Statistical errors and parametric correlations of covariant energy density functionals

Anatoli Afanasjev
Mississippi State University

1. Motivation and introduction
2. Systematic uncertainties: brief review
3. Statistical errors in prediction of physical observables
4. Parametric correlations
5. Conclusions

In collaboration with S. Abgemava (MSU), A. Taninah (MSU)

Approximations in the modelling of nuclear many-body problem.

General approach (DFT level)

- Non-relativistic Schrodinger equation: Skyrme and Gogny DFT
- Relativistic Dirac equation: covariant DFT (CDFT)

Range of interaction

Zero range
- point coupling models in CDFT (no mesons)
- Skyrme DFT

Finite range
- meson exchange models in CDFT
- Gogny DFT

Effective density dependence

CDFT :
- explicit (DD-ME2, DD-PC1)
- non-linear (through the powers of mesons) (NL1, NL3*)

Skyrme and Gogny DFTs: different prescriptions for density dependence

Theoretical errors/uncertainties in description/predictions of physical observables

Systematic errors/uncertainties - **apply to a set of the functionals**
- related to the choice of the basic physics behind the functional

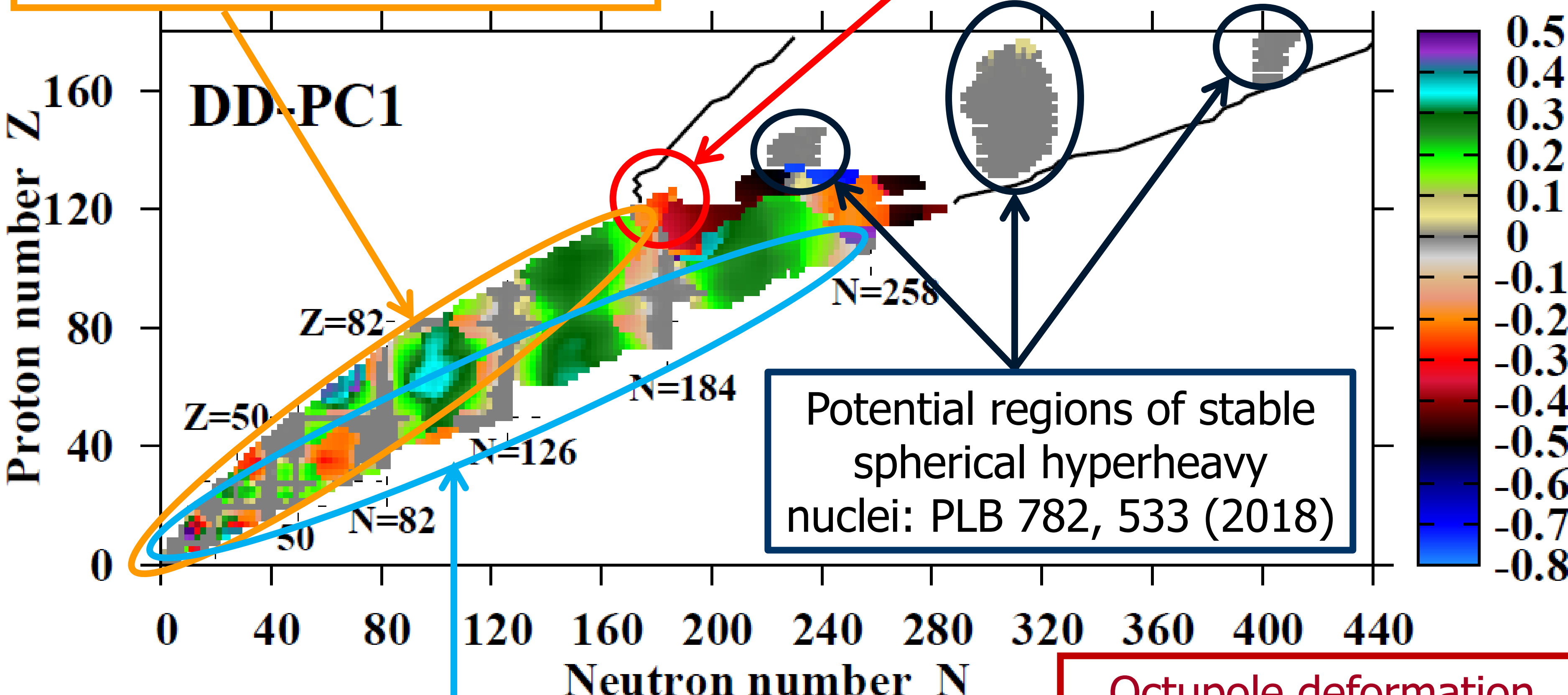
Statistical errors/uncertainties - **apply only to a given functional**
- due to choice of experimental data and the selection of adopted errors in the fitting protocol (the latter is to a degree subjective especially for the quantities of different dimensions)

1. S. Brandt, Data analysis. Statistical and Computational Methods for Scientists and Engineers. (Springer International Publishing, Switzerland, 2014).
2. J. Dobaczewski et al, J. Phys. G **41** (2014) 074001

Systematic uncertainties in physical observables

Global performance of CEDFs:
PRC 89, 054320 (2014),
PRC 93, 054310 (2016)

Superheavy nuclei: ground states and fission barriers: PRC 92,054310 (2015), PRC 95, 054324 (2017)

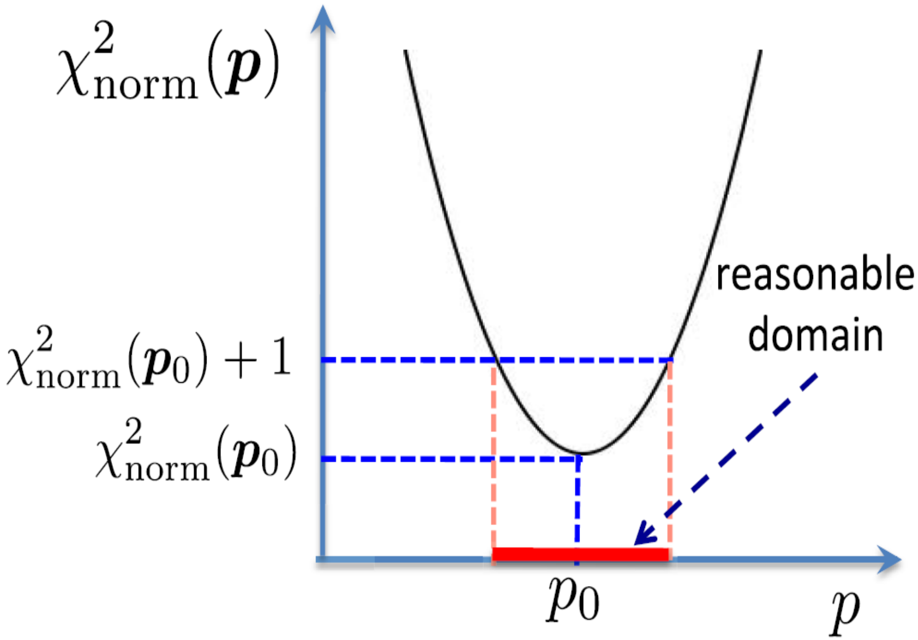


Potential regions of stable spherical hyperheavy nuclei: PLB 782, 533 (2018)

Neutron-rich nuclei and two-neutron drip line:
PLB 726, 680 (2013), PRC 89, 054310 (2015),
PRC 91, 014324 (2015), PRC 93, 054310 (2016)

Octupole deformation (global study):
PRC 93, 054310 (2016),
PRC 96, 024301 (2017)

Definition of statistical errors



J. Dobaczewski et al, J. Phys. G,**41** (2014) 074001

$$\chi^2_{norm}(\mathbf{p}) = \frac{1}{s}\sum_{i=1}^{N_{type}}\sum_{j=1}^{n_i}\left(\frac{O_{i,j}(\mathbf{p})-O^{exp}_{i,j}}{\Delta O_{i,j}}\right)^2$$

$\mathcal{O}_i(\boldsymbol{p})$ stands for the calculated values

$\mathcal{O}_i^{\rm exp}$ for experimental data,

$\Delta\mathcal{O}_i$ for adopted errors

$$\Delta\mathcal{O}_i^2 = \left(\Delta\mathcal{O}_i^{\rm exp}\right)^2 + \left(\Delta\mathcal{O}_i^{\rm num}\right)^2 + \left(\Delta\mathcal{O}_i^{\rm the}\right)^2$$

small small subjective

$$s = \frac{\chi^2_{norm}(\mathbf{p}_0)}{N_{data}-N_{par}}$$

Birge factor (global scale factor)

For p_i in a "reasonable domain"

$$\sigma = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(O(p_i)-O(p_0)\right)^2}$$

The procedure

1. Generate the functional variations by means of Monte-Carlo procedure
2. Define the parameter hyperspace
3. For simplicity use non-linear meson exchange functionals since they have the smallest number of parameters → thus the smallest volume of parameter hyperspace

$$\mathcal{L} = \bar{\psi}\left[\gamma\cdot(i\partial - g_\omega\omega - g_\rho\vec{\rho}\vec{\tau} - eA) - m - g_\sigma\sigma\right]\psi$$
$$+ \frac{1}{2}(\partial\sigma)^2 - U(\sigma) - \frac{1}{4}\Omega_{\mu\nu}\Omega^{\mu\nu} + \frac{1}{2}m_\omega^2\omega^2$$
$$- \frac{1}{4}\vec{R}_{\mu\nu}\vec{R}^{\mu\nu} + \frac{1}{2}m_\rho^2\vec{\rho}^2 - \frac{1}{4}F_{\mu\nu}F^{\mu\nu}$$

$$U(\sigma) = \frac{1}{2}m_\sigma^2\sigma^2 + \frac{1}{3}g_2\sigma^3 + \frac{1}{4}g_3\sigma^4$$

