Optimization and sensitivity analysis for the UNEDF family of functionals

Workshop on "Recent developments in nuclear density functional models"
Saclay, Nov. 24-28, 2014

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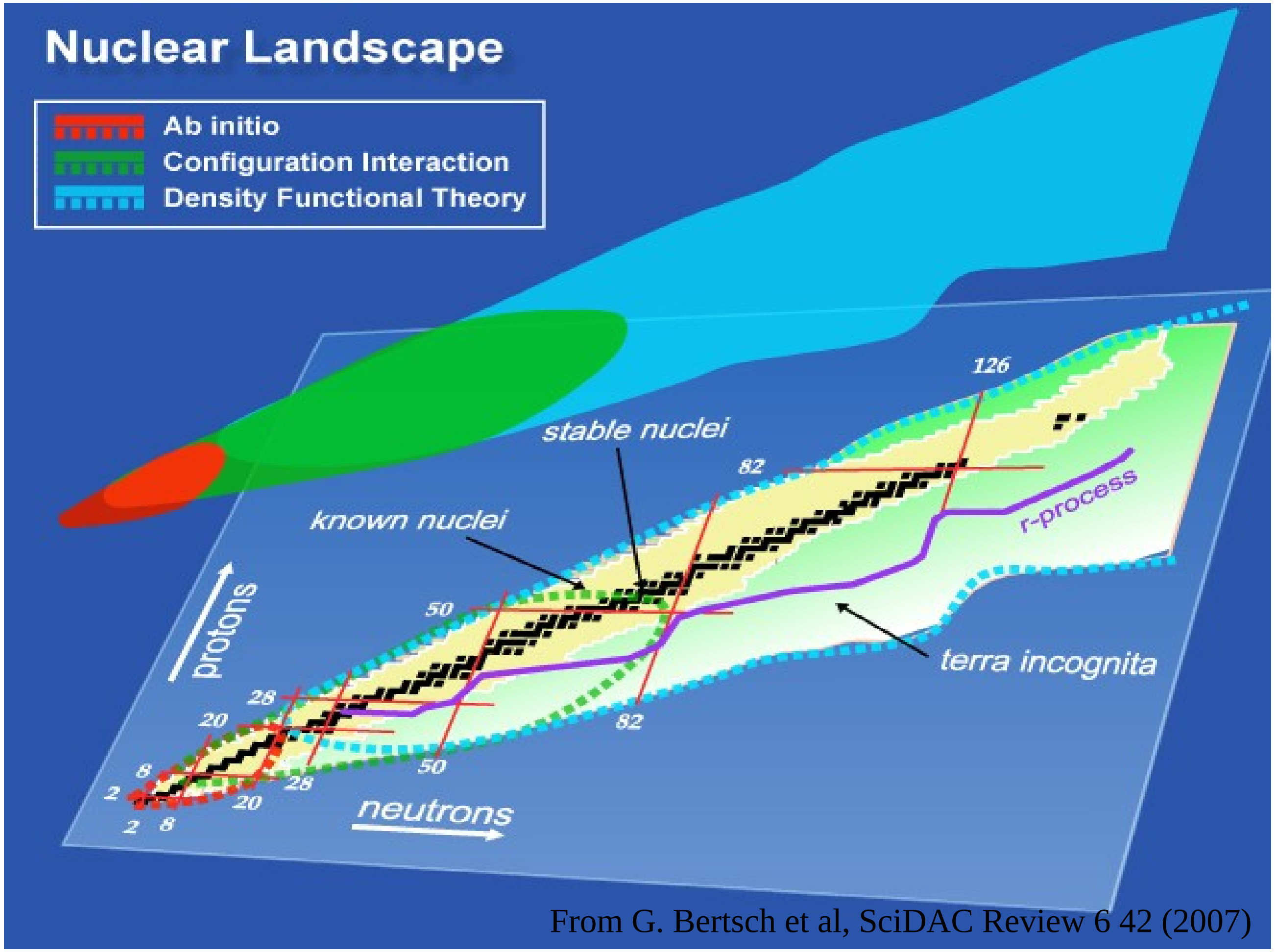
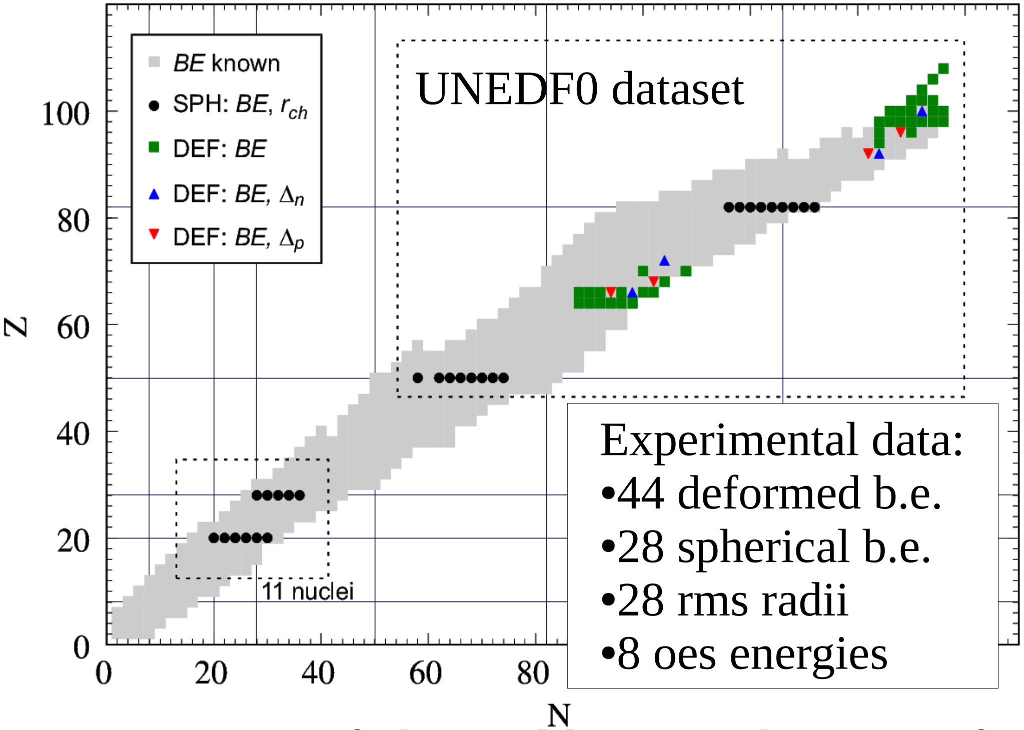
The nuclear landscape

- Nuclear density functional theory (DFT) is applicable throughout the whole nuclear chart
- The key ingredient of the DFT is the energy density functional (EDF)
- Parameters of the EDF model needs to be optimized to experimental input
- What about parameter uncertainties (and uncertainties of predicted observables)?
- Predictive power of the model?



From G. Bertsch et al, SciDAC Review 6 42 (2007)

Energy density optimization: UNEDF0 and UNEDF1



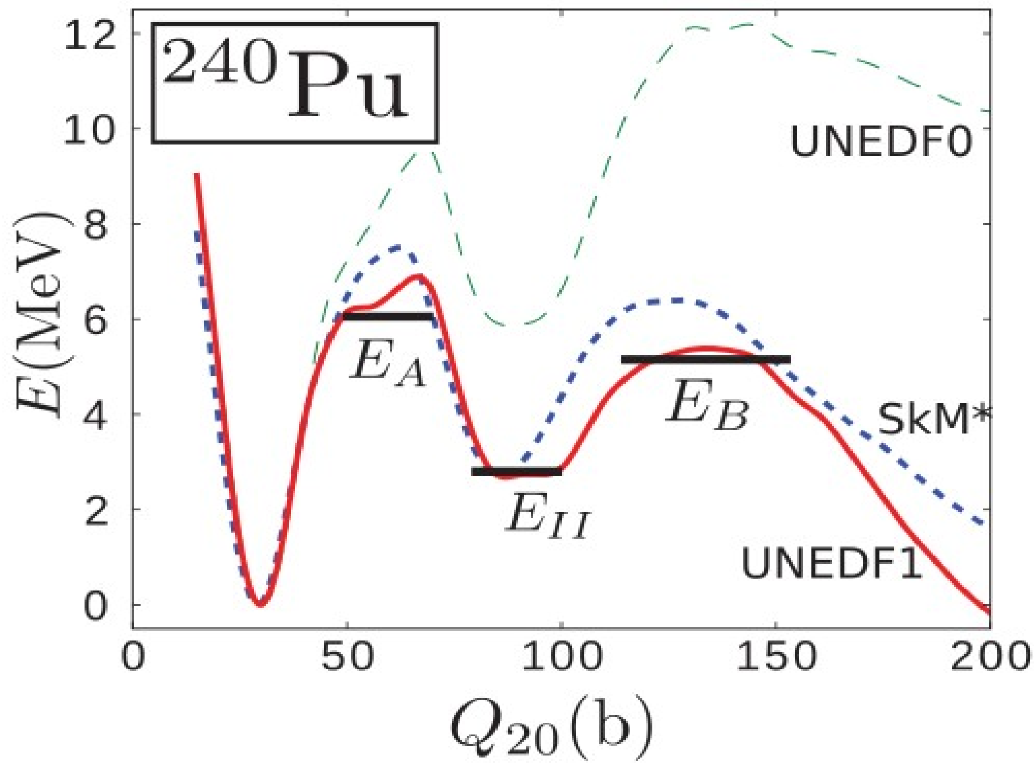
Experimental data:
- 44 deformed b.e.
- 28 spherical b.e.
- 28 rms radii
- 8 oes energies

UNEDF0: M. K., T. Lesinski, J. Moré, W. Nazarewicz, J. Sarich, N. Schunck, M. V. Stoitsov, S. Wild, PRC 82, 024313 (2010)

UNEDF1: M. K., J. McDonnell, W. Nazarewicz, P.-G. Reinhard, J. Sarich, N. Schunck, M. V. Stoitsov, S. Wild, PRC 85, 024304 (2012)

- Optimization of Skyrme-like ED with respect of 12 parameters at axially deformed HFB level

$$\rho_c, E^{NM}/A, K^{NM}, a^{NM}_{sym}, L^{NM}_{sym}, M_s^{-1}$$
$$C_0^{\rho\Delta\rho}, C_1^{\rho\Delta\rho}, V_0^n, V_0^p, C_0^{\rho\nabla J}, C_1^{\rho\nabla J}$$



- UNEDF1 was the first parameterization which was systematically optimized at the deformed HFB level for fission studies
- UNEDF1 included data on 4 fission isomers states (^{226}U, ^{238}U, ^{240}Pu, ^{242}Cm)

Energy density optimization: UNEDF2

- Optimization of Skyrme-like ED with respect of 14 parameters at deformed HFB level: Tensor terms now included

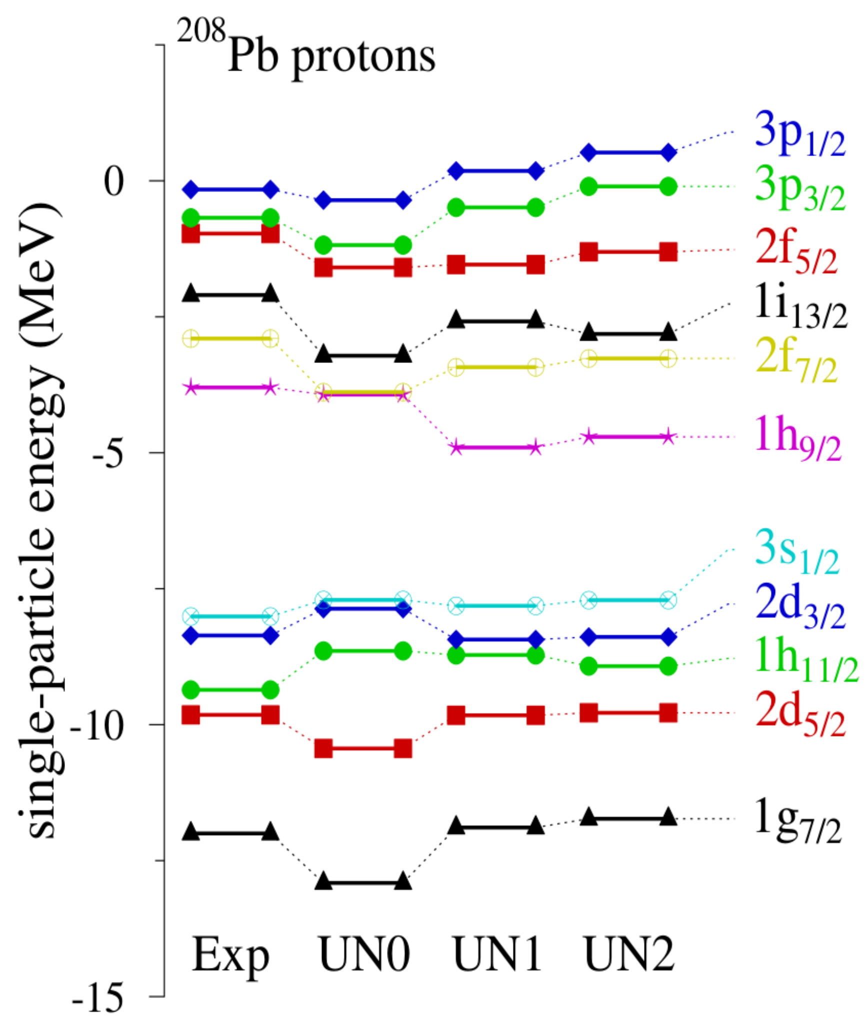
$$\rho_c, E^{NM}/A, K^{NM}, a_{sym}^{NM}, L_{sym}^{NM}, M_s^{-1}$$
$$C_0^{\rho\Delta\rho}, C_1^{\rho\Delta\rho}, V_0^n, V_0^p, C_0^{\rho\nabla J}, C_1^{\rho\nabla J}, \boxed{C_0^J, C_1^J}$$

