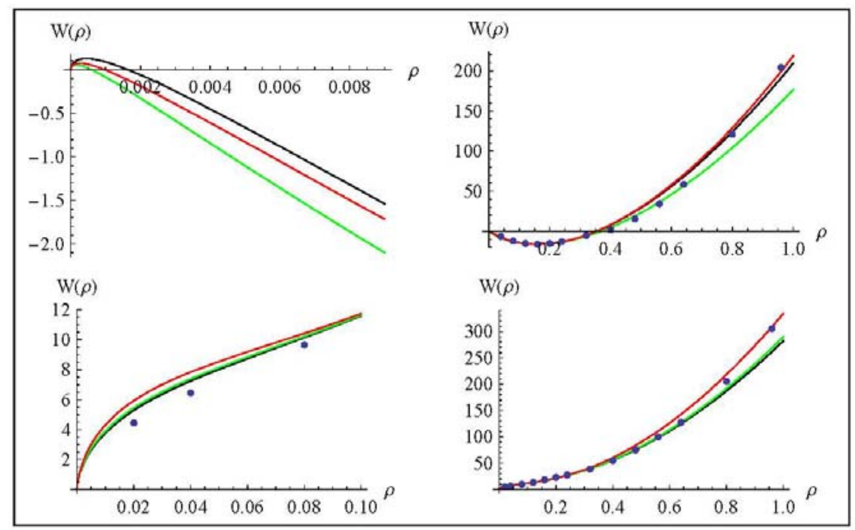


G_{DME}=1496.98

gamma=0.5G=3631.



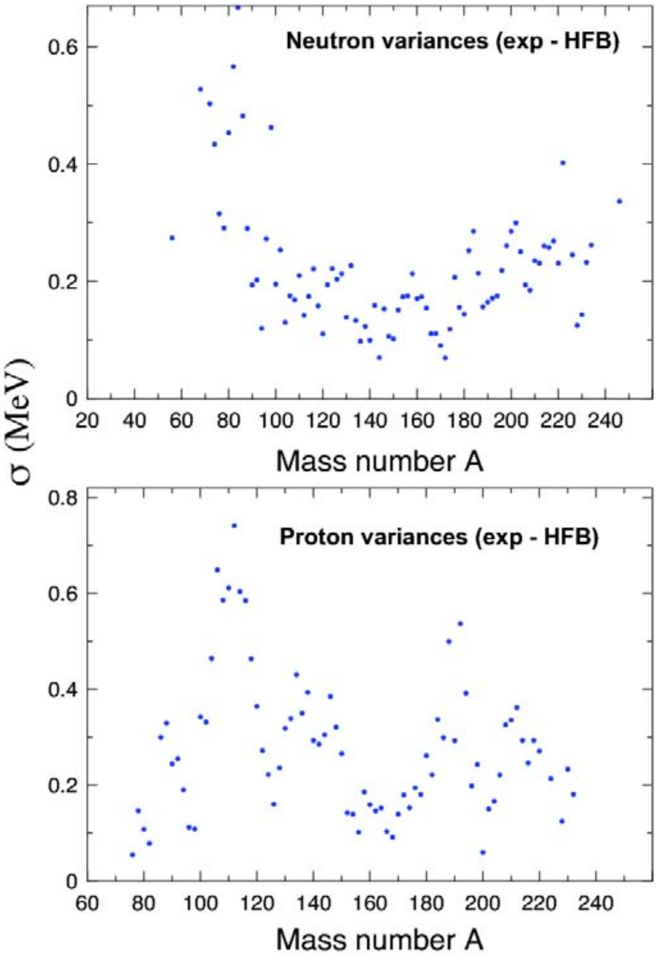
gamma=0.0001G=-1744.9



Odd-even mass differences from self-consistent mean field theory

G.F. Bertsch,[1] C.A. Bertulani,[2] W. Nazarewicz,[3,4,5] N. Schunck,[3,4] and M.V. Stoitsov[3,4,6]