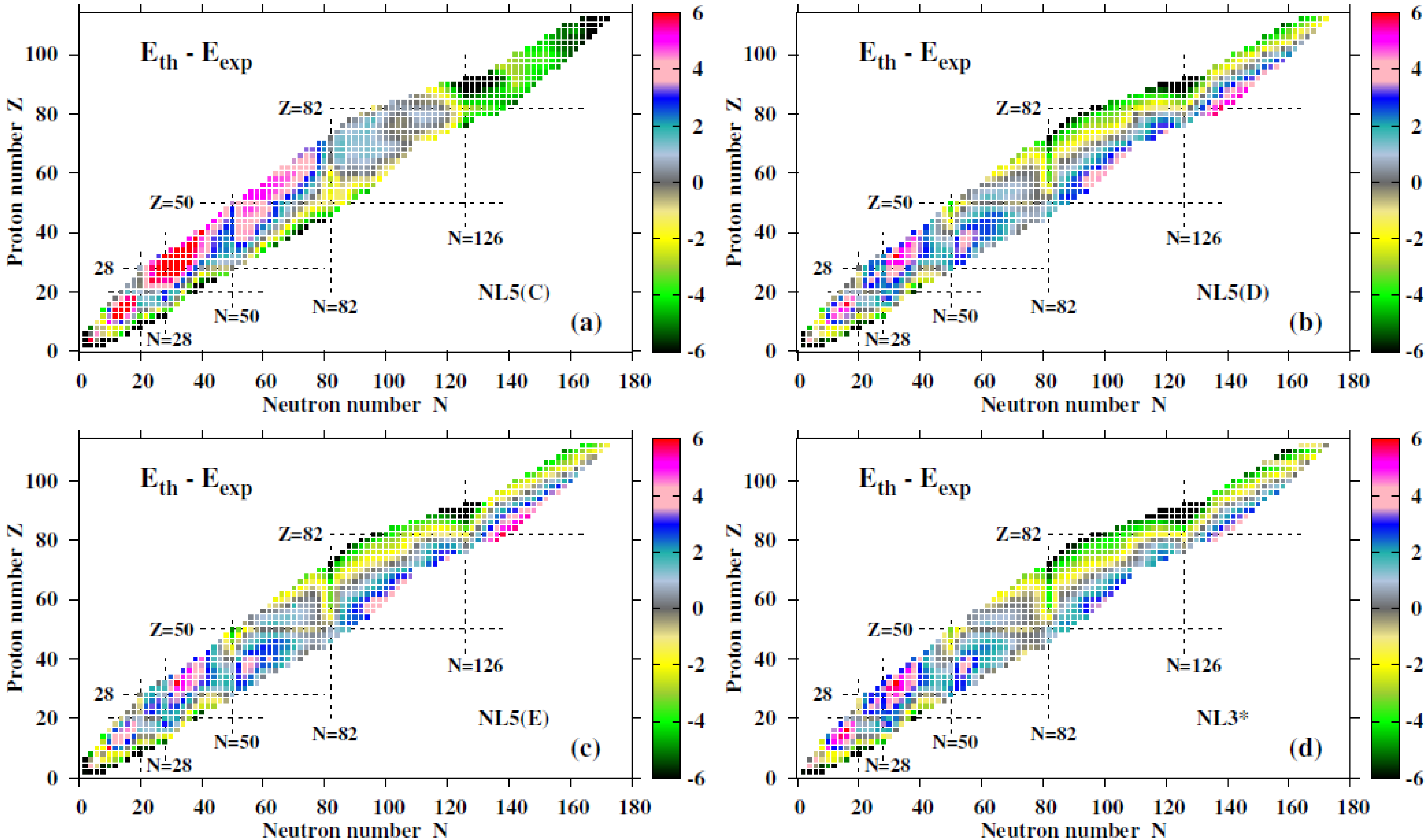
6 parameters: m_σ, g_σ, m_ω, g_ρ, g_2, g_3

The NL5(*) functionals: the fitting protocols

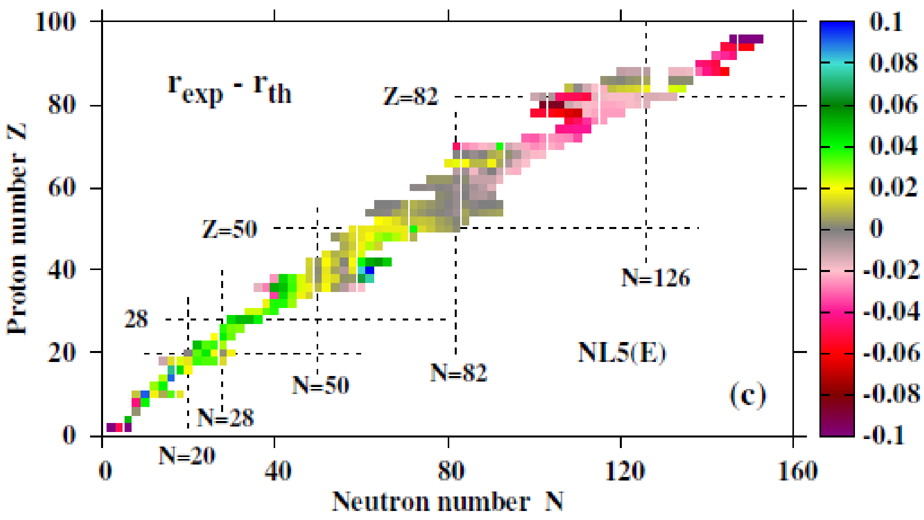
	NL5(A)	NL5(B)	NL5(C)	NL5(D)	NL5(E)
1. Parameters					
m_σ	516.993054	503.253177	502.481217	503.122989	503.298890
g_σ	10.165747	9.896631	9.900244	10.187753	10.263955
g_ω	12.658290	12.457831	12.489590	12.940276	13.052487
g_ρ	4.277136	4.202553	4.318575	4.589814	4.582673
g_2	- -8.350509	-10.925997	-10.821667	-10.858440	-10.976703
g_3	- -19.260373	-28.502727	-28.27378	-30.993091	-32.006687
2. Nuclear matter properties					
E/A	-16.25	-16.20	-16.24	-16.29	-16.27
ρ_0	0.146	0.150	0.150	0.150	0.150
K_0	318.42	259.22	260.673	256.50	252.96
J	34.92	34.92	35.925	38.87	38.93
L_0	108.85	108.33	112.31	123.98	124.96
2. Penalty function contributions					
χ^2_{total}	343.901	367.822	273.014	74.973	85.049
χ^2_{total}/degree	14.95	15.99	12.41	3.9459	3.698
χ^2_{NM} (%)	8.120 (2.3 %)	2.626 (0.5 %)	3.842 (1.1 %)	4.434 (5.3 %)	3.625 (3.5 %)
χ^2_{E} ((%)	128.318 (37.3 %)	145.727 (39.6 %)	111.550 (40.9 %)	55.221 (73.7 %)	51.231 (60.2 %)
χ^2_{Rch} (%)	34.231 (9.9 %)	18.363 (5.0 %)	16.124 (5.9 %)	15.318 (20.4 %)	16.802 (19.7 %)
χ^2_{Nskin} (%)	173.235 (50.4 %)	201.105 (54.6 %)	141.498 (51.8 %)	0 (0.0 %)	13.390 (15.7 %)
$\chi^2_{Nskin(Zr)}$(%)	76.071 (22.1 %)	86.591 (23.5 %)	0 (0.0 %)	0 (0.0 %)	1.178 (1.4 %)

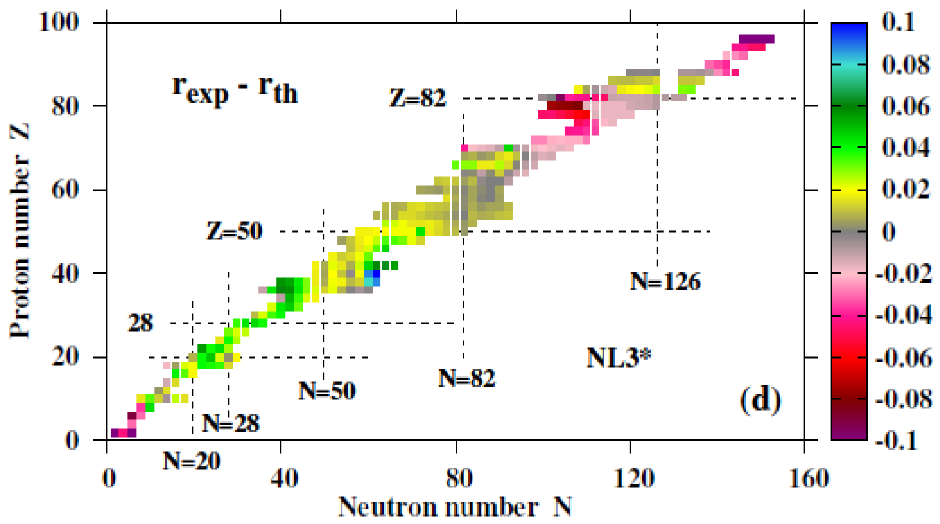
Adopted error	10% for K_0	2.5% for K_0			
Neutron skins (adopted err.)	4 (5%)	4 (5%)	3 (5%)	0	4 (exp.)
	NL3*-like				