- Single particle energies included in the optimization. These were handled with blocked HFB calculations

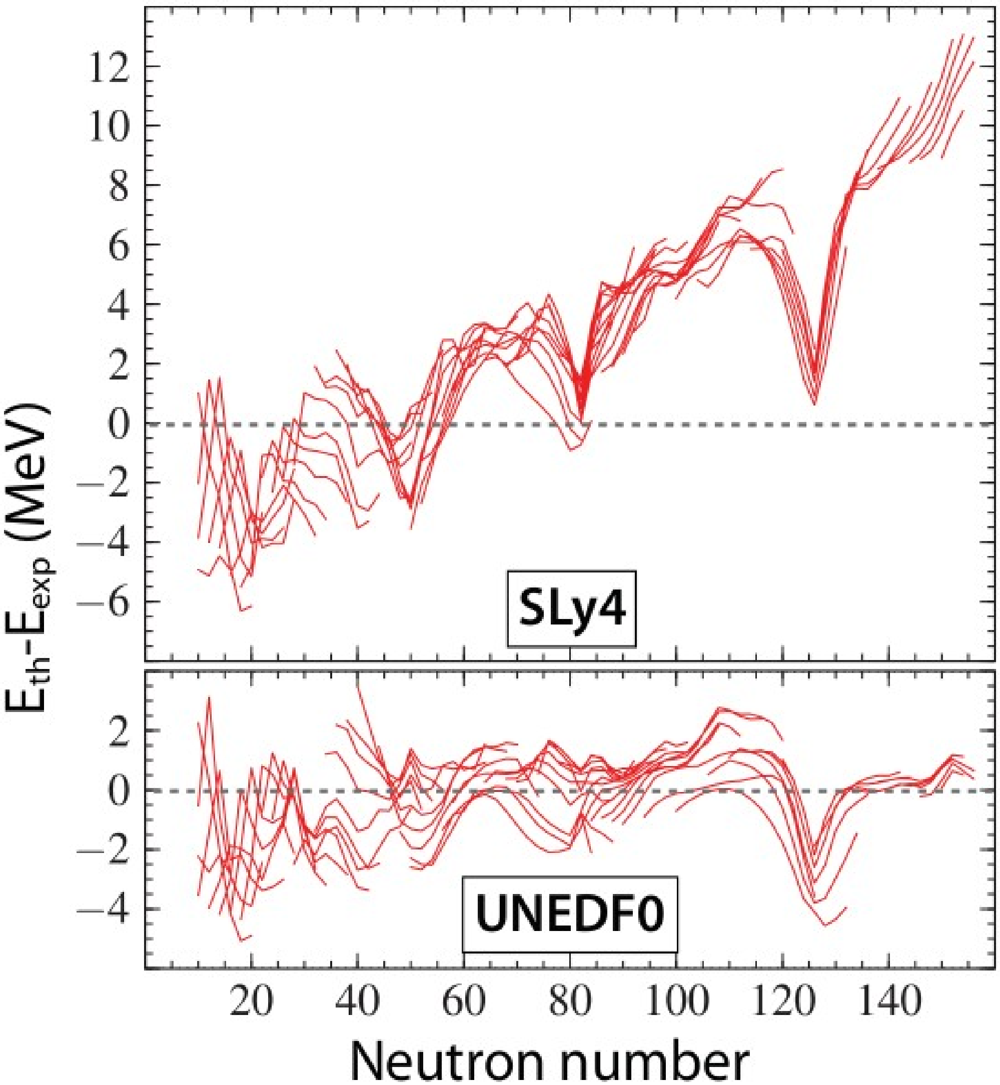
$$E_{\text{s.p.}}^{(\text{part.})} = E_{\text{bl}}(A+1) - E(A)$$
$$E_{\text{s.p.}}^{(\text{hole})} = E(A) - E_{\text{bl}}(A-1)$$

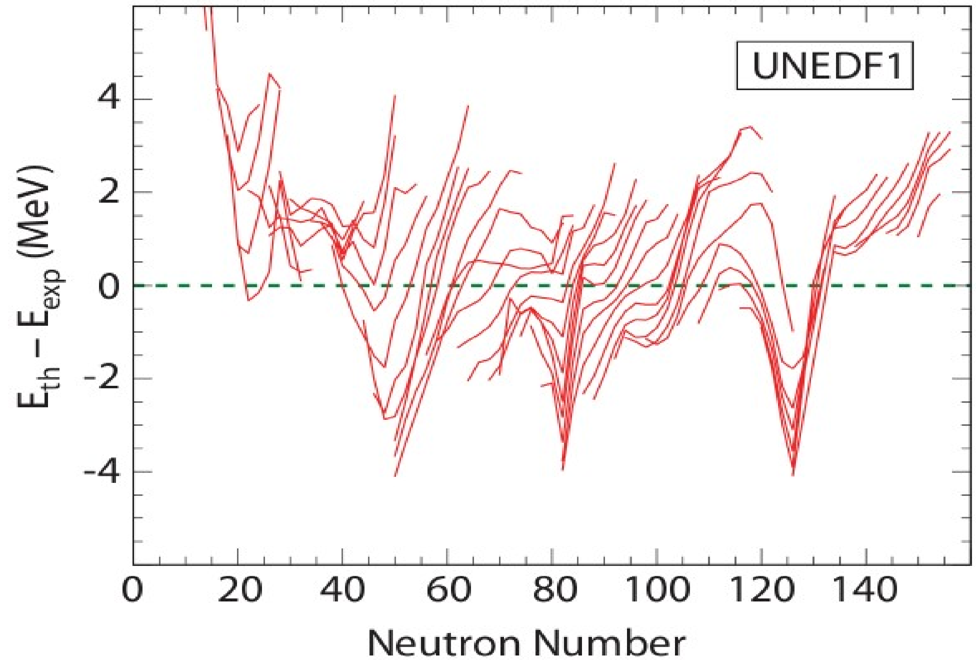
- Generally, UNEDF2 gives no or only marginal improvement over to UNEDF1
  $\Rightarrow$ Need to go to novel EDFs

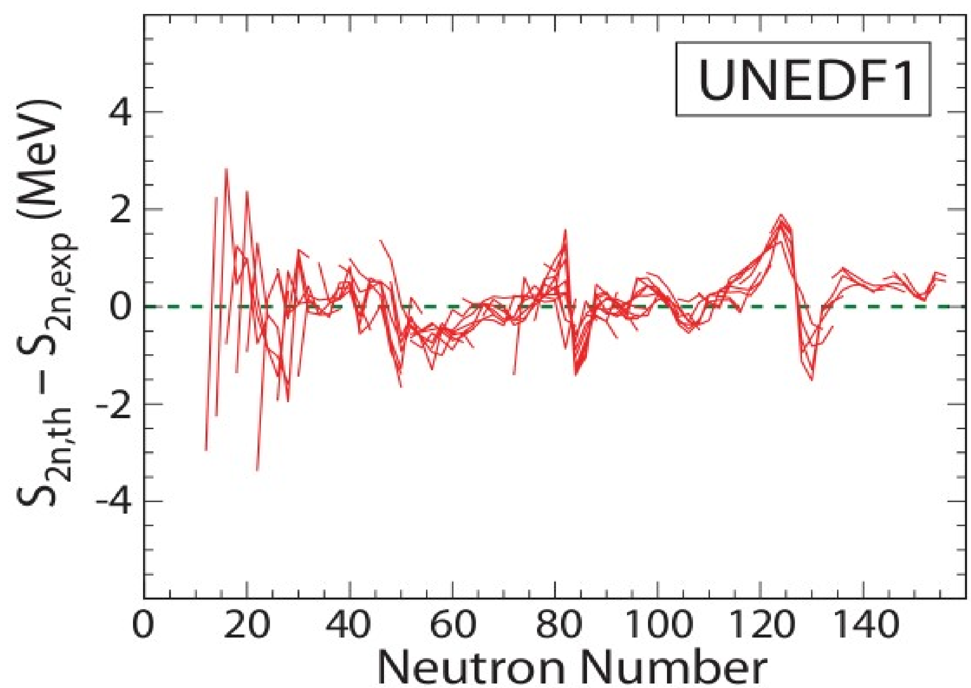
UNEDF2: M.K., J. McDonnell, W. Nazarewicz, E. Olsen, P.-G. Reinhard, J. Sarich, N. Schunck, S.M. Wild, D. Davesne, J. Erler, A. Pastore, Phys. Rev. C 89 054314 (2014)



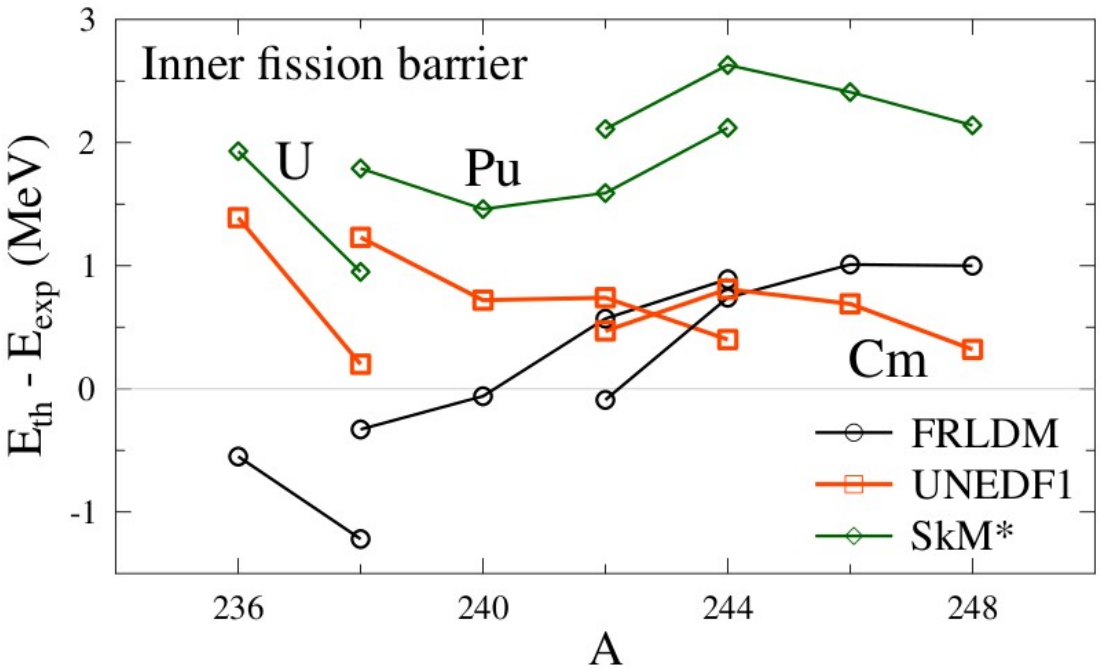
Predictions with UNEDF0,1 EDFs: Existing exp. data