[1] *Institute for Nuclear Theory and Dept. of Physics, University of Washington, Seattle, Washington*
[2] *Department of Physics, Texas A&M University-Commerce, Commerce, Texas 75429, USA*
[3] *Department of Physics and Astronomy, University of Tennessee, Knoxville, TN 37996, USA*
[4] *Oak Ridge National Laboratory, P.O. Box 2008, Oak Ridge, TN 37831, USA*
[5] *Institute of Theoretical Physics, Warsaw University, ul.Hoża 69, PL-00681 Warsaw, Poland*



As expected, best agreement for well deformed rare earths and actinides whose properties vary smoothly with particle number

Largest deviations around shell closures and in the regions of shape coexistence (A=90 for neutrons and A=110 and 190 for protons) where dynamic shape fluctuations are known to strongly impact masses

- There is a weak preference for a surface-peaked n-n pairing, which might be attributable to many-body effects
- A larger strength is required in the proton pairing channel than in the neutron pairing channel
- Pairing strengths adjusted to the isotope chains are too weak to give a good overall fit to the mass differences
- The results supports the recent attempts to directly parametrize the pairing functional in terms of isovector densities

TOWARDS A UNIVERSAL NUCLEAR ENERGY DENSITY FUNCTIONAL

Isovector Density Dependent Contact Pairing Force

$$v_{pair}(1,2) = \frac{1-\mathrm{P}_\sigma}{2}\mathrm{V}_0\, \mathrm{g}_{\tau 3}[\rho,\rho_1]\,\delta(\mathbf{r}_1-\mathbf{r}_2).$$

$$\rho_1(r) = (\rho_\mathrm{n}-\rho_\mathrm{p}),\ \rho(r) = (\rho_\mathrm{n}+\rho_\mathrm{p})$$

Hiroyuki Sagawa (SLYS)

$$\mathrm{g_n}[\rho,\rho_1] = 1-(1-\beta)\eta_\mathrm{s}\left(\frac{\rho}{\rho_0}\right)^{\alpha_\mathrm{s}} - \beta\eta_\mathrm{n}\left(\frac{\rho}{\rho_0}\right)^{\alpha_\mathrm{n}}$$

$$\mathrm{g_p}[\rho,\rho_1] = 1-(1+\beta)\eta_\mathrm{s}\left(\frac{\rho}{\rho_0}\right)^{\alpha_\mathrm{s}} + \beta\eta_\mathrm{n}\left(\frac{\rho}{\rho_0}\right)^{\alpha_\mathrm{n}}$$