Global performance of the NL5(*) functionals: binding energies



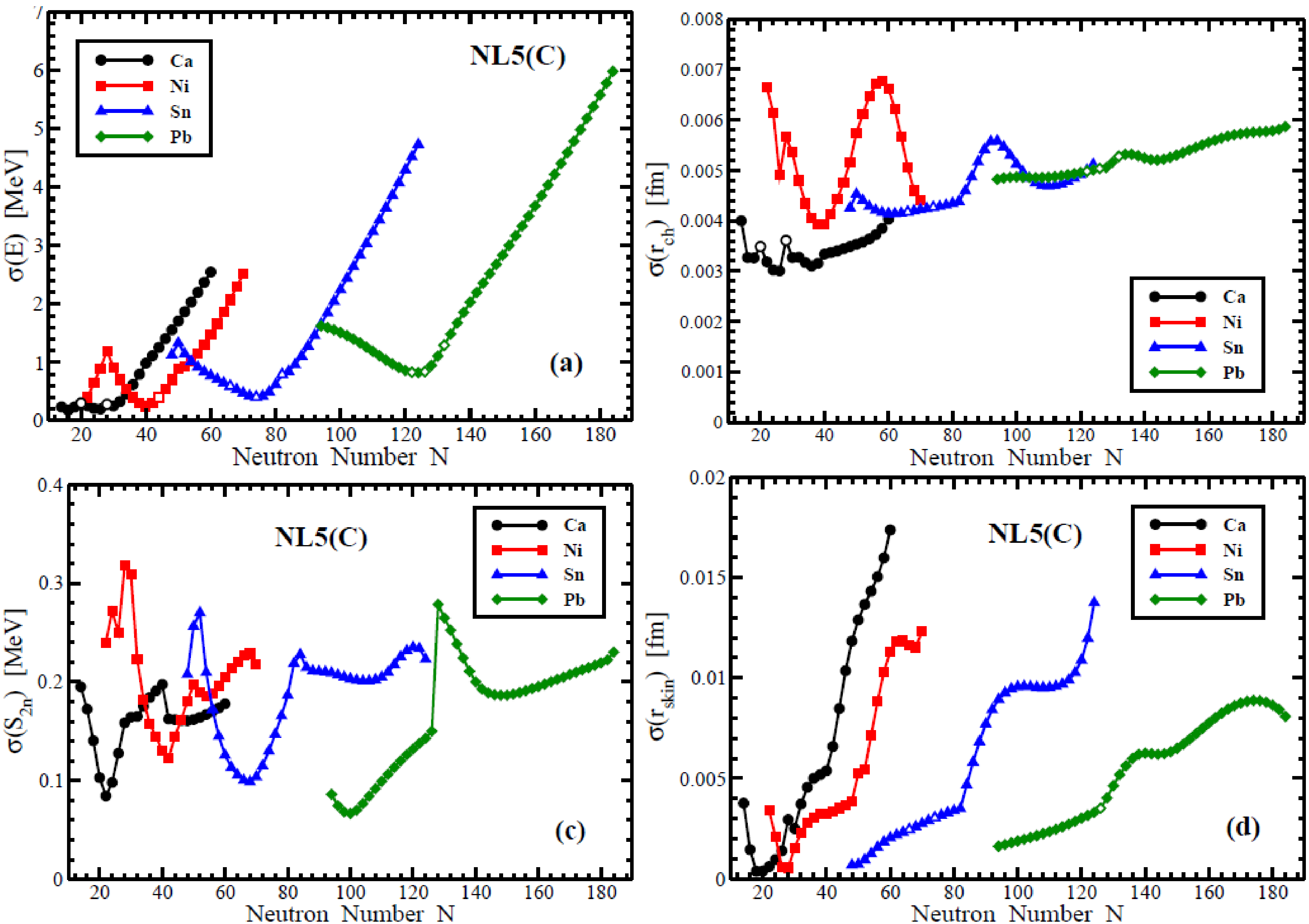
Global performance of the NL5(*) functionals: charge radii and summary





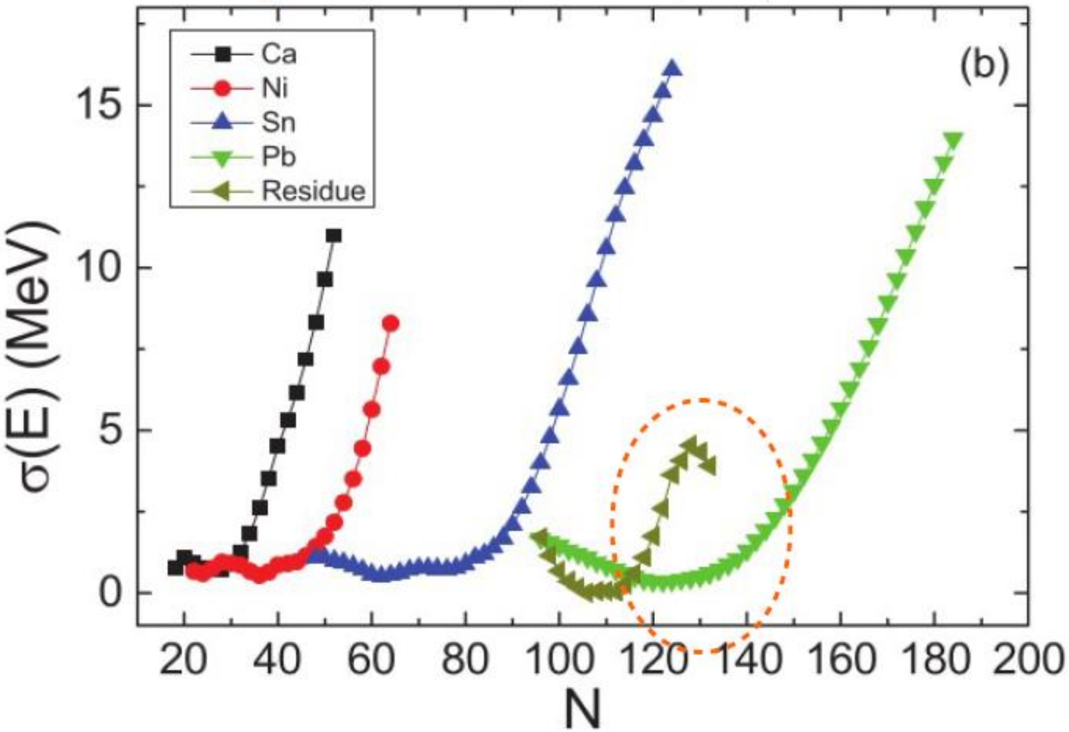
CEDF	measured	measured+estimated			charge radii	
	ΔE_{rms} [MeV]	ΔE_{rms} [MeV]	$\Delta(S_{2n})_{rms}$ [MeV]	$\Delta(S_{2p})_{rms}$ [MeV]	$\Delta(r_{ch})_{rms}$ [fm]	$\Delta(r_{ch})_{rms}$ [fm]
1	2	3	4	5	6	7
NL5(C)	3.41	3.71	1.37	1.54	0.040	0.0284
NL5(D)	2.83	2.90	1.22	1.29	0.041	0.0277
NL5(E)	2.73	2.81	1.23	1.29	0.042	0.0288
NL3*	2.96	3.00	1.23	1.29	0.041	0.0283

Statistical errors in the masses, two-neutron separation energies, charge radii and neutron skins