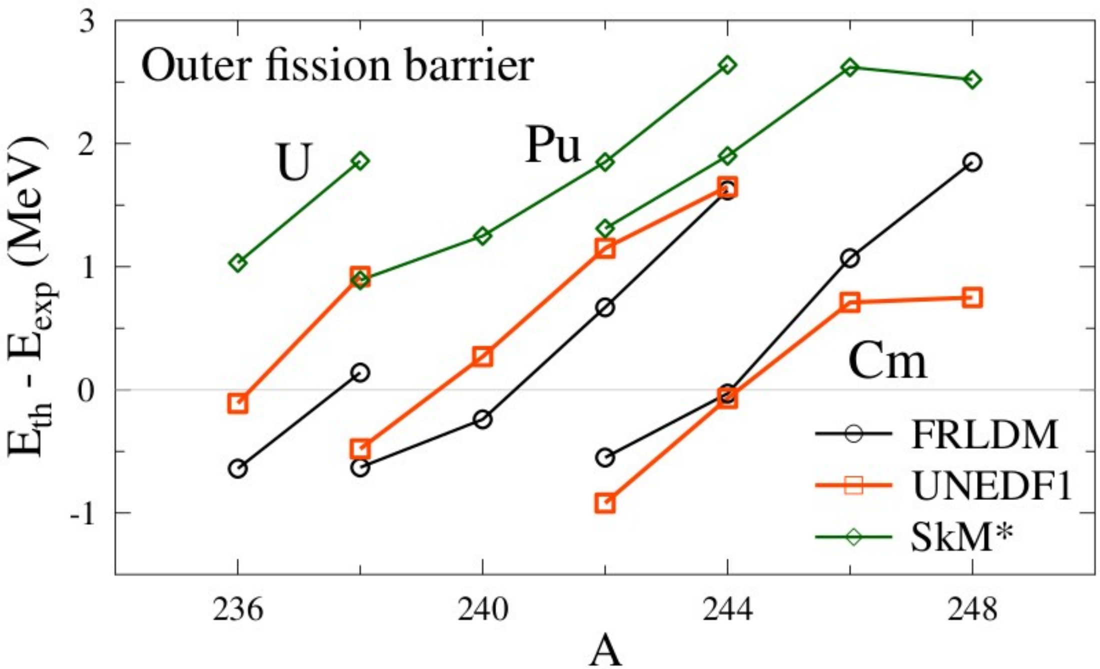






Fission properties of UNEDF1



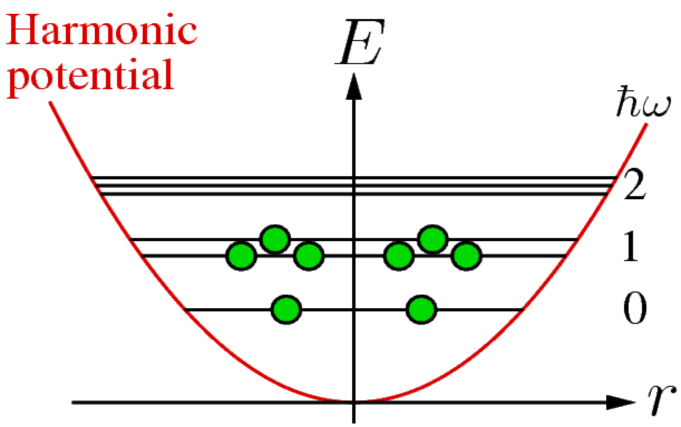


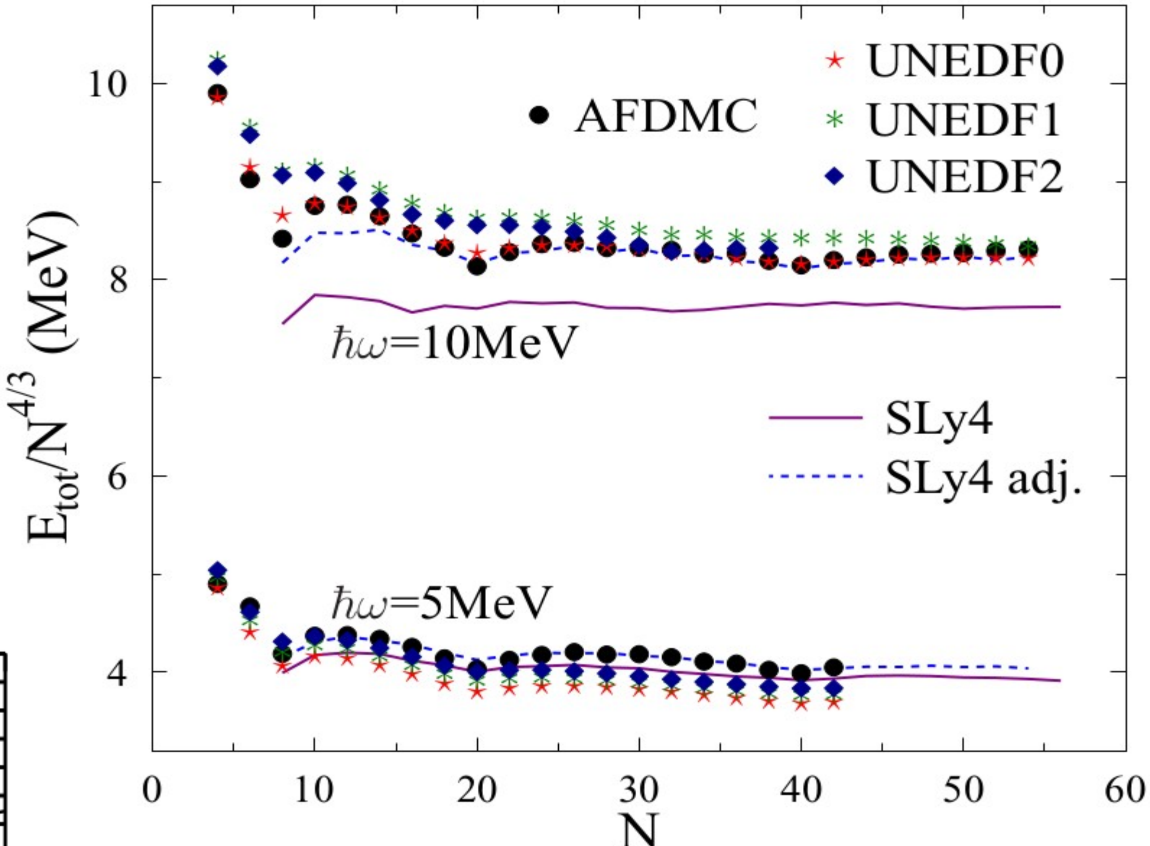
Liquid drop coefficients of UNEDF0 and UNEDF1 (in MeV)

	a_{vol}	a_{sym}	$a_{sym}^{(2)}$	a_{surf}	a_{curv}	a_{ssym}
UNEDF0	−16.056	30.543	4.418	18.7	7.1	−44
UNEDF1	−15.800	28.987	3.637	16.7	8.8	−29

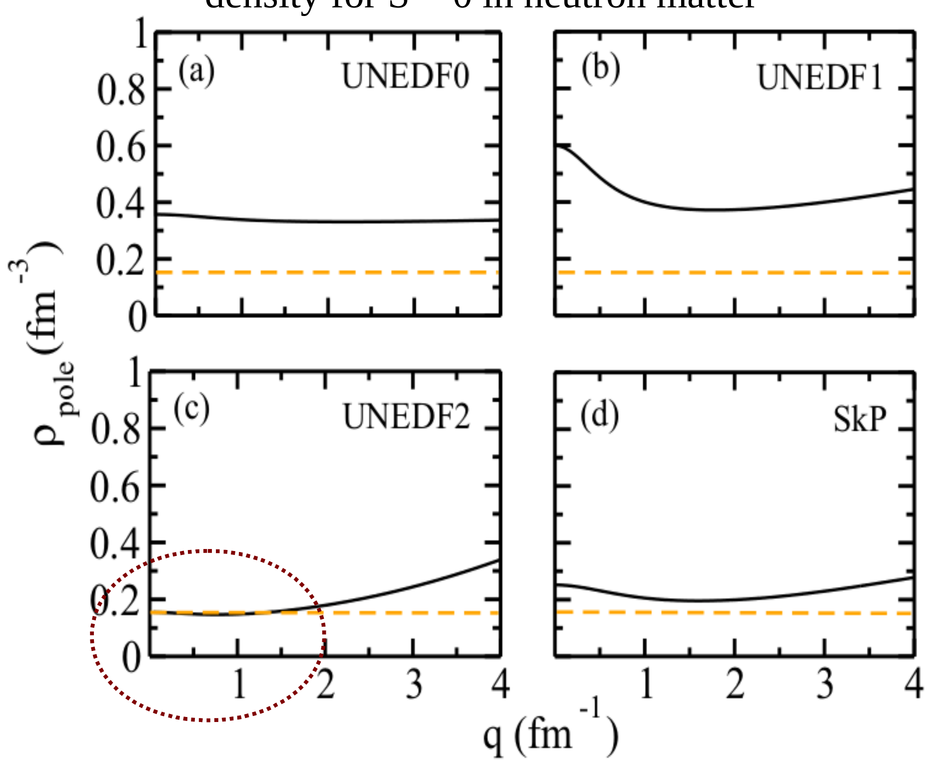
- Inclusion of fission isomer data allowed to constrain UNEDF1 EDF to reproduce fission properties in actinide region reasonably well
- Surface symmetry energy notably different between UNEDF0 and 1

Predictions with UNEDF EDFs: Neutron droplets



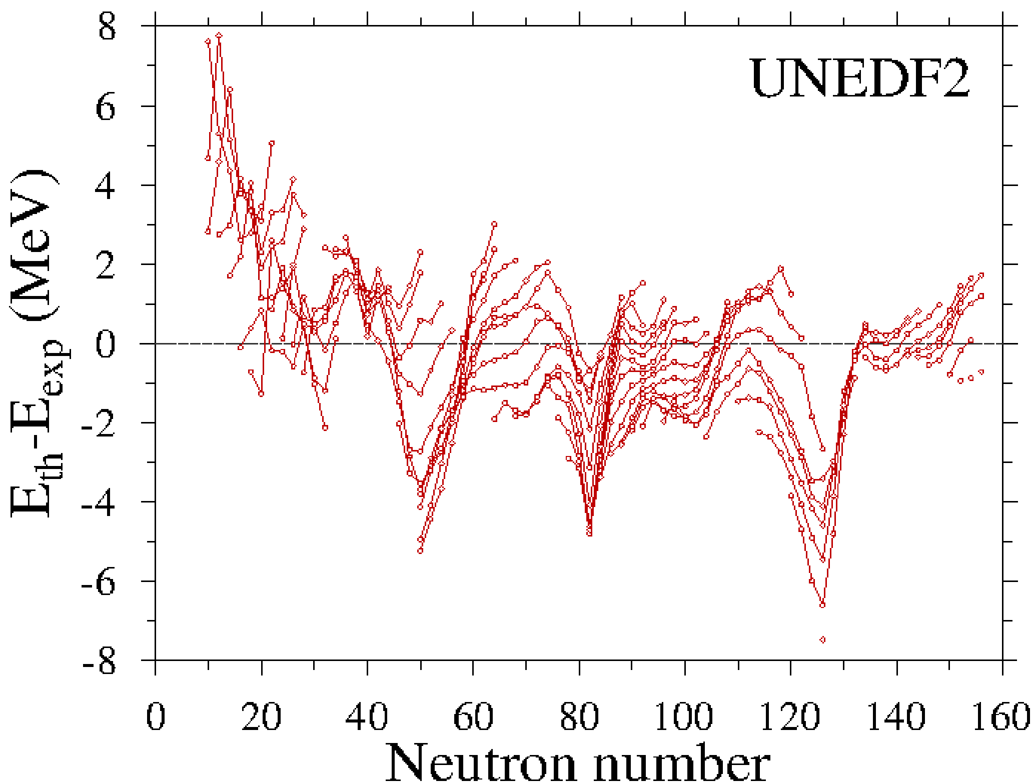


Position of the lowest critical density for S = 0 in neutron matter

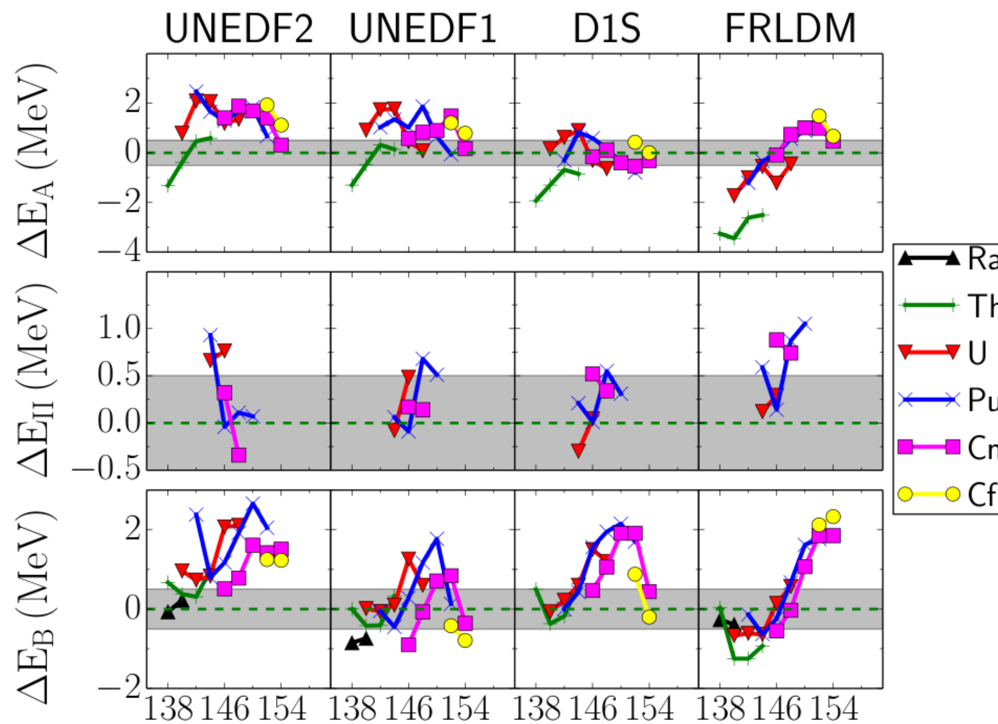


- Neutron droplets allow to test various many-body methods in controlled environment
- UNEDF EDFs reproduce AFDMC ab-initio results (av8' +UIX) reasonably well
- With UNEDF2, instability in dense neutron matter shows up in heavy droplets