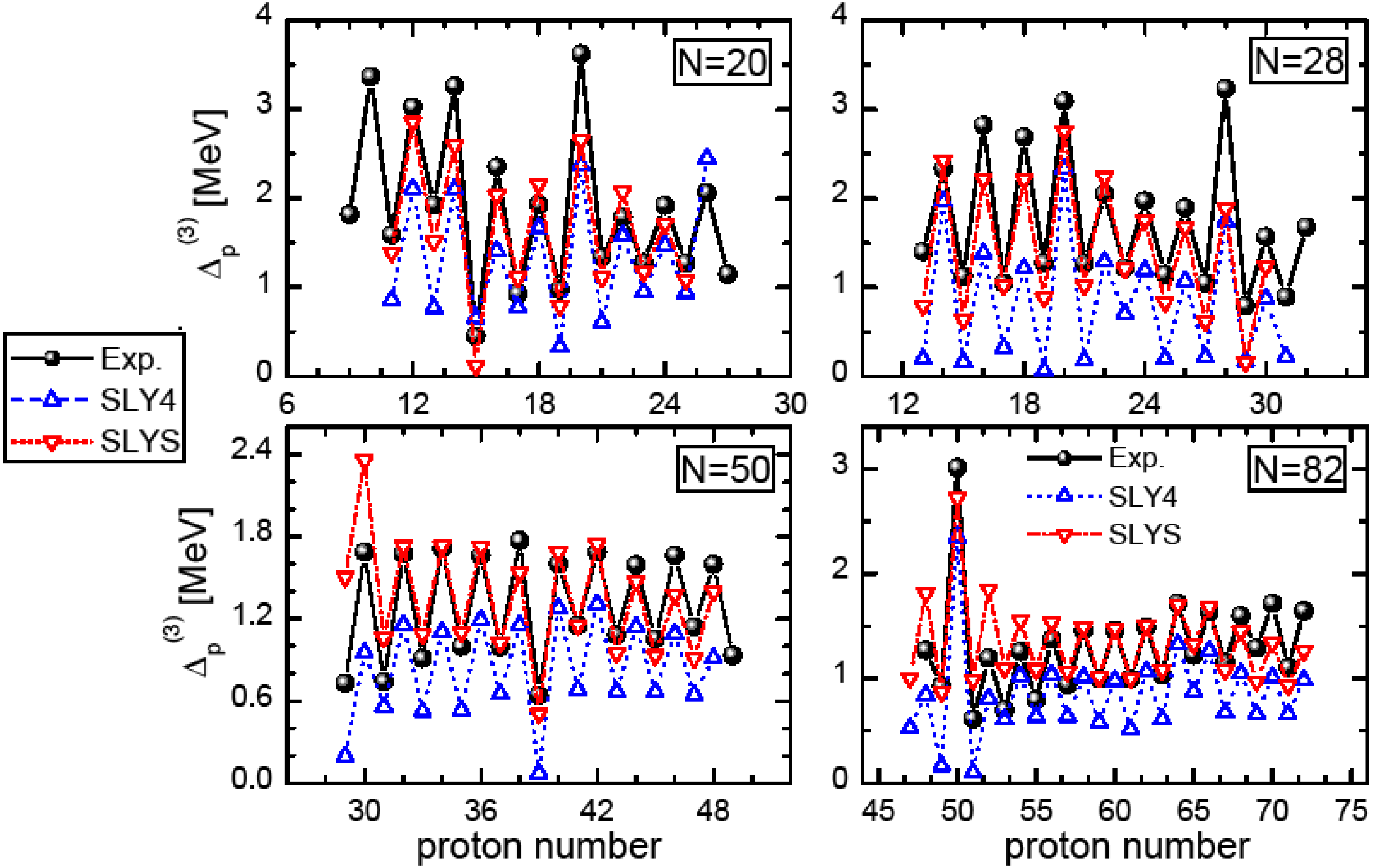
$$\beta(r) = \rho_1(r)/\rho(r),\ \eta_\mathrm{s} = 0.664,\ \alpha_\mathrm{s} = 0.522,\ \eta_\mathrm{n} = 1.01,\ \alpha_\mathrm{n} = 0.525,\ \rho_0 = 0.16 fm^{-3}$$

Masayuki Yamagami (SLYY)

$$\mathrm{g}_{\tau_3}[\rho,\rho_1] = 1-\frac{1}{2}\left(\frac{\rho}{\rho_0}\right)-\frac{\tau_3}{4}\left(\frac{\rho_1}{\rho_0}\right)-\frac{5}{2}\left(\frac{\rho_1}{\rho_0}\right)^2$$

Isovector Density Dependent Contact Pairing Force

(preliminary results)



TOWARDS A UNIVERSAL NUCLEAR ENERGY DENSITY FUNCTIONAL

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

1. Mass Table Calculations
2. Optimal parameters of the functional
3. Improving the functional
4. Visualization and development tools

Visualization and Development Tools

Mass Table Explorer

http://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
- Saves data and images in many formats

On-Line Version

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

Subversion Control System (SVN)

http://massexplorer.org/websvn/

- http://massexplorer.org/svn/FitDME
- http://massexplorer.org/svn/HFBTHO
- http://massexplorer.org/svn/HFODD
- http://massexplorer.org/svn/MPI_HFODD

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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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- Map of the Nuclides
- D1S Gogny
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ORNL/UTK
M. Kortelainen
T. Lesinski
J. McDonnell
W. Nazarewicz
N. Nikolov
J.C. Pei
N. Schunck

ANL
J. Moré
J. Sarich
S. Wild

Ohio State University
Dick Furnstahl

NSCL/MSU
S.K. Bogner

Warsaw/Jvyäskylä
J. Dobaczewski

University of Washington
G. Bertsch

Texas A&M Commerce
C. Bertulani

University of Aizu
H. Sagawa