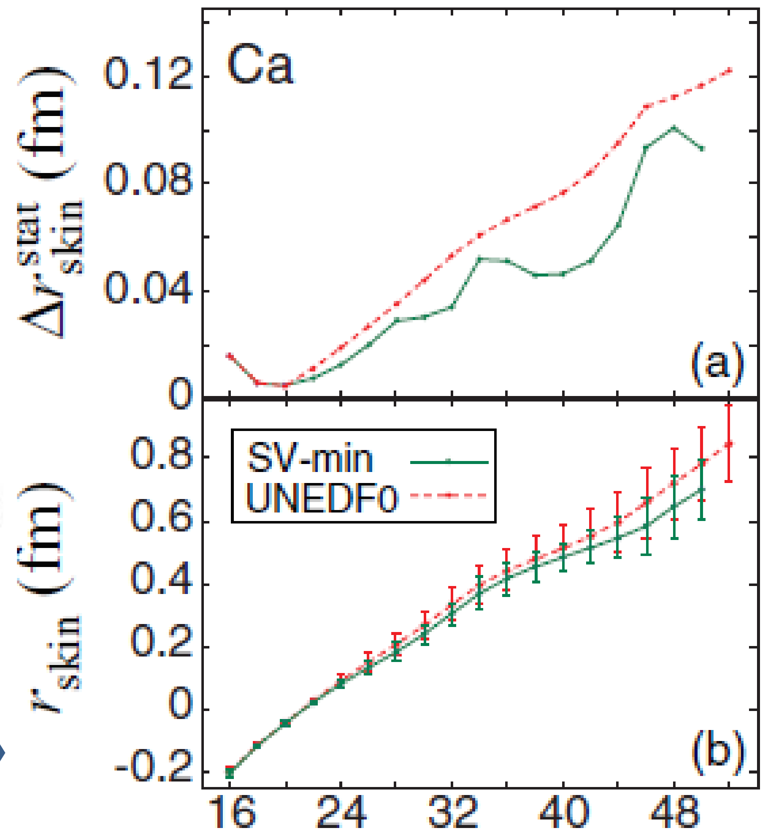


For comparison - statistical errors in Skyrme DFT

Y. Gao, J. Dobaczewski, M. K., J. Toivanen, D. Tarpanov, PRC87, 034324 (2013)

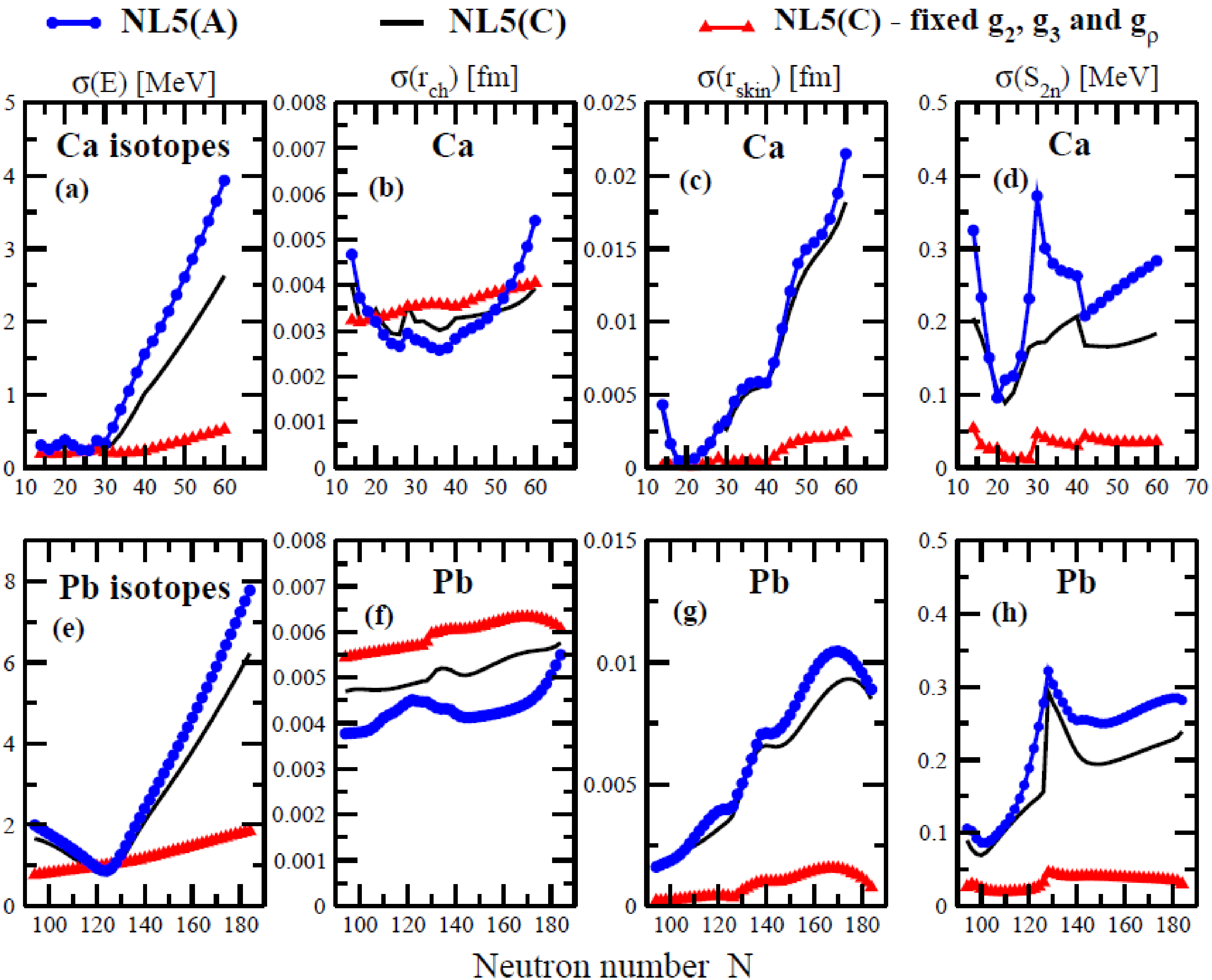


Nucleus	$\Delta r^{\rm stat}_{\rm skin}$	
	UNEDF0	SV-min
^{208}Pb	0.058	0.037
^{48}Ca	0.035	0.026

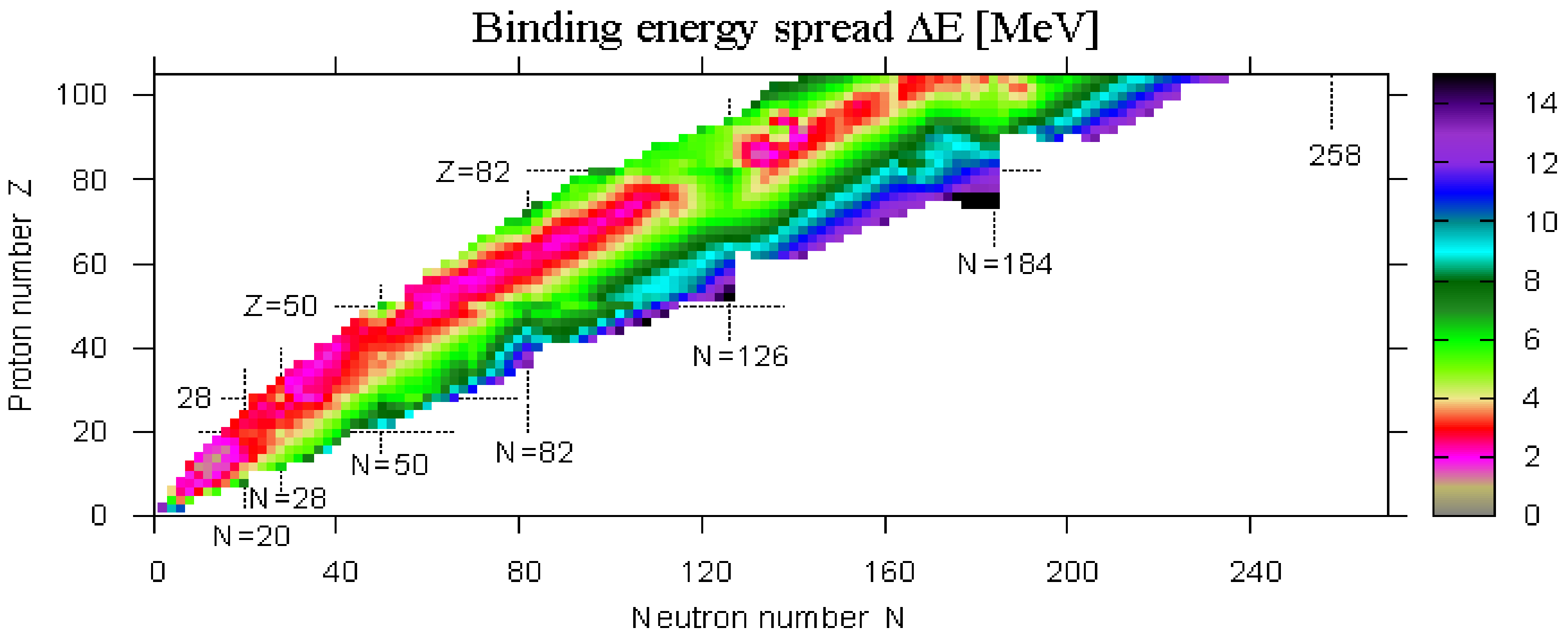


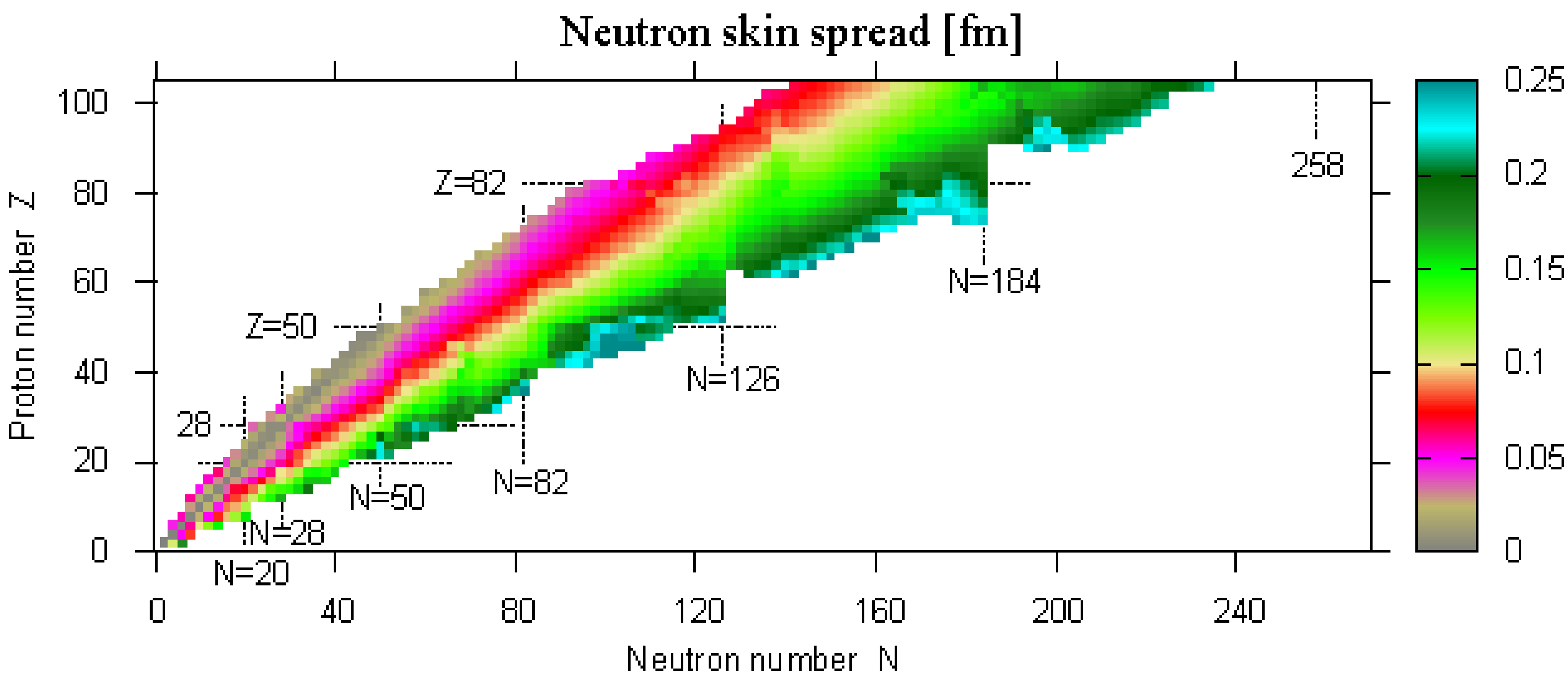
M. Kortelainen et al, PRC 88, 031305(R) (2013)

Statistical errors: dependence on fitting protocol and on “loose” parameters.