Predictions with UNEDF2 EDF: Existing exp. data



Residuals of inner (E_A) barrier, fission isomer (E_{II}) and outer (E_B) barrier



Observable	UNEDF0	UNEDF1	UNEDF2
E	1.428	1.912	1.950
E $(A < 80)$	2.092	2.566	2.475
E $(A \geq 80)$	1.200	1.705	1.792
S_{2n}	0.758	0.752	0.843
S_{2n} $(A < 80)$	1.447	1.161	1.243
S_{2n} $(A \geq 80)$	0.446	0.609	0.711
S_{2p}	0.862	0.791	0.778
S_{2p} $(A < 80)$	1.496	1.264	1.309
S_{2p} $(A \geq 80)$	0.605	0.618	0.572

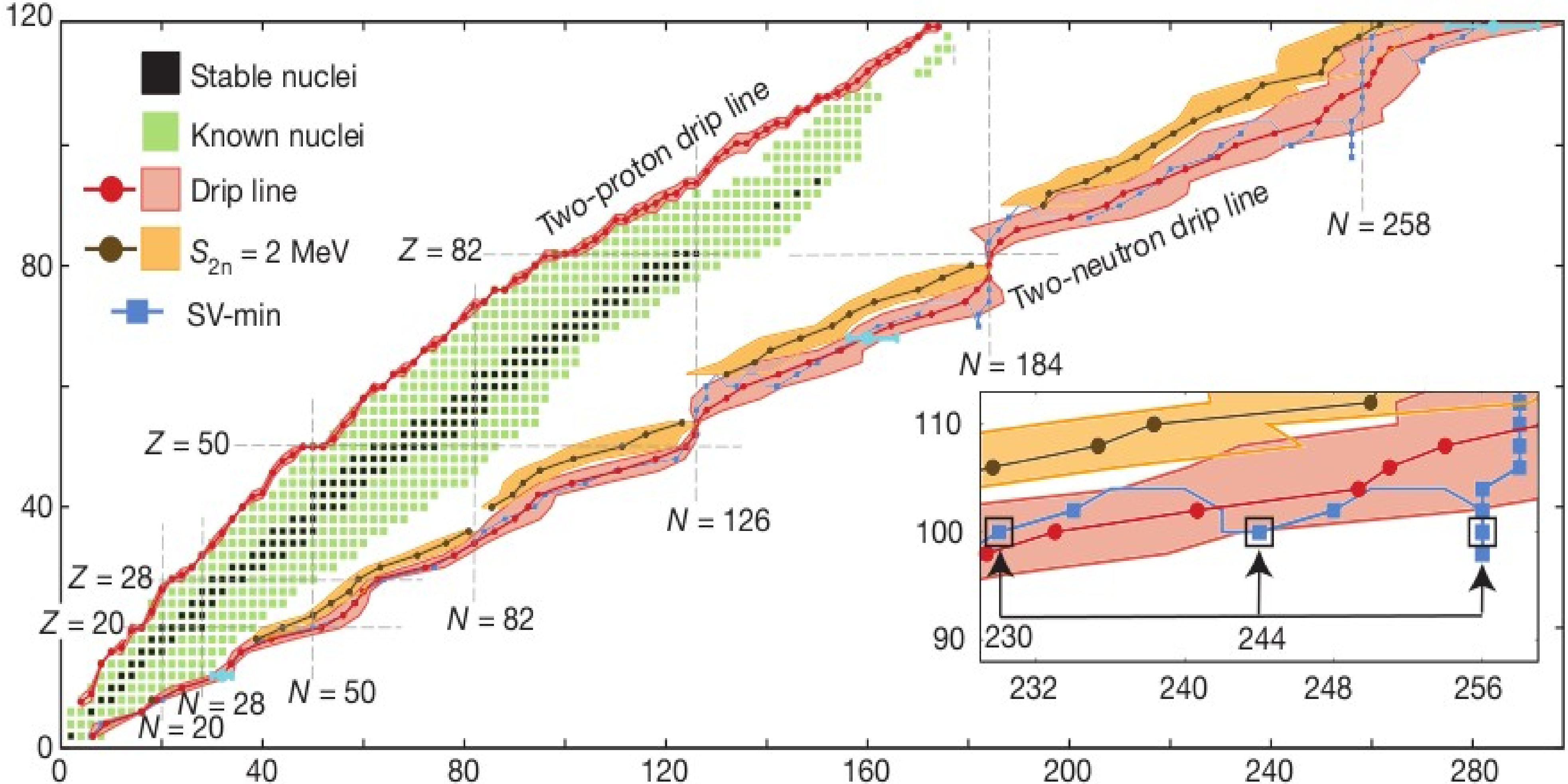
TABLE IX. RMSDs of s.p. energies from empirical values of Ref. [53] (in MeV).

Nuclei	UNEDF0	UNEDF1	UNEDF2
All	1.42	1.38	1.38
Light	1.80	1.72	1.74
Heavy	0.94	0.97	0.95

What about extrapolation to experimentally unknown region?

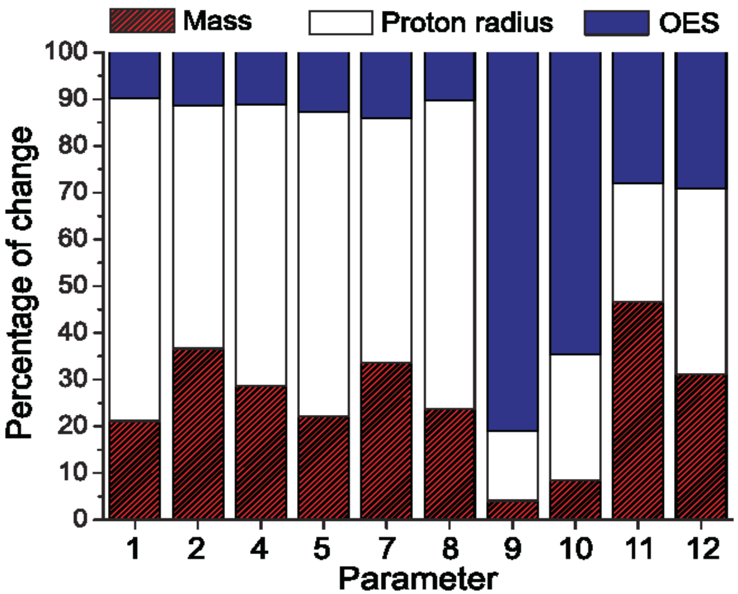
Assessing theoretical uncertainties

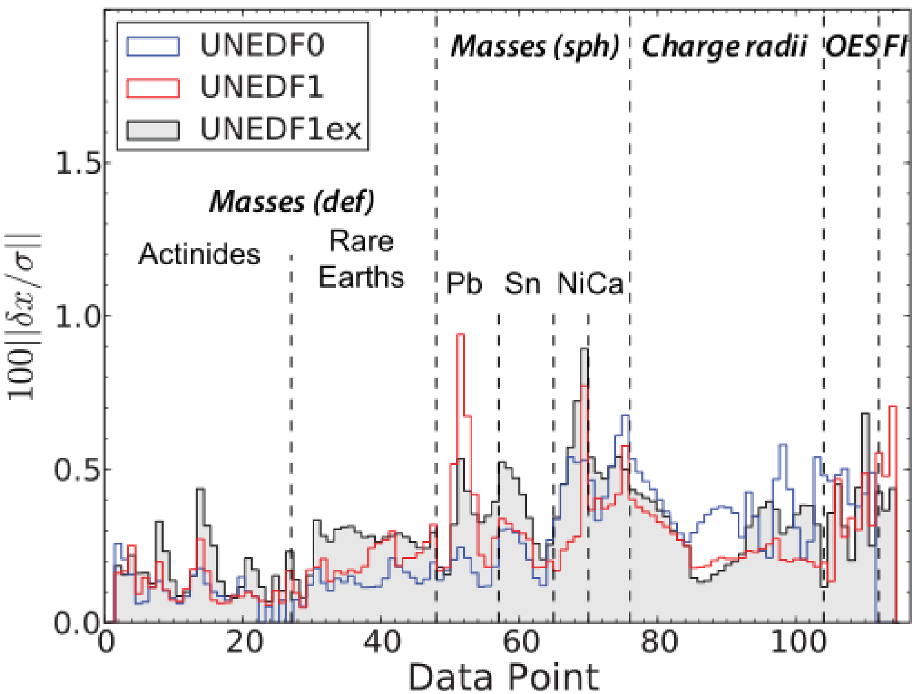
J. Erler, N. Birge, M. Kortelainen, W. Nazarewicz, E. Olsen, A.M. Perhac, M. Stoitsov, Nature 486, 509-512 (2012)



