Energy density optimization: UNEDF2

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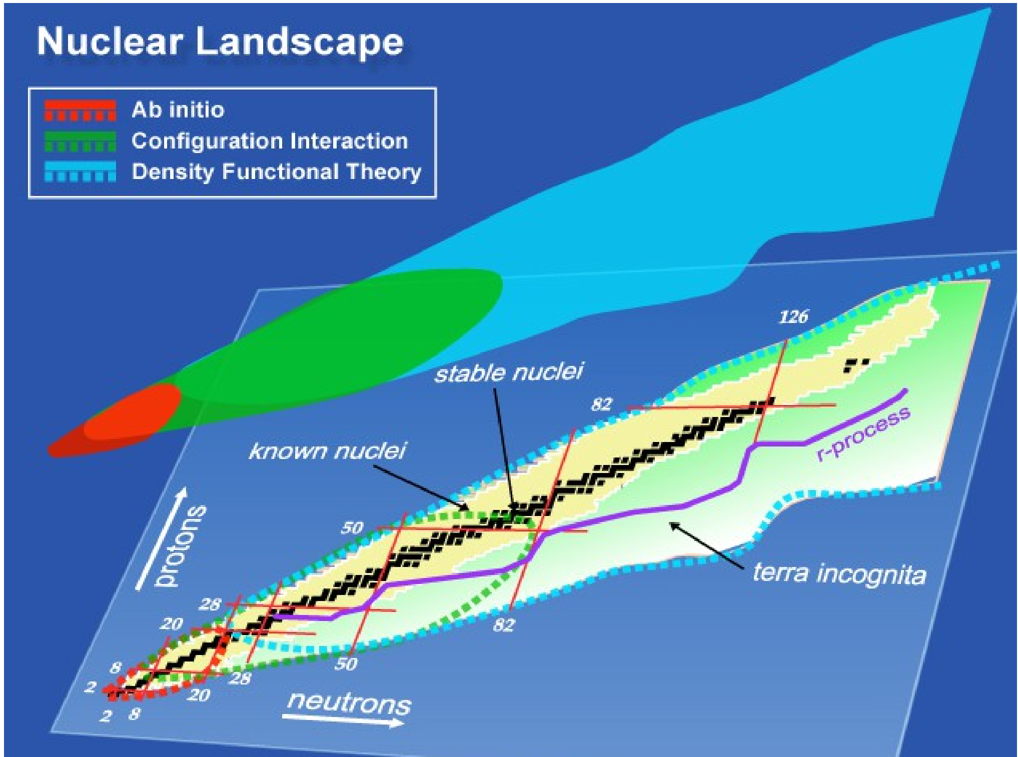
Skyrme energy density

$$H_t^{even}(r) = C_t^{\rho}\rho_t^2 + C_