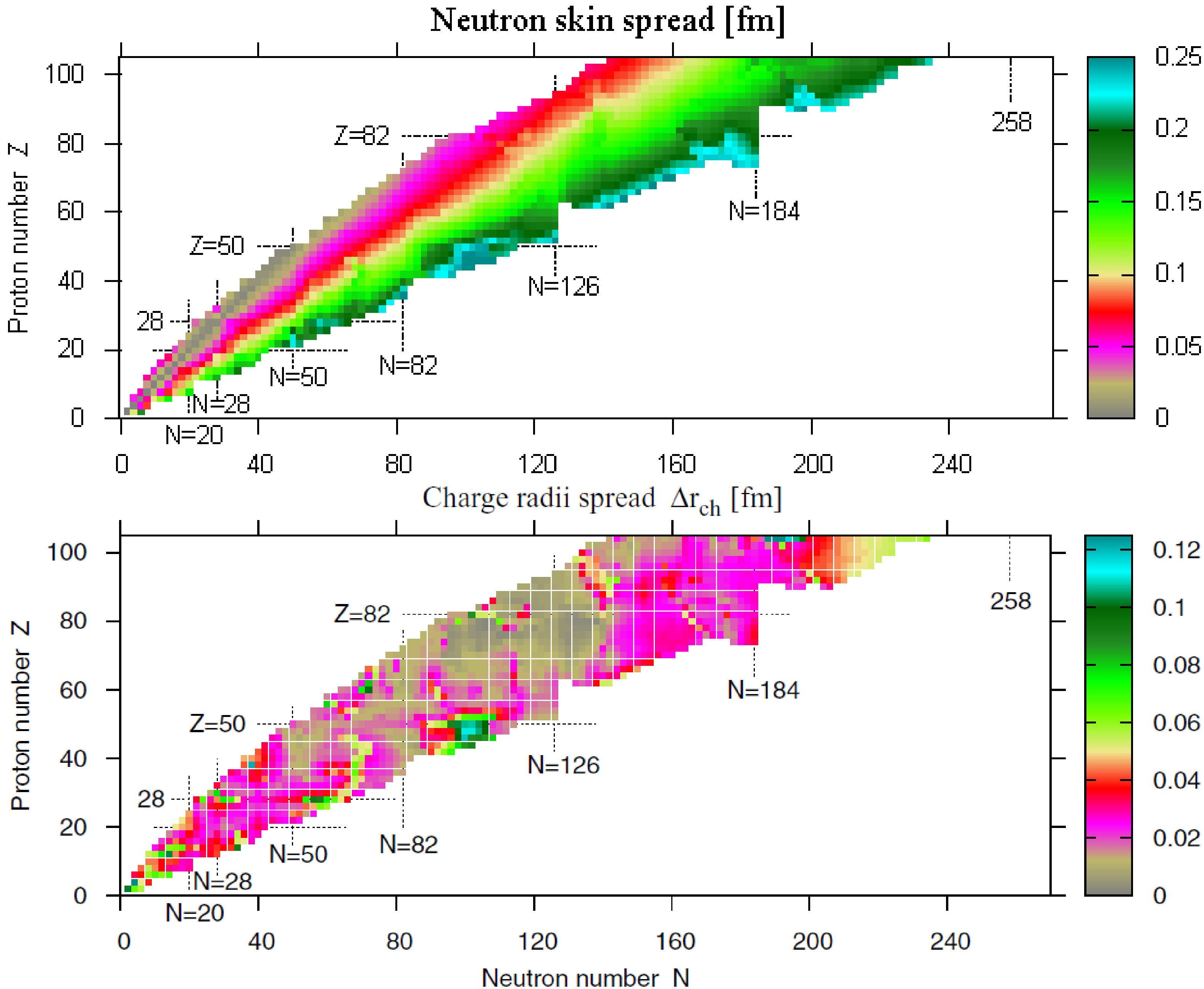
Statistical errors versus systematic uncertainties





S. Agbemava, AA, D. Ray and P. Ring,
PRC 89, 054320 (2014)

Statistical errors versus systematic uncertainties

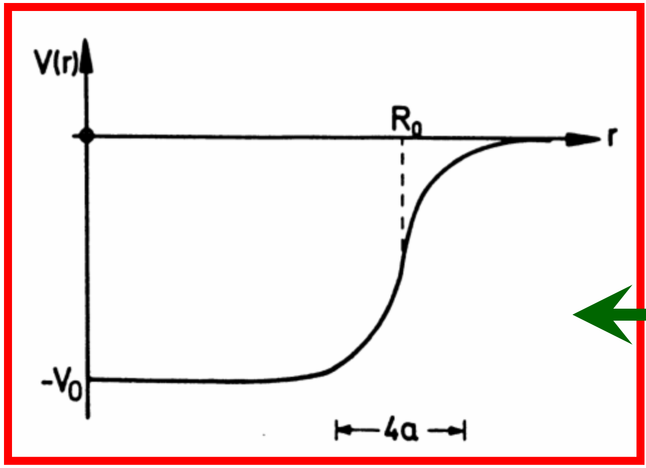


S. Agbemava, AA, D. Ray and P. Ring, PRC 89, 054320 (2014)

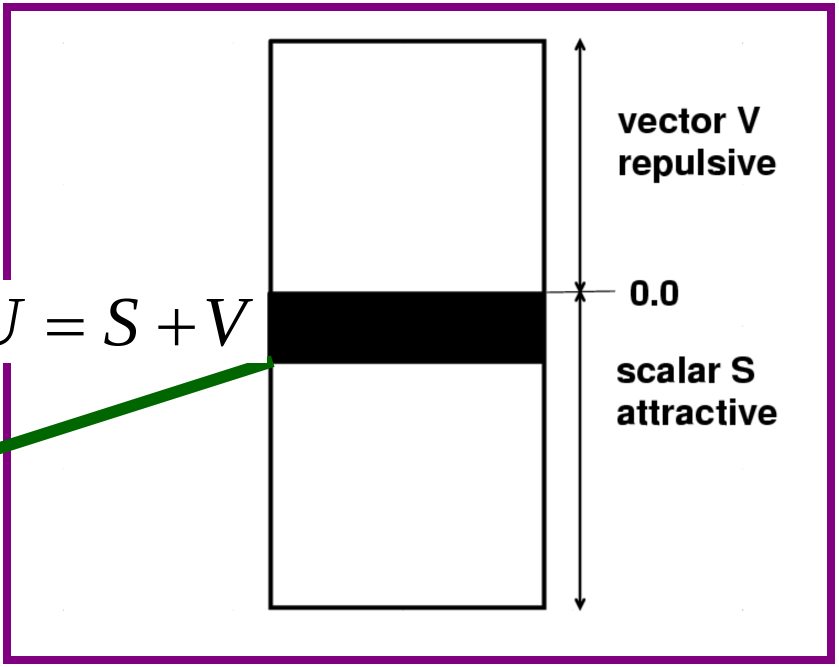
CDFT in a "nutshell"

$$V(\mathbf{r}) = g_{\omega}\omega(\mathbf{r})$$

U – nucleonic potential



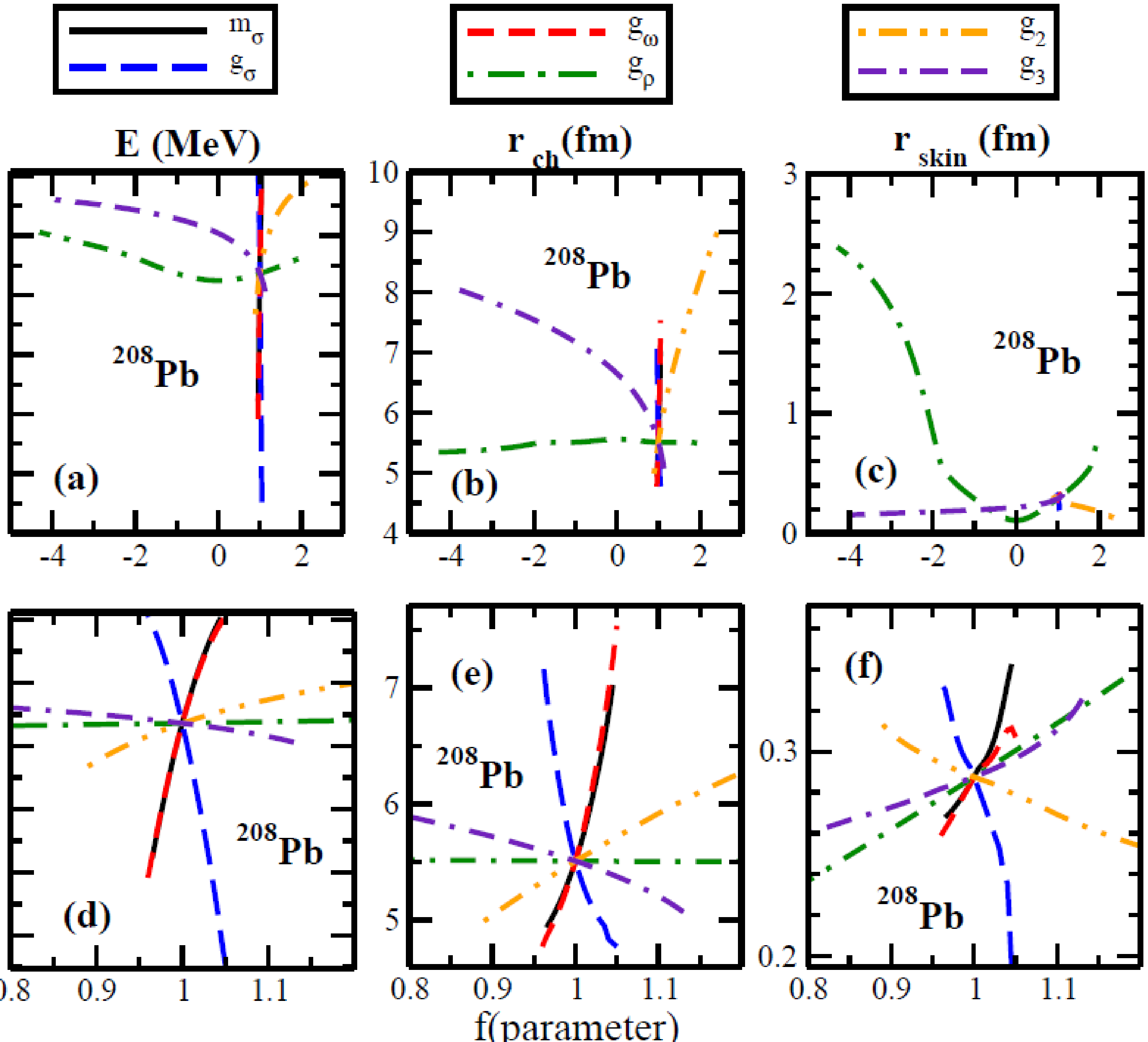
$$U = S + V$$



V ~ 350 MeV/nucleon
S ~ - 400 MeV/nucleon
U ~ - 50 MeV/nucleon

$$S(\mathbf{r}) = g_{\sigma}\sigma(\mathbf{r})$$

Variation of physical observables in ^{208}Pb with a change of a single parameter



$$f_i = \frac{par_i}{par_i^{opt}}$$

Variation of physical observables in ^{208}Pb with a change of a single parameter