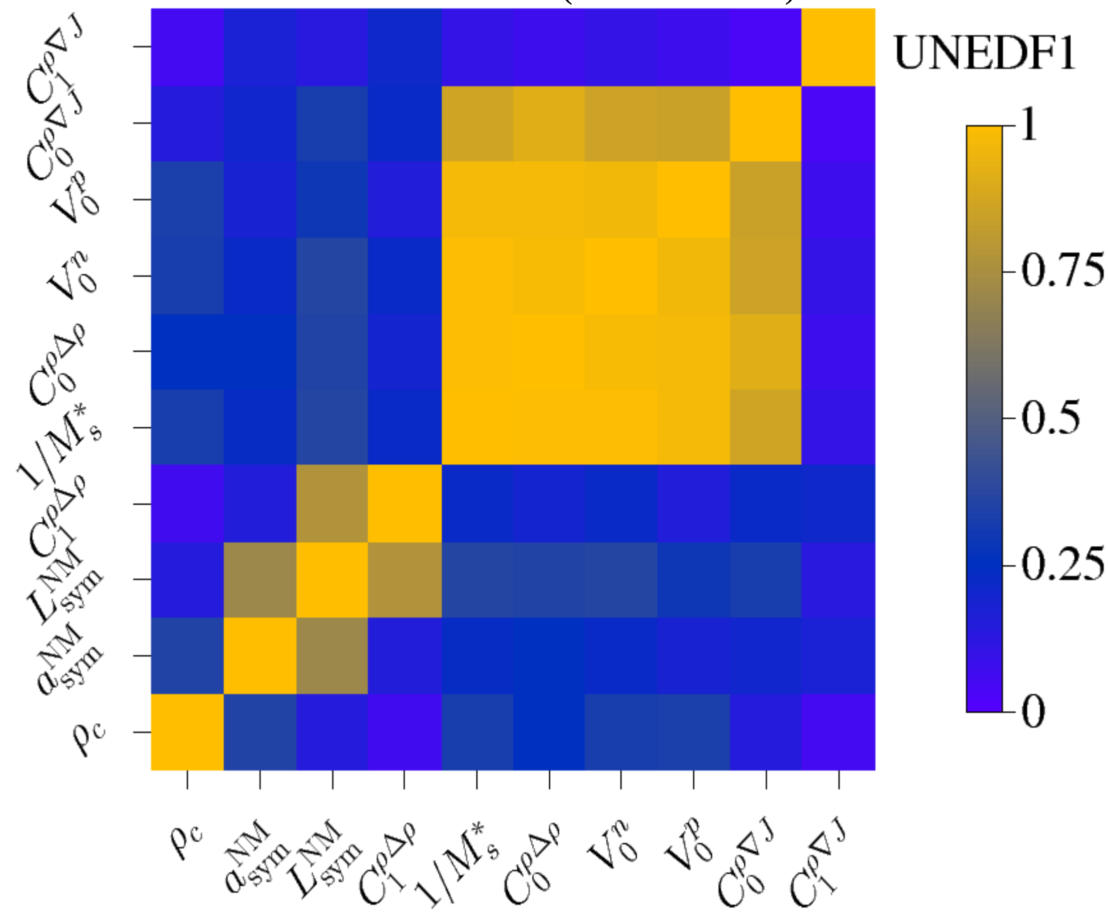
Sensitivity analysis

UNEDF0



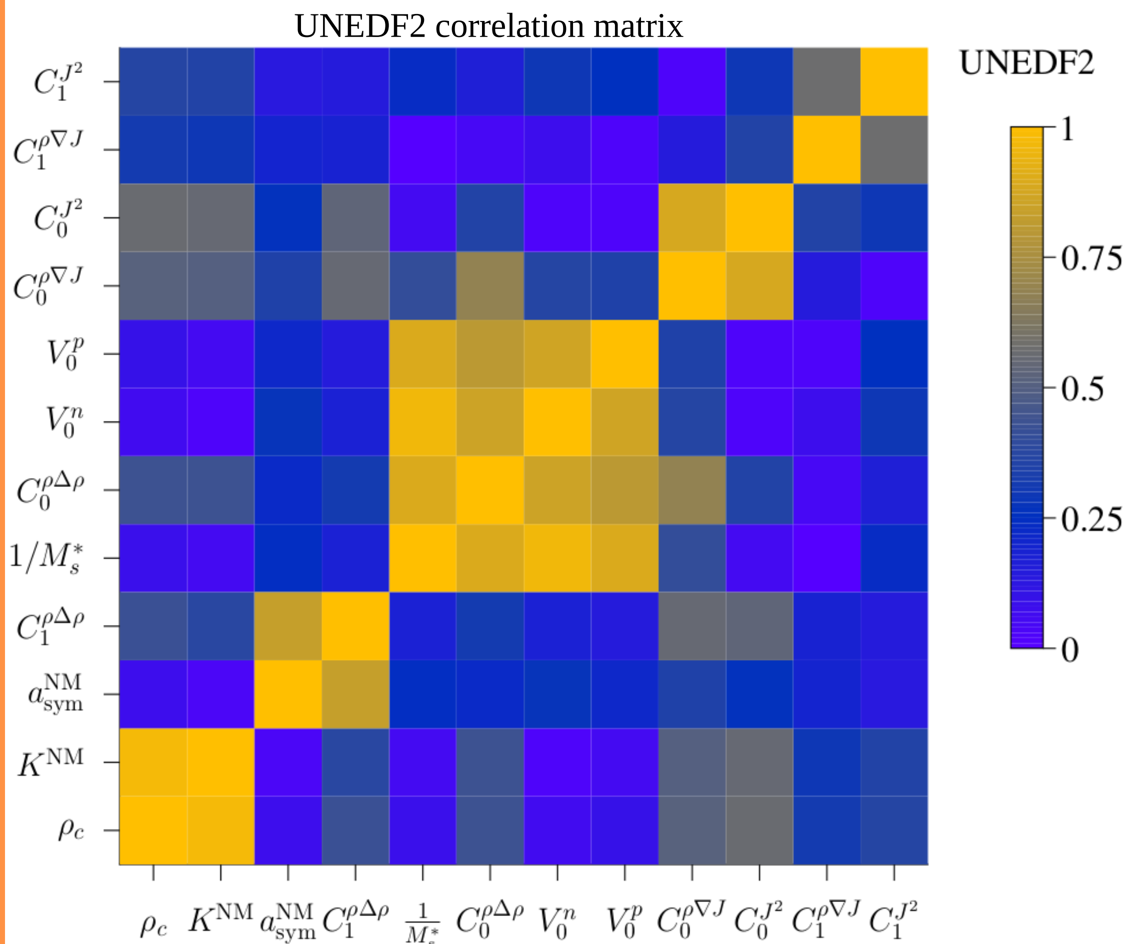


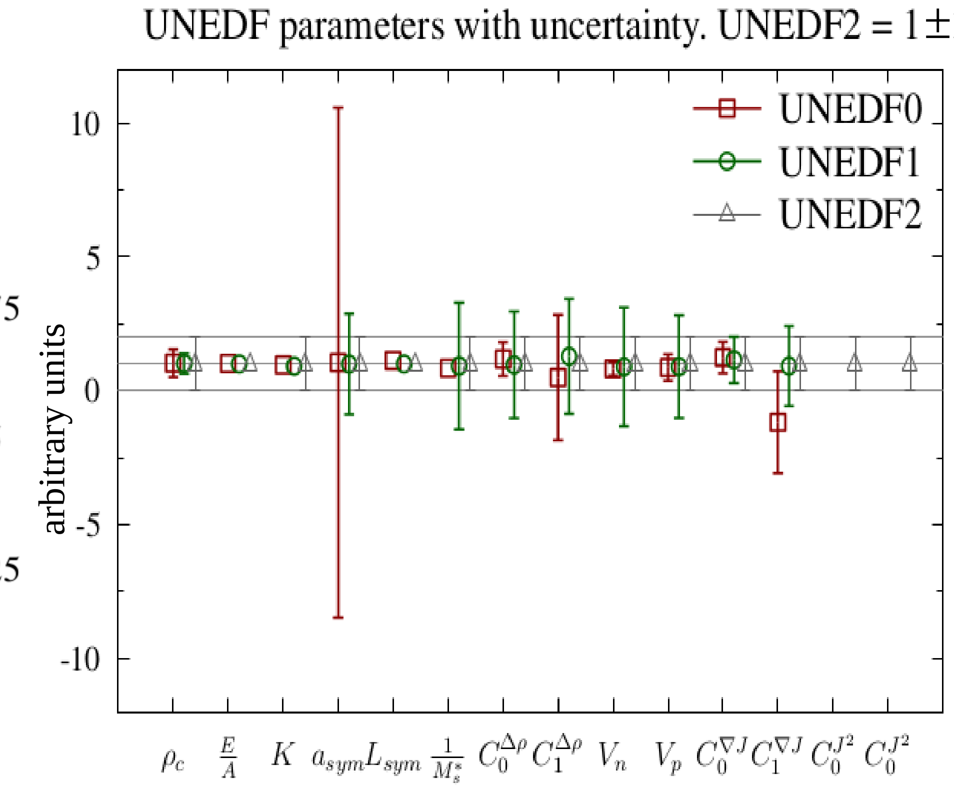
UNEDF1 correlation matrix (absolute values)

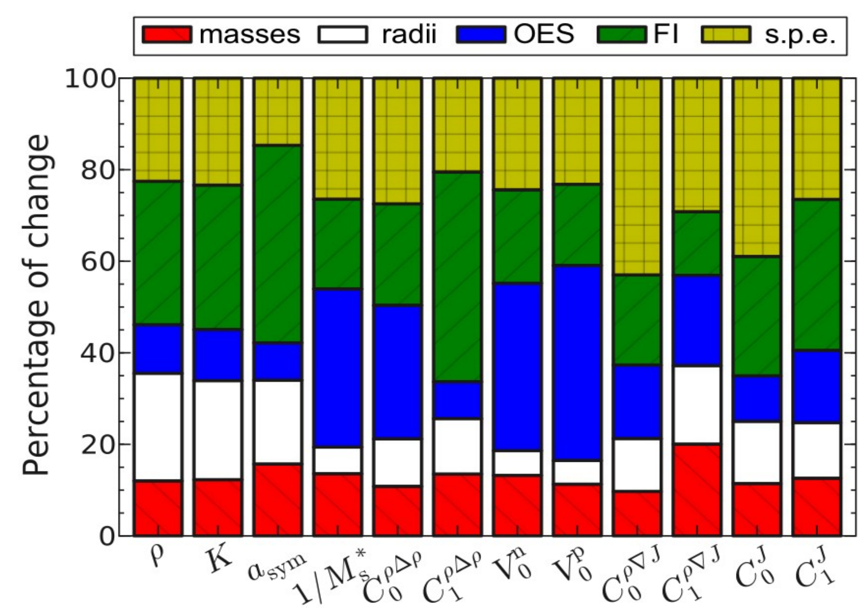


- With UNEDF0, 1 and 2, a complete sensitivity analysis was done for the obtained minimum
- Gives standard deviations and correlations of optimized EDF parameters (covariance matrix)

UNEDF2 sensitivity analysis







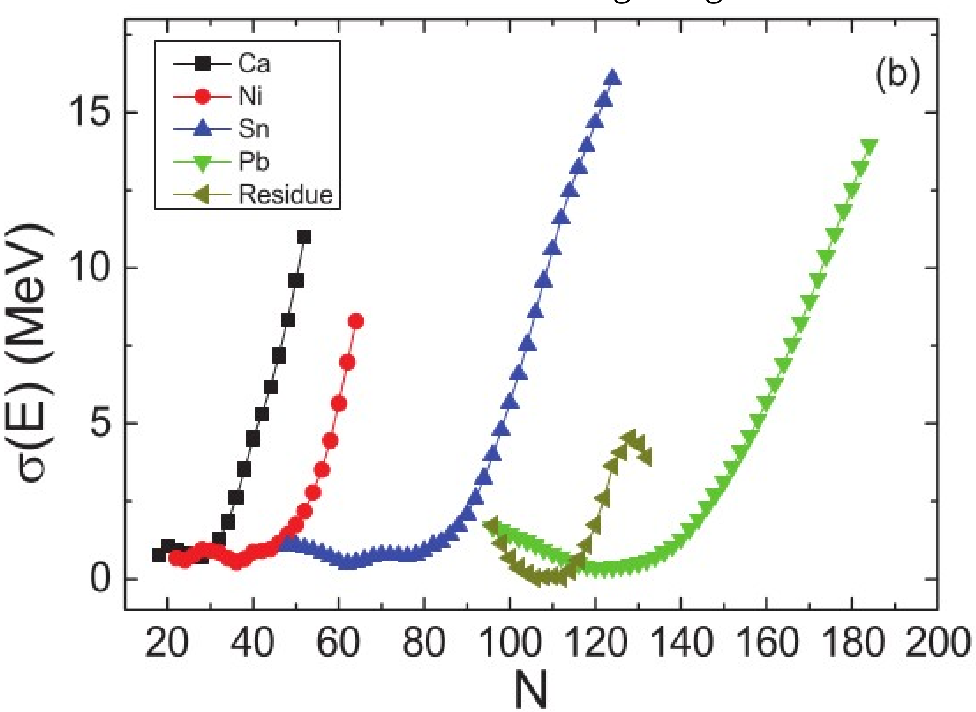
- UNEDF2 sensitivity analysis shows that UNEDF2 is better constrained that UNEDF0,1
- Indicates that major improvements not possible

Propagation of uncertainties

$$\sigma_y^2 = \sum_{i,j} \mathrm{Cov}(x_i, x_j) \left[\frac{\partial y}{\partial x_i} \frac{\partial y}{\partial x_j} \right]$$

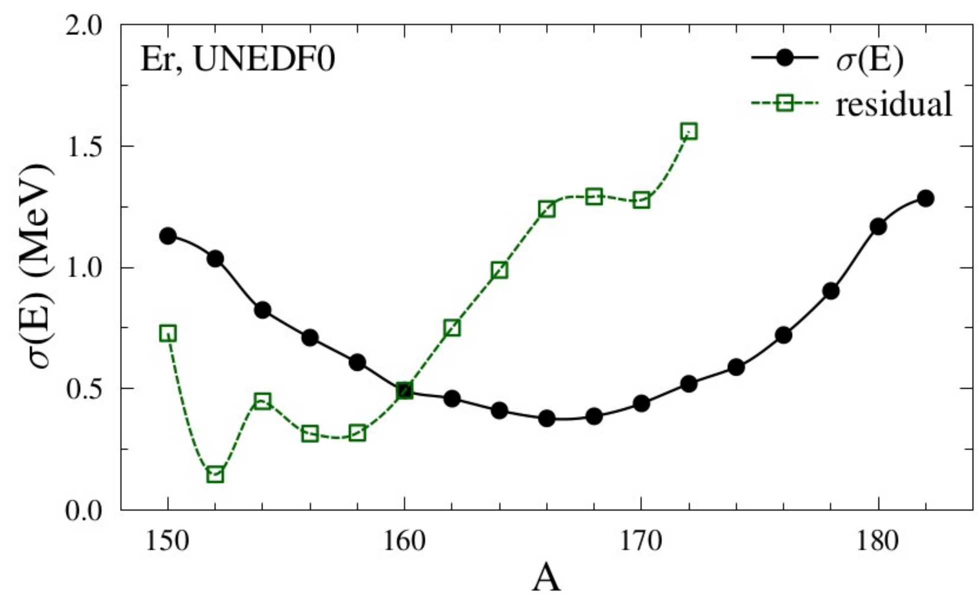
Y. Gao, J. Dobaczewski, M. Kortelainen, J. Toivanen, and D. Tarpanov, Phys. Rev. C 87, 034324 (2013)

Statistical error of binding energies



- One way to assess model uncertainties is to calculate propagated uncertainties
- Requires the covariance matrix of model parameters
- Gives statistical uncertainty (but not systematic uncertainty)
- With UNEDF0, the general tendency is that uncertainties increase when going further away from the valley of stability

M. K., to appear in J.Phys.G, arXiv:1409.1413



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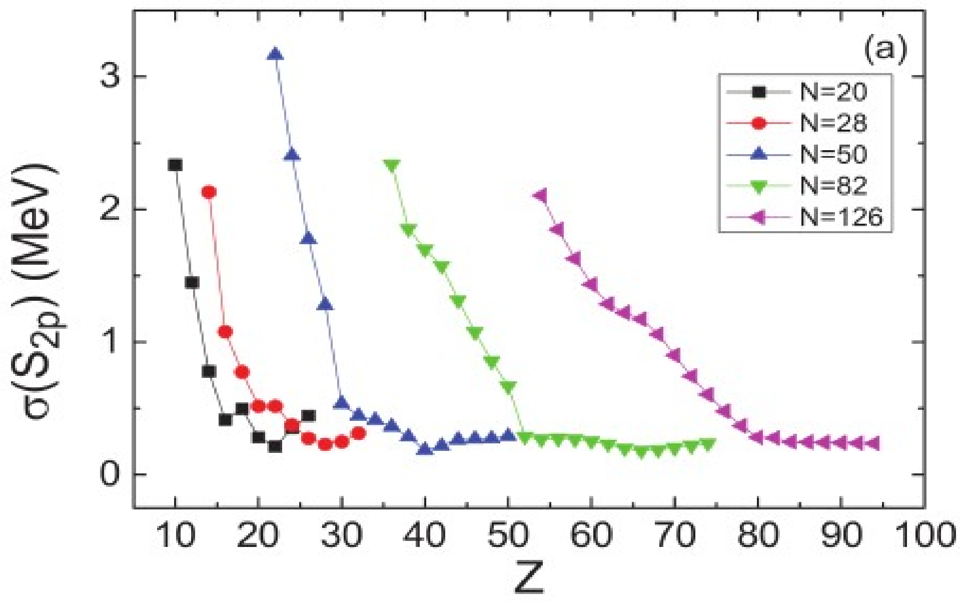

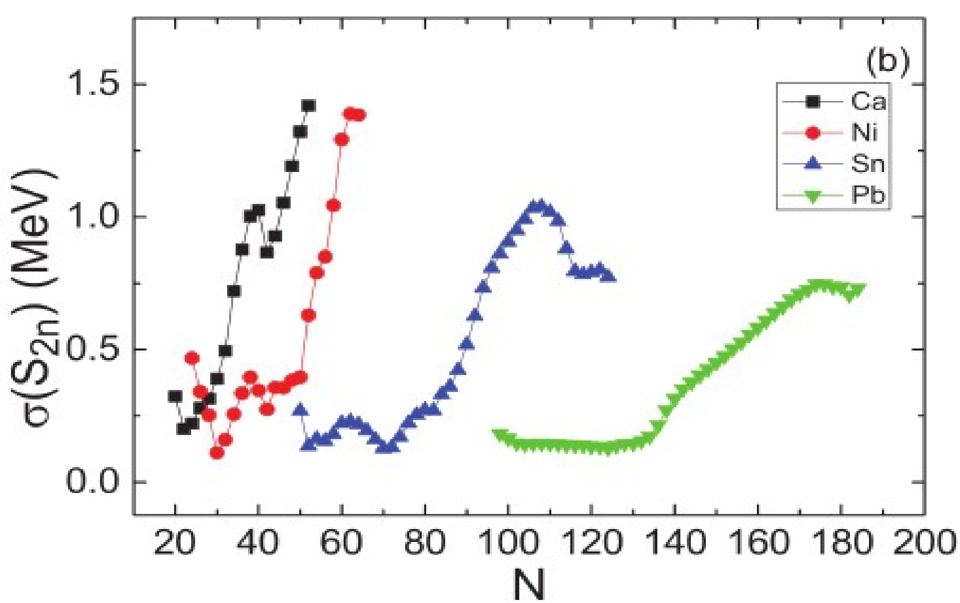

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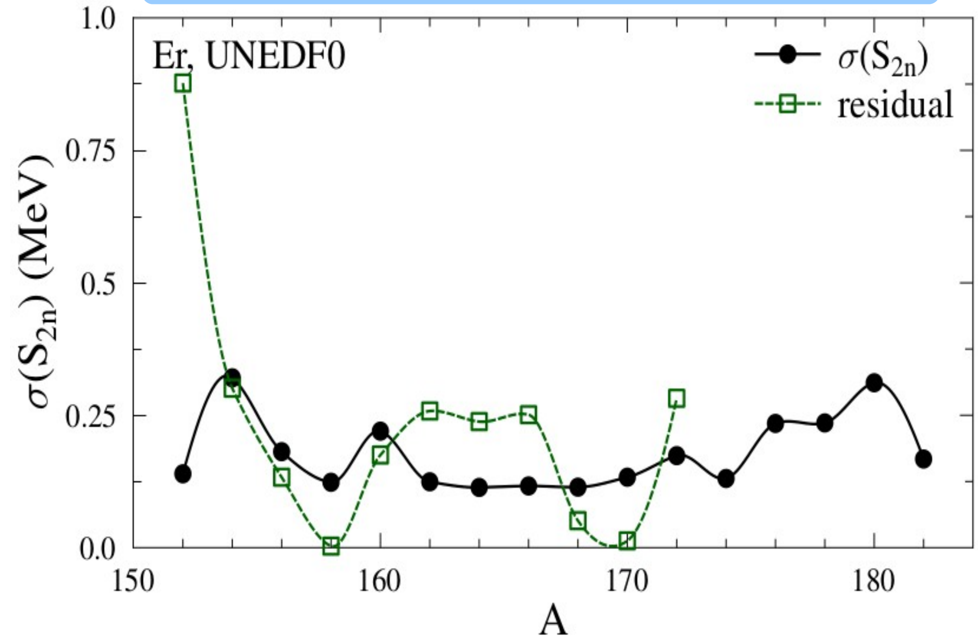
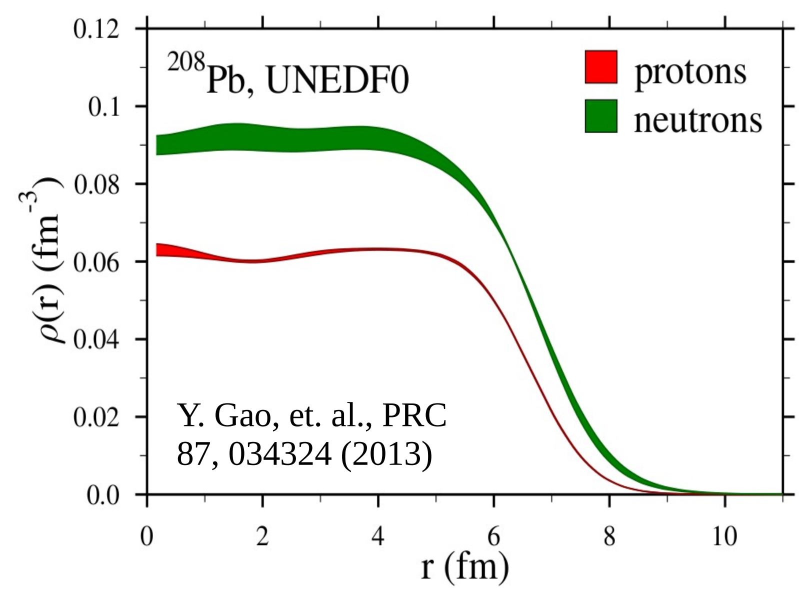
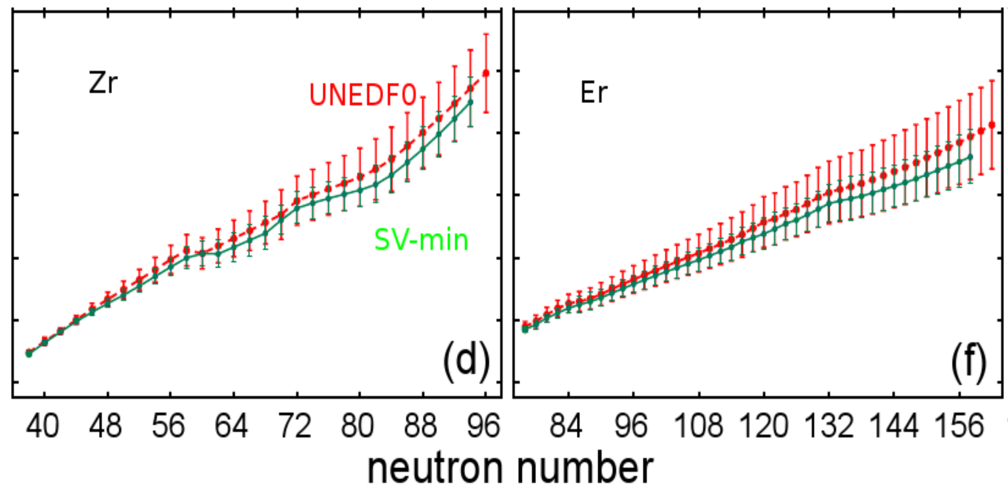


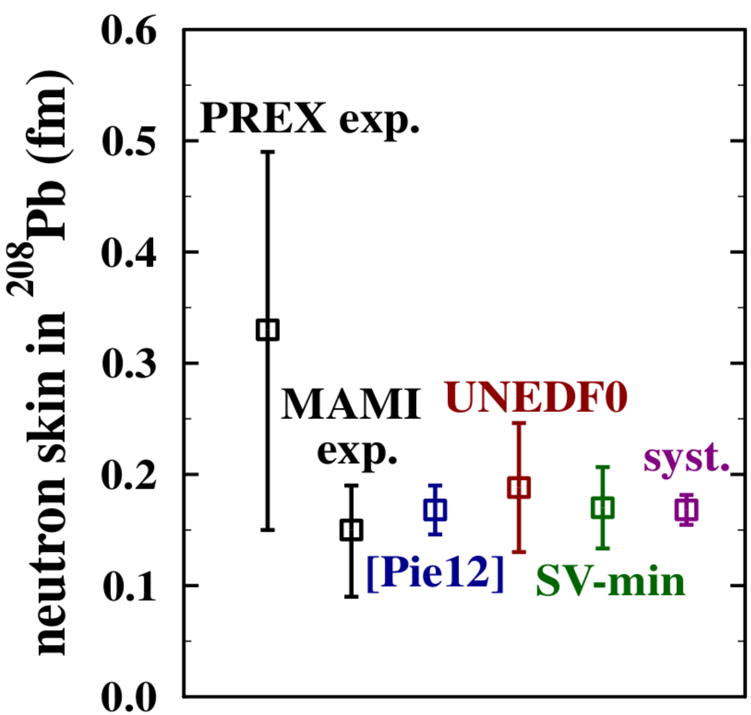


Neutron skin thickness

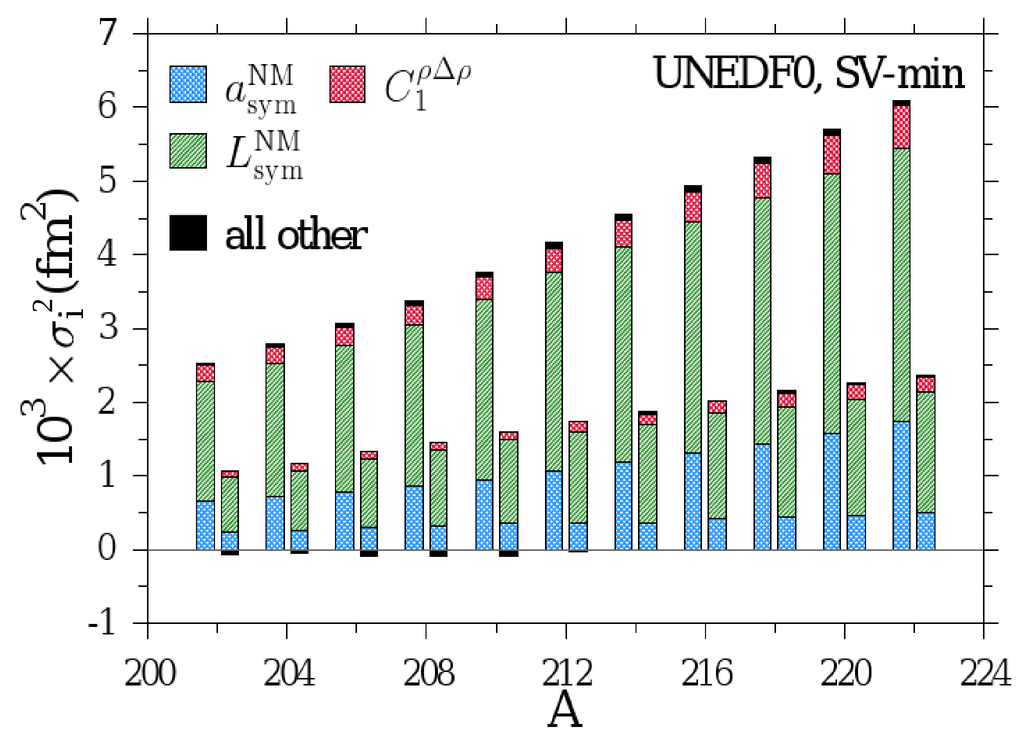
- ^{208}Pb neutron skin thickness was measured in PREX and MAMI experiments
- Experimental error bar in PREX larger than model uncertainties
- Statistical uncertainty larger compared to the systematic uncertainties
- Statistical uncertainty comes mostly from the uncertainty related to the density dependence of the symmetry energy