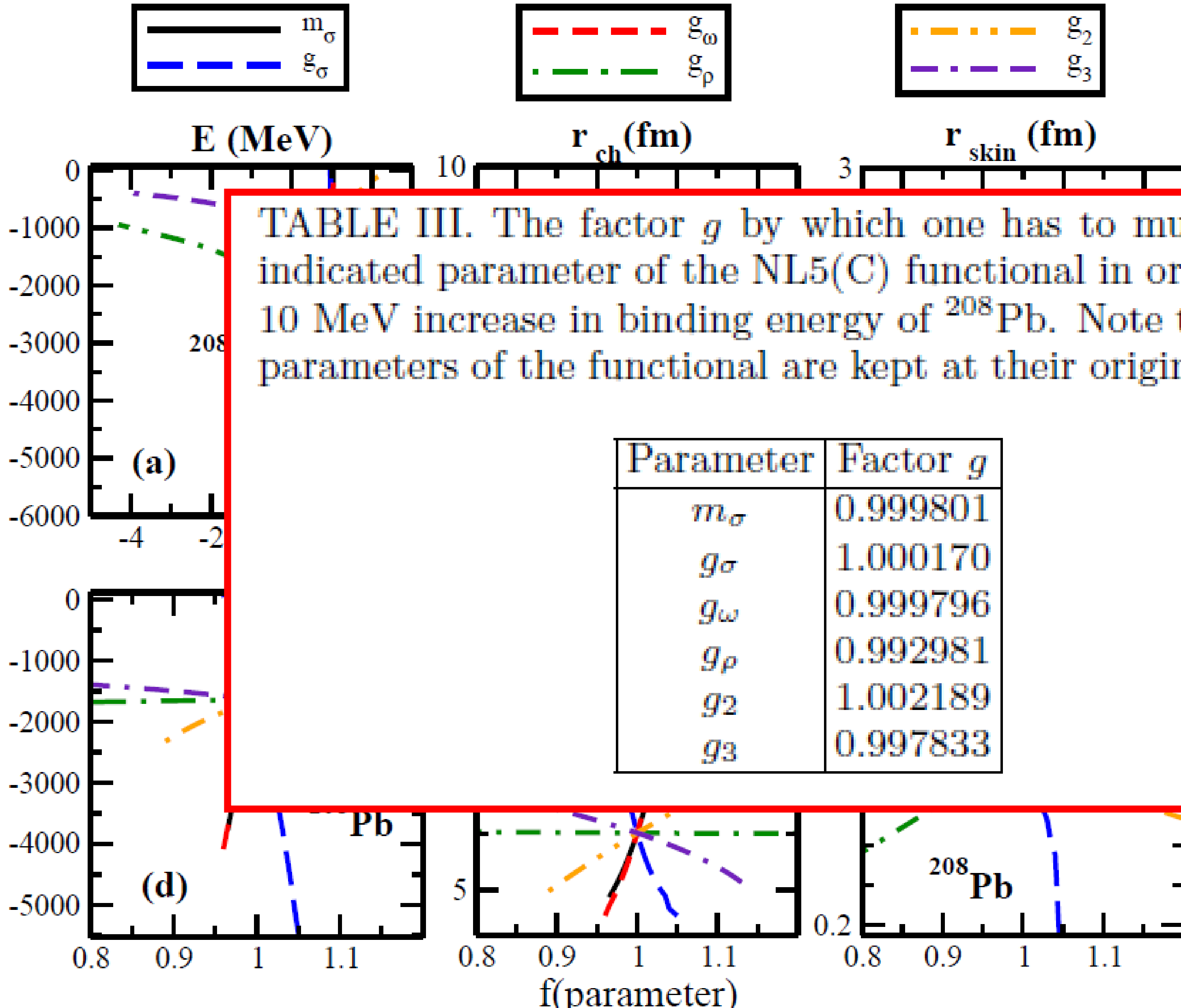
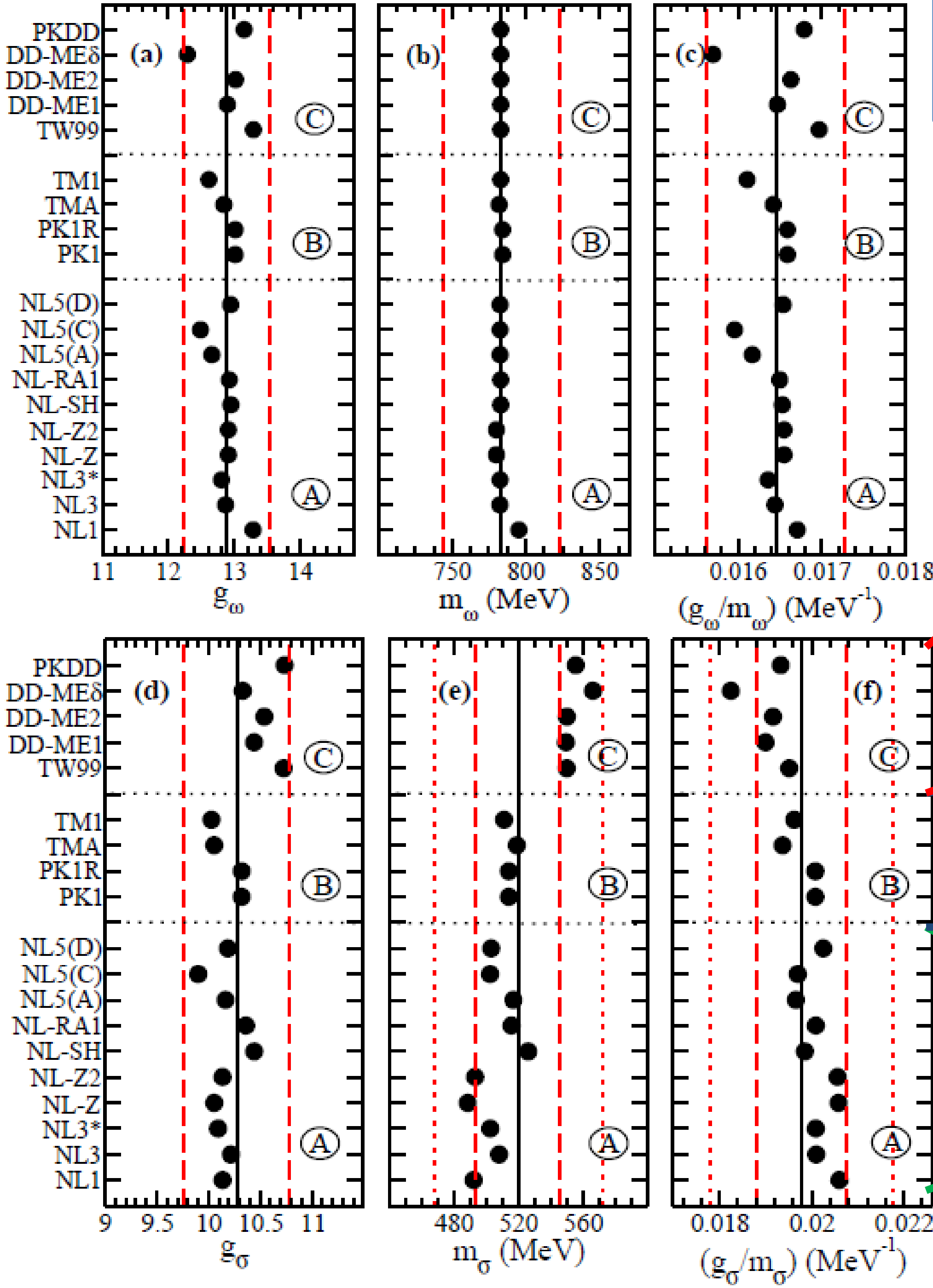


TABLE III. The factor g by which one has to multiply the indicated parameter of the NL5(C) functional in order to get 10 MeV increase in binding energy of ^{208}Pb. Note that other parameters of the functional are kept at their original values.

Parameter	Factor g
m_σ	0.999801
g_σ	1.000170
g_ω	0.999796
g_ρ	0.992981
g_2	1.002189
g_3	0.997833

Localization of the parameters in the parameter hyperspace



Blue line – mean value of set of presented functionals

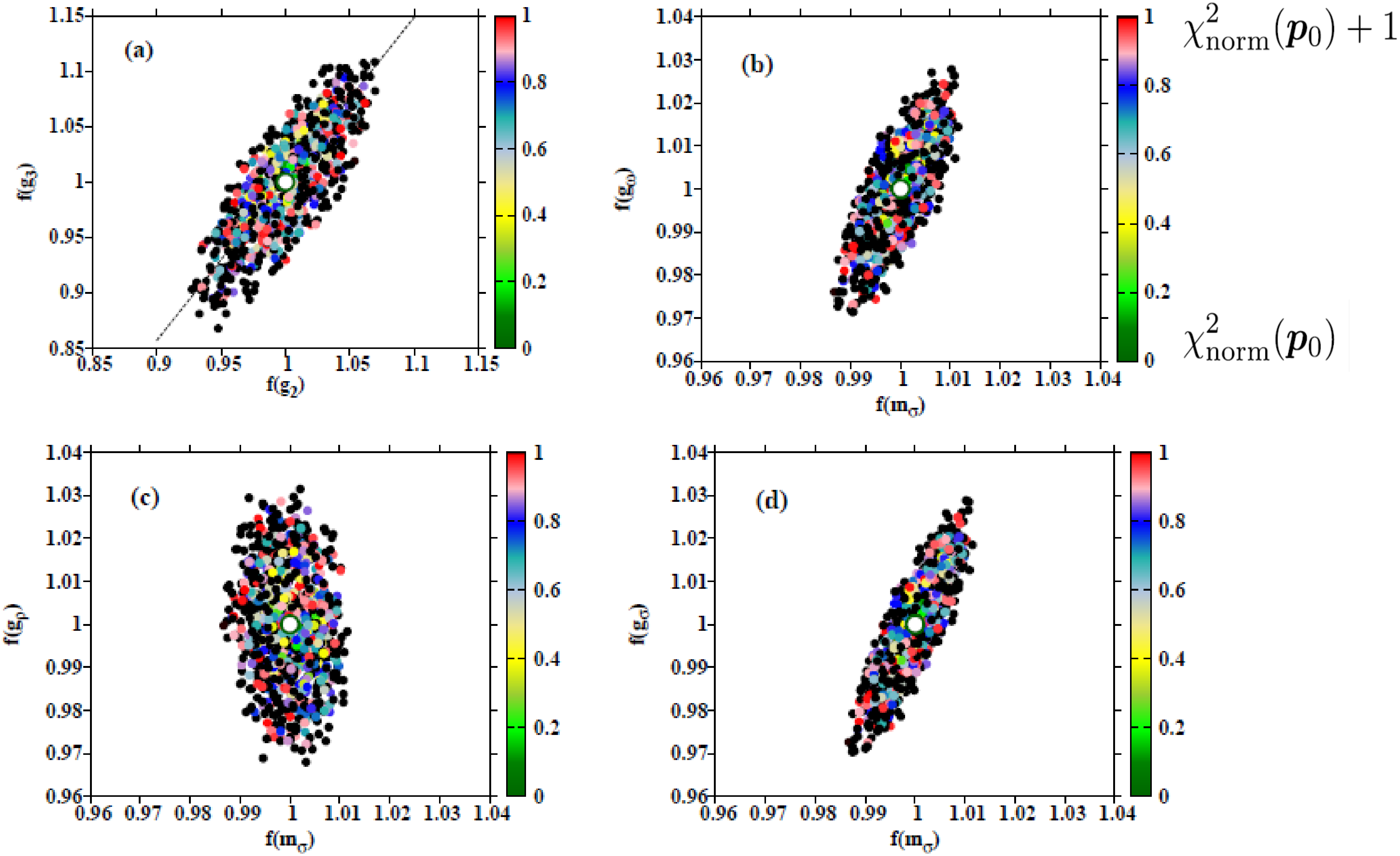
Red dashed and dotted lines show 5% and 10% deviation bands with respect of these mean values