M. Kortelainen, J. Erler, N. Birge, Y. Gao, W. Nazarewicz, E. Olsen, Phys Rev. C 88, 031305(R) (2013)





[Pie12] = J. Piekarewicz, et. al., PRC 85, 041302(R) (2012)



Future directions?

Energy density functional

DME-based functionals with enriched density dependency

+ Relatively easy to implement
+ Computationally comparable to Skyrme
- Density dependency (prohibits beyond mean field calculations)
- Zero-range

Functionals with higher order and/or many-body terms

+ Computationally comparable to Skyrme
- Could have many new parameters to be optimized
- Zero-range

Finite-range functionals

+ Finite range (provides natural cut-off)
- Computationally more expensive

Optimization and post-optimization

Data-set for EDF parameter optimization

? Type of data to include
? Weights of the data points

Uncertainties of EDF parameters and predictions

? Effect of input data-set
? Effect of the type of the EDF

Conclusions

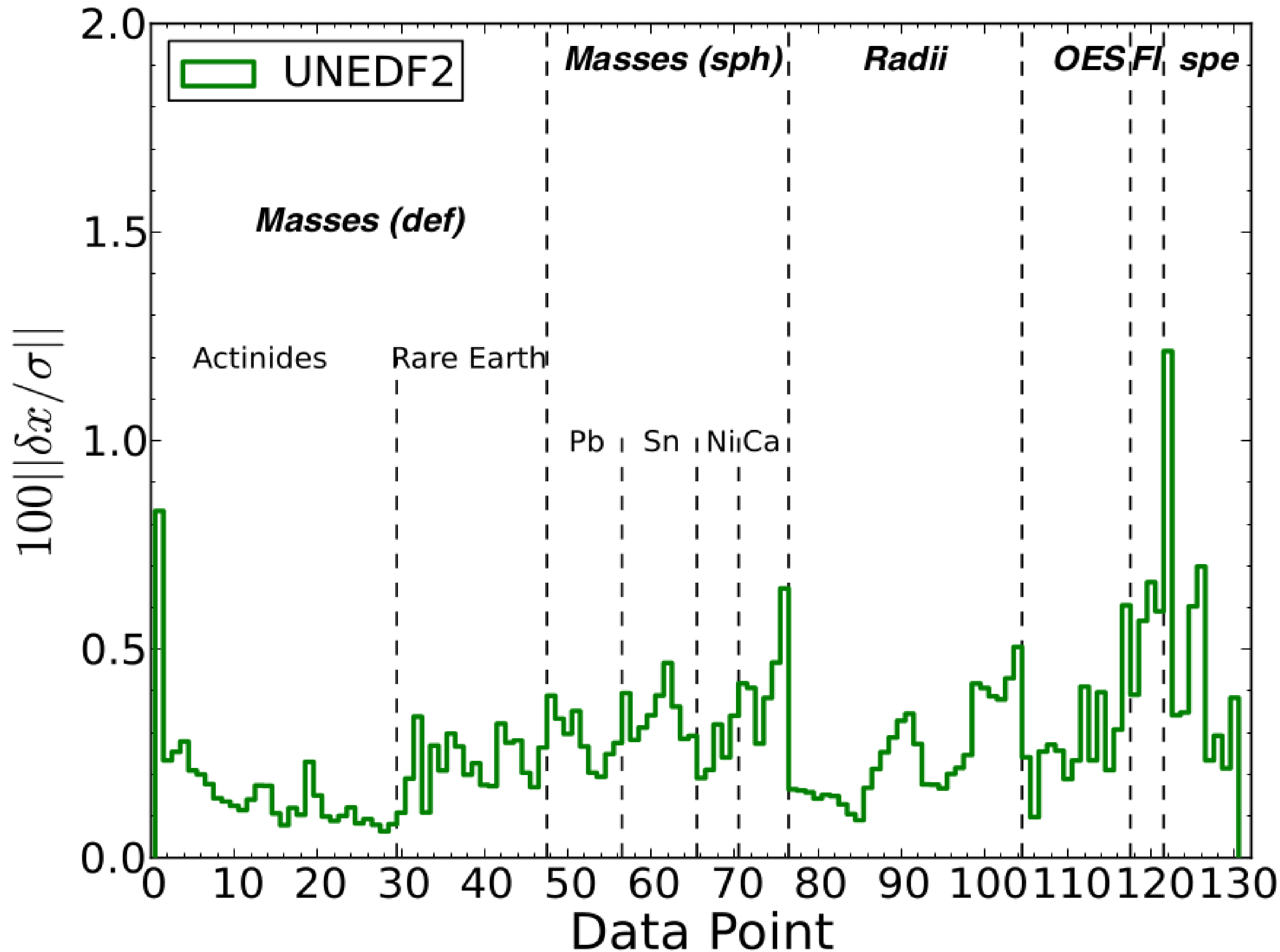
- UNEDF0, 1 and 2 presents a optimization scheme of Skyrme-like EDF, which includes progressively more experimental data
- Sensitivity analysis shows that further major improvements from UNEDF2 are unlikely
- Generally, Skyrme-like EDF models can not be improved much. Need to go novel EDFs. This conclusion is also supported by several other studies.
- To assess the predictive power of the EDF model, sensitivity analysis is mandatory: Should be a standard post-optimization tool with the future EDF optimization schemes.
- Propagated uncertainties gives statistical uncertainties of predictions. Important when judging predictive power of the EDF model

Backup slides

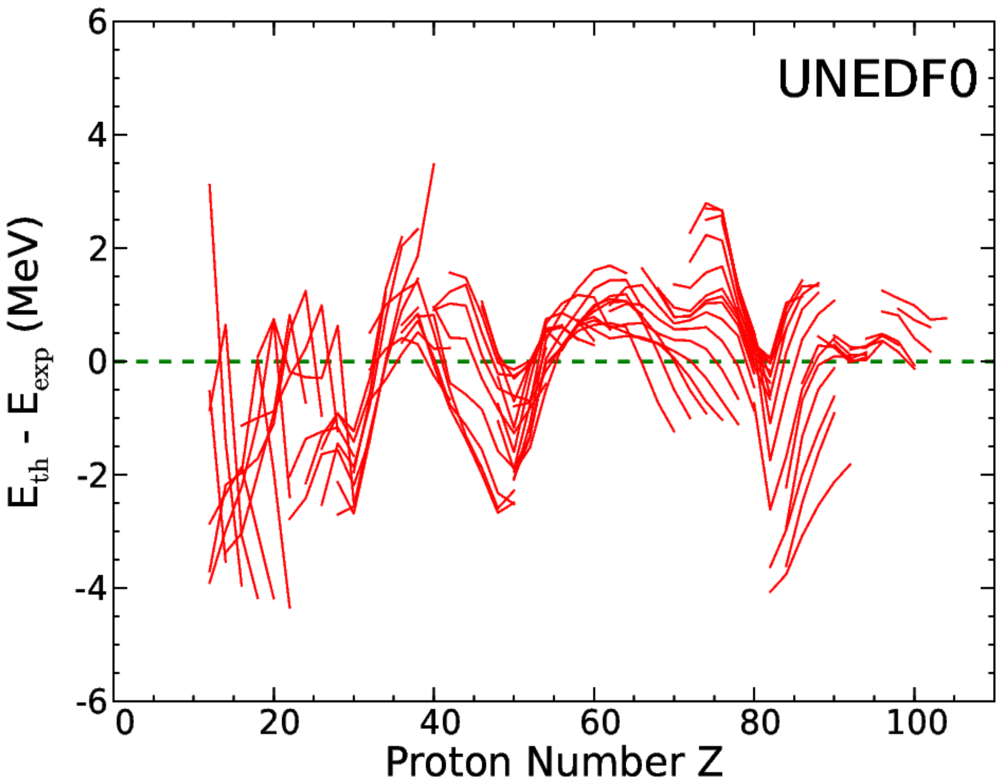
UNEDF2 parameters

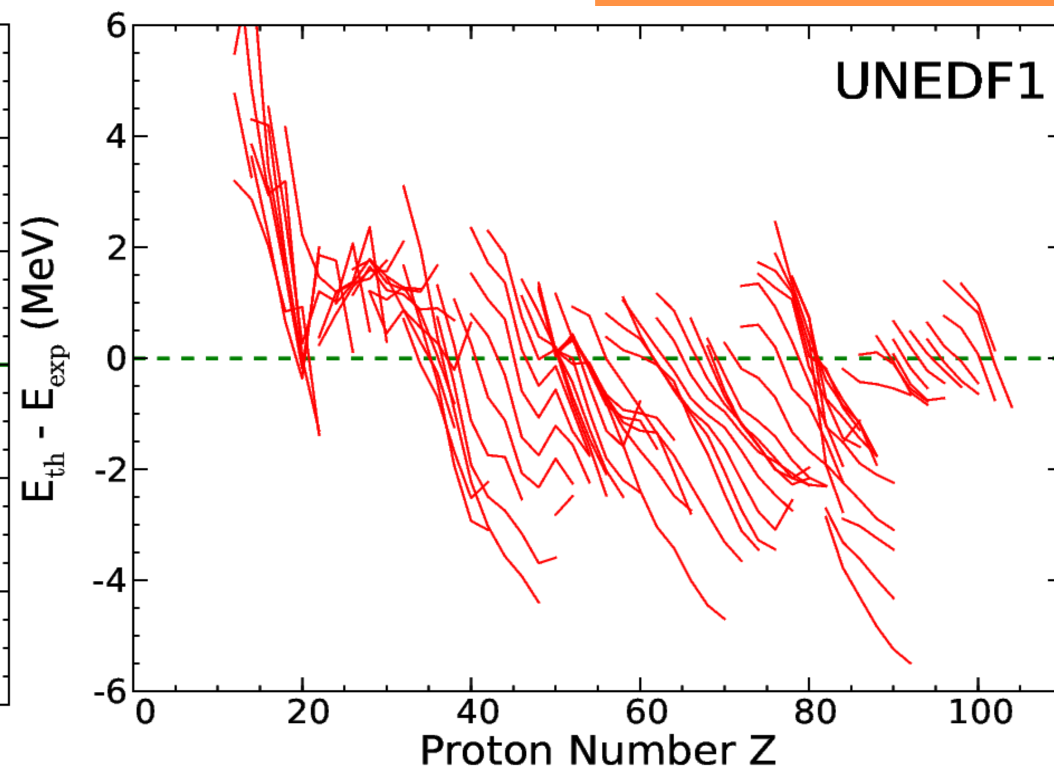
x	$\hat{x}^{(\text{fin.})}$	σ	95% CI
ρ_c	0.15631	0.00112	[0.154, 0.158]
E/A	−15.8		
K	239.930	10.119	[223.196, 256.663]
a_{sym}	29.131	0.321	[28.600, 29.662]
L	40.0		
$1/M_s^*$	1.074	0.052	[0.988, 1.159]
$C_0^{\rho\Delta\rho}$	−46.831	2.689	[−51.277, −42.385]
$C_1^{\rho\Delta\rho}$	−113.164	24.322	[−153.383, −72.944]
V_0^n	−208.889	8.353	[−222.701, −195.077]
V_0^p	−230.330	6.792	[−241.561, −219.099]
$C_0^{\rho\nabla J}$	−64.309	5.841	[−73.968, −54.649]
$C_1^{\rho\nabla J}$	−38.650	15.479	[−64.246, −13.054]
C_0^{JJ}	−54.433	16.481	[−81.687, −27.180]
C_1^{JJ}	−65.903	17.798	[−95.334, −36.472]

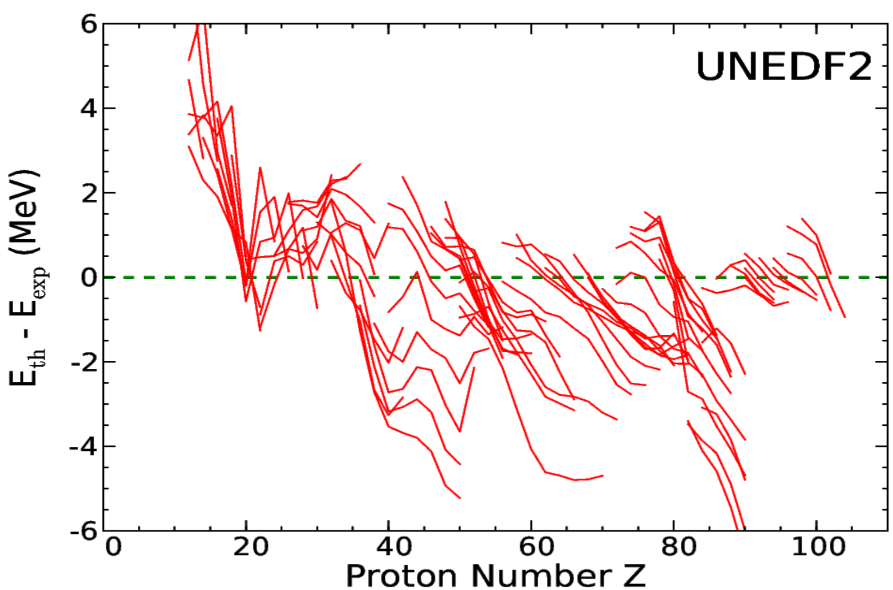
UNEDF2: effect of data point



UNEDF0,1,2 binding energies

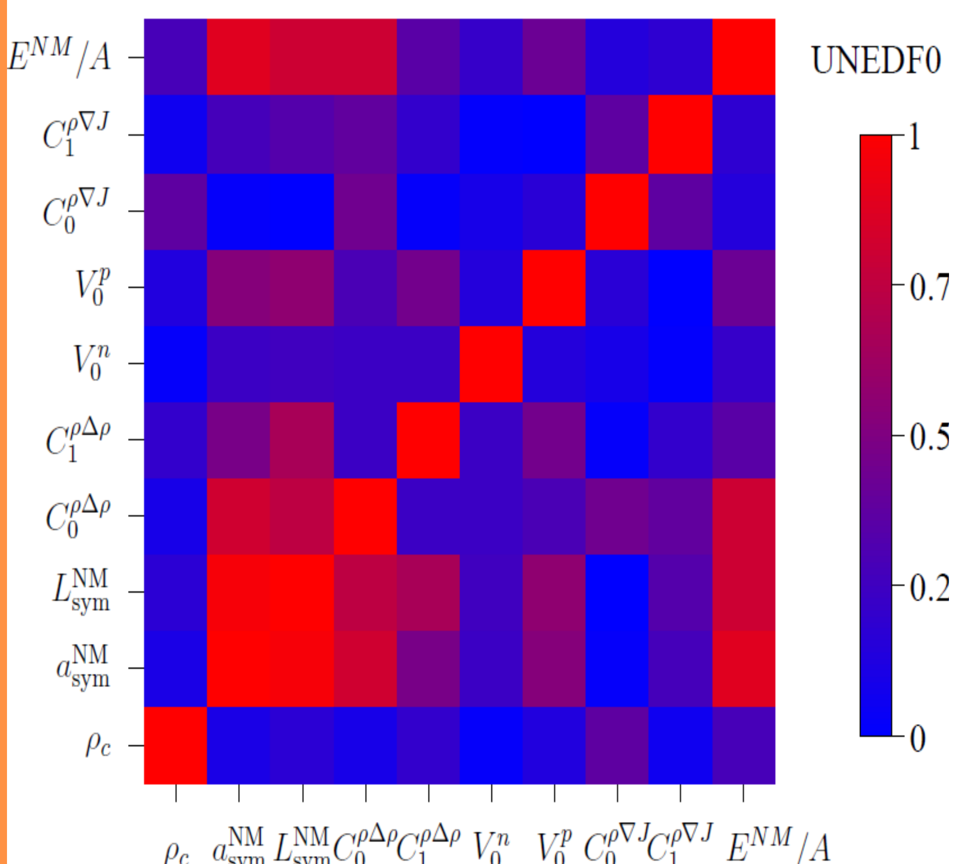


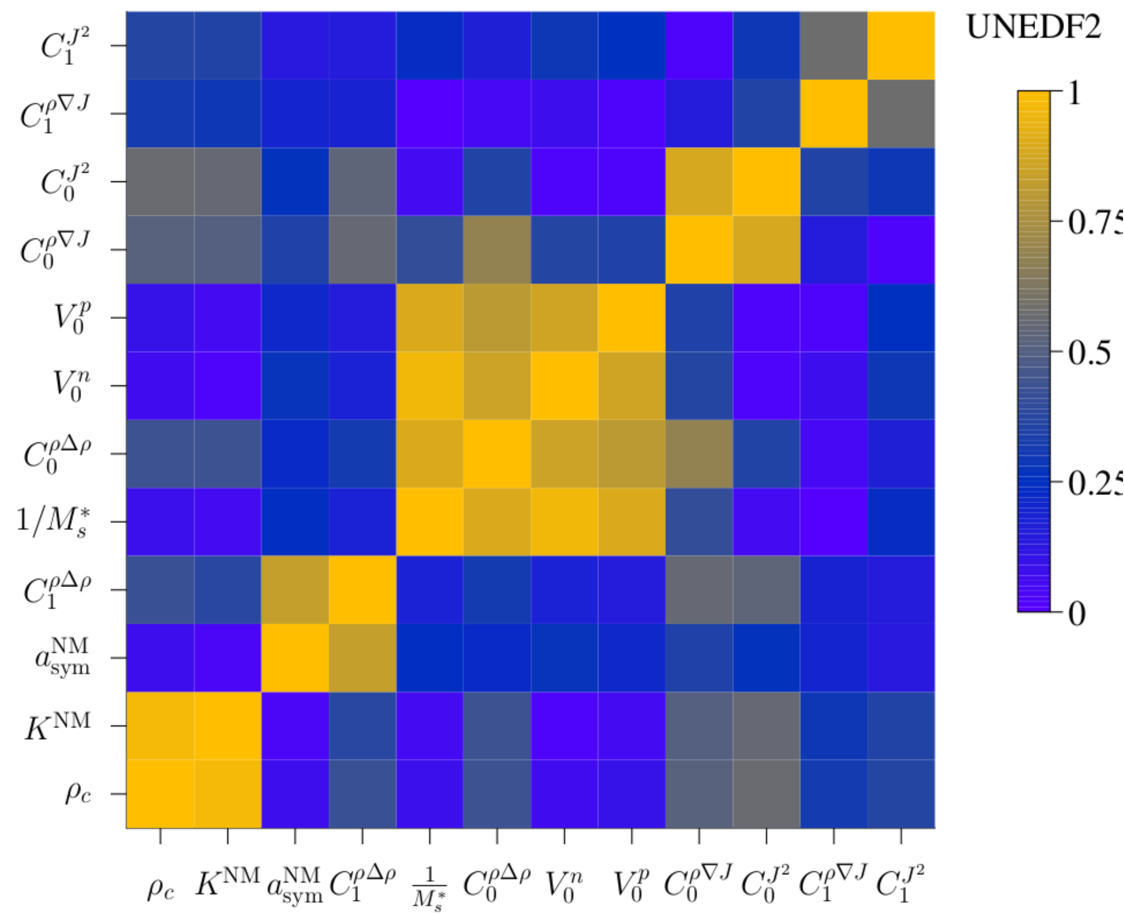




χ^2 and UNEDF0,2 correlation matrix

$$\chi^2(\mathbf{x}) = \frac{1}{n_d - n_x} \sum_{i=1}^{D_T} \sum_{j=1}^{n_i} \left(\frac{s_{i,j}(\mathbf{x}) - d_{i,j}}{w_i} \right)^2$$





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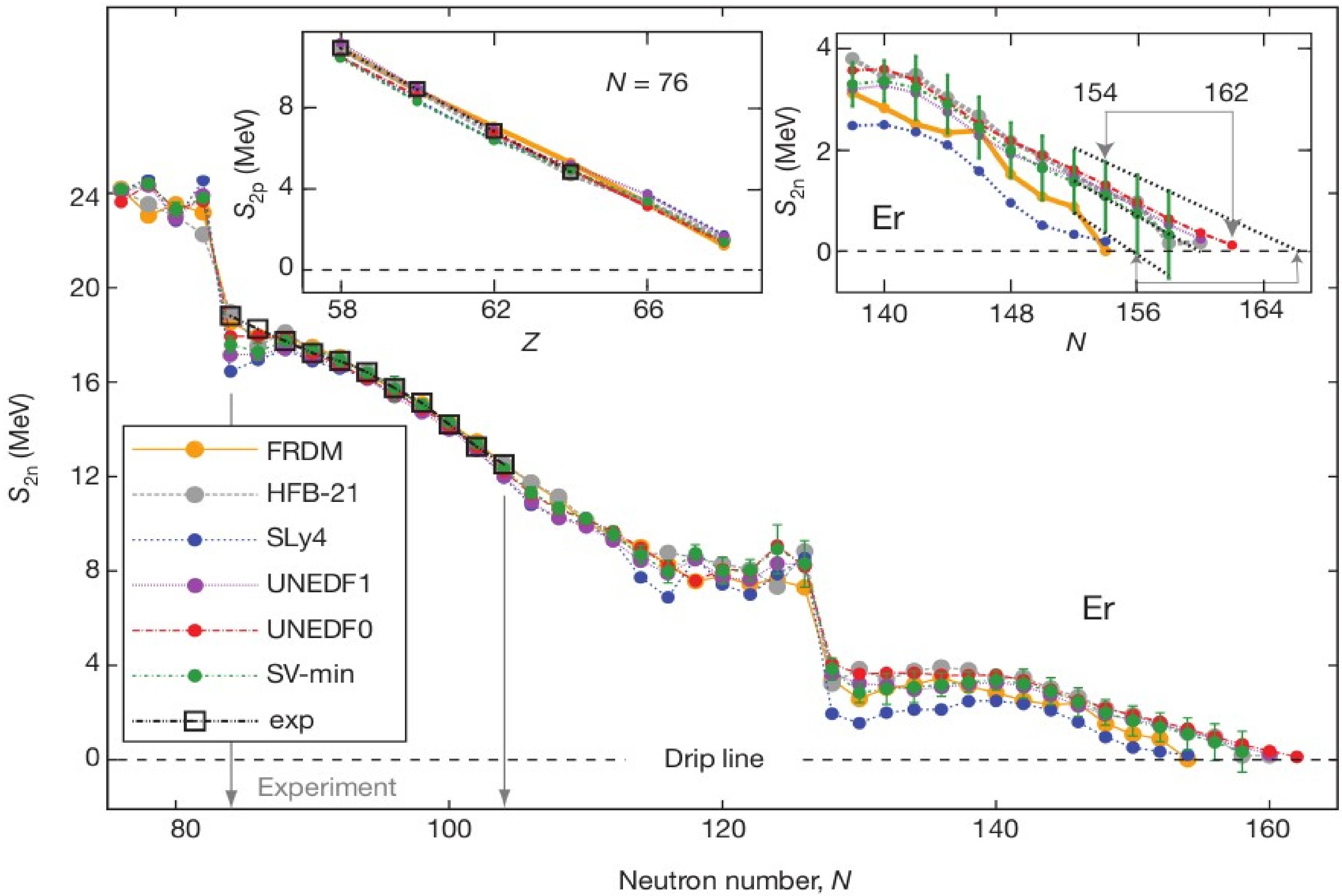

Uncertainties of neutron skin thickness

M.K., arXiv:1409.1413, to appear in JPhysG