Density dependence for meson-nucleon couplings for σ-, ω- (ρ-) mesons

Non-linear self-coupling for σ-, ω- (ρ-) mesons

Non-linear self-coupling only for σ-meson

Parametric correlations: NL5(C) functional

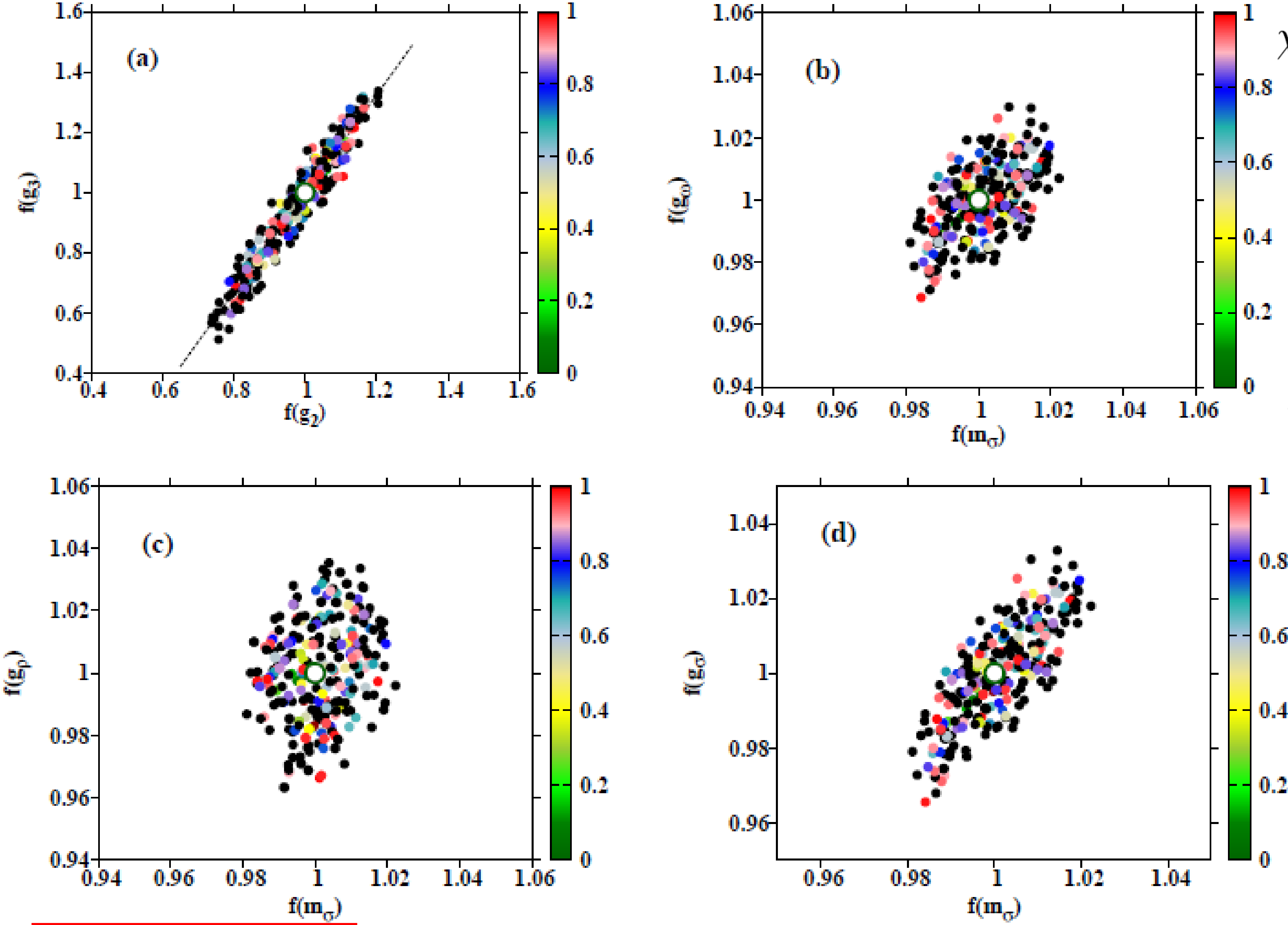


$$f_i = \frac{par_i}{par_i^{opt}}$$

$$f(g_3) = a f(g_2) + b$$

$$a = 1.461276$$
$$b = -0.458276$$

Parametric correlations: NL5(A) functional



$\chi^2_{\mathrm{norm}}(\boldsymbol{p}_0)+1$

$\chi^2_{\mathrm{norm}}(\boldsymbol{p}_0)$

$$f_i = \frac{par_i}{par_i^{opt}}$$

$$f(g_3) = a f(g_2) + b$$

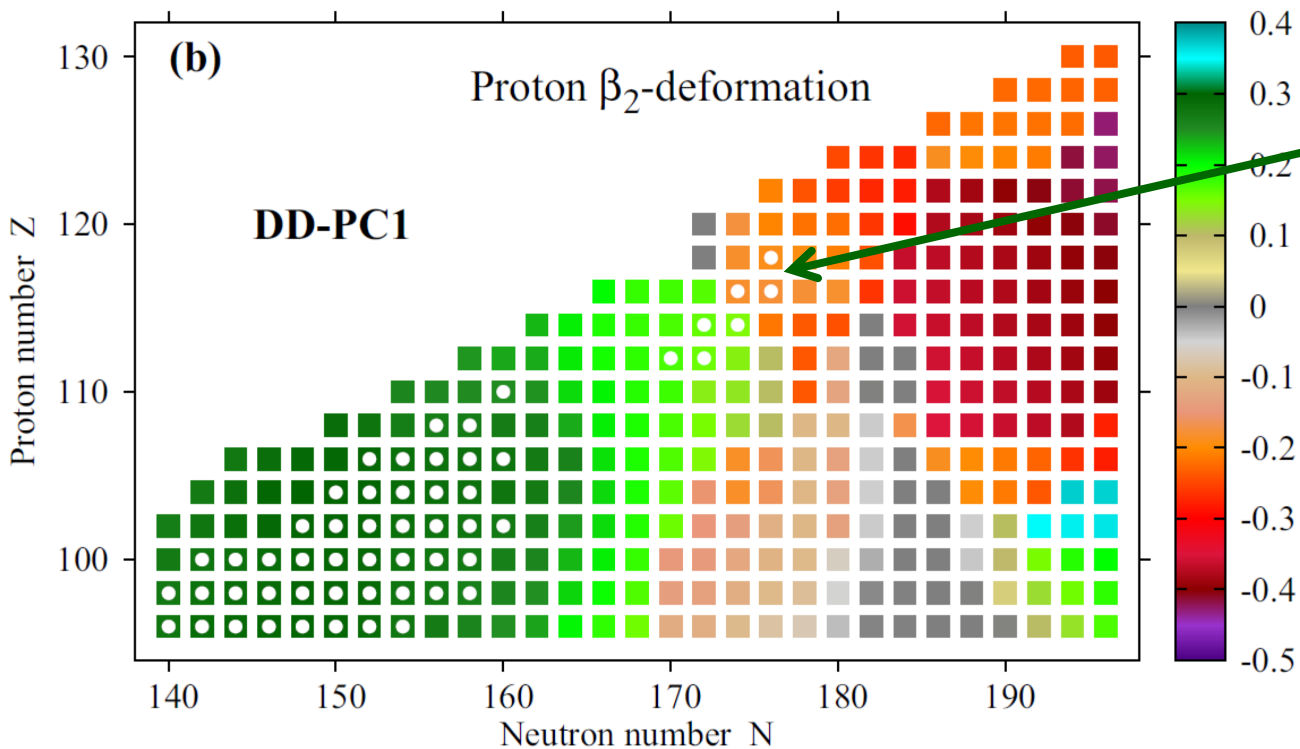
$$a = 1.643$$
$$b = -0.64693$$

Skyrme and Gogny ED functionals: less localized in the parameter space

Parameters	UNEDF0 [81]	UNEDF1 [82]	SLy4 [84]	SKM* [85]	BSk28 [83]	BSk29 [83]
$t_0[MeV\,fm^3]$	-1883.68781034	-2078.32802326	-2488.91	-2645.00	-3988.86	-3970.40
$t_1[MeV\,fm^5]$	277.50021224	239.40081204	486.82	410.00	395.769	394.880
$t_2[MeV\,fm^5]$	608.43090559	1575.11954190	-546.39	-135.00		
$t_3[MeV\,fm^{3+3\alpha}]$	13901.94834463	14263.64624708	13777.0	15595.0	22774.4	22649.3
$t_4[MeV\,fm^{5+3\beta}]$					-100.000	-100.000
$t_5[MeV\,fm^{5+3\gamma}]$					-150.000	-150.000
x_0	0.00974375	0.05375692	0.834	0.09	0.928026	0.964850
x_1	-1.77784395	-5.07723238	-0.344	0.00	0.0274980	-0.0047741
x_2	-1.67699035	-1.36650561	-1.000	0.00		
$t_2x_2[MeV\,fm^5]$					-1388.61	-1388.95
x_3	-0.38079041	-0.16249117	1.354	0.00	1.09482	1.14453

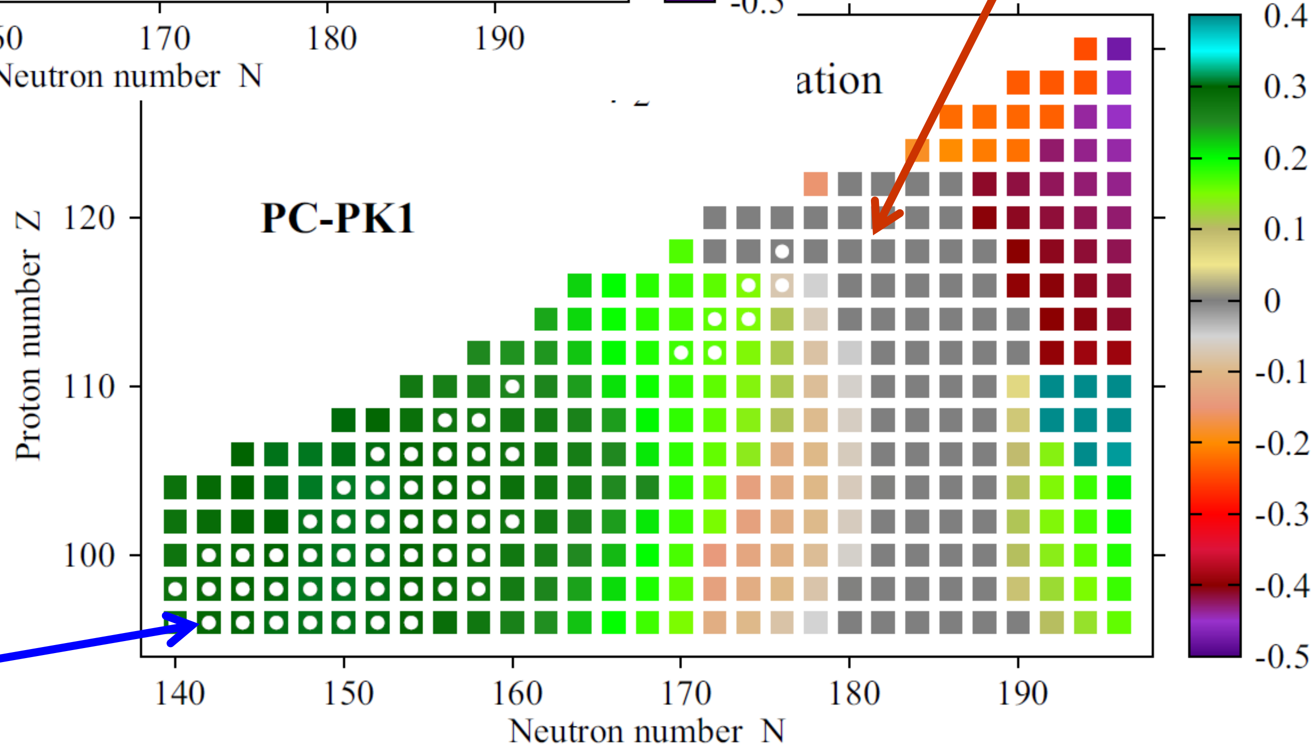
Parameters	D1S[78]		D1[80]		D1M[79]	
μ_i (fm)	0.7	1.2	0.7	1.2	0.5	1.0
W_i [MeV]	-1720.30	103.64	-402.4	-21.30	-12797.57	490.95
B_i [MeV]	1300.00	-163.48	-100.0	-11.77	14048.85	-752.27
H_i [MeV]	-1813.53	162.81	-496.2	37.27	-15144.43	675.12
M_i [MeV]	1397.60	-223.93.	-23.56	-68.81	11963.89	-693.57
t_0 [MeV]	1390.6		1350.0		1562.22	
x_0	1		1		1	
α	1/3		1/3		1/3	
W_{LS} [MeV]	-130.0		115.0		115.56	

DD-PC1:
Experimental
Z=116, 118
nuclei are oblate



PC-PK1:
Experimental
Z=118 nucleus
is spherical

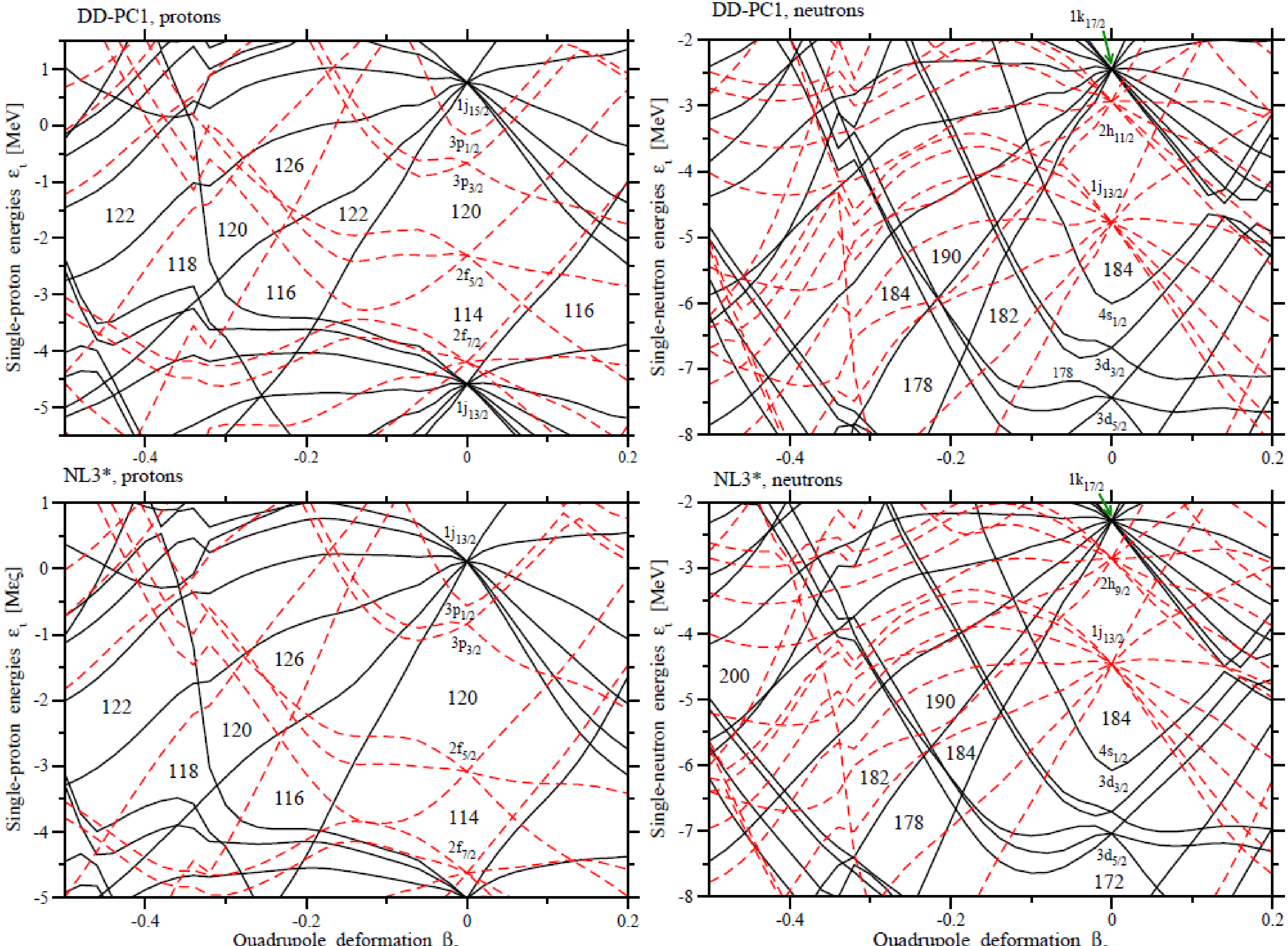
Other experimental
SHE are prolate



Open circles –
experimentally
observed nuclei

S. Agbemava et al, PRC **92**, 054310 (2015)

The source of oblate shapes – the low density of s-p states



S. Agbemava et al, PRC **92**, 054310 (2015)

Statistical errors in the description of absolute and relative single-particle energies in $^{304}120$

Neutron			Proton		
Orbital	$\bar{e}_\nu$	$\sigma(e_\nu)$	Orbital	$\bar{e}_\pi$	$\sigma(e_\pi)$
$4s_{1/2}$	-6.372	0.077	$2f_{5/2}$	-2.418	0.121
Neutron Fermi level			Proton Fermi level		
$1j_{13/2}$	-5.195	0.136	$3p_{3/2}$	-0.302	0.132

Neutron			Proton		
Orbital pairs (m, j)	$\overline{\Delta e_\nu}$	$\sigma(\Delta e_\nu)$	Orbital pairs (m, j)	$\overline{\Delta e_\pi}$	$\sigma(\Delta e_\pi)$
$3d_{5/2}$ - $3d_{3/2}$	0.322	0.005	$1i_{13/2}$ - $2f_{7/2}$	0.247	0.082
$3d_{3/2}$ - $4s_{1/2}$	0.642	0.011	$2f_{7/2}$ - $2f_{5/2}$	1.486	0.035
below neutron Fermi level			below proton Fermi level		
$4s_{1/2}$ - $1j_{13/2}$	1.177	0.102	$2f_{5/2}$ - $3p_{3/2}$	2.116	0.030
$1j_{13/2}$ - $2h_{11/2}$	1.917	0.107	$3p_{3/2}$ - $3p_{1/2}$	0.318	0.006

$$\Delta e_i(m, j) = e_i(m) - e_i(j)$$

Conclusions

1. Statistical errors for different classes of physical observables are substantially lower than systematic ones for covariant density functionals.

2. Parametric correlations emerge for "loosely" defined parameters. Seen in NL5(*), DD-ME2 and PC-PK1

3. Functionals have to be checked for parametric correlations and they have to be removed to make parameters really independent.

→ Question: How many independent parameters could be defined by the models/fitting protocols in use?

Submitted to PRC, see also nuclear theory archieve arXiv: 1811.11473

This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Nuclear Physics under Award No. DE-SC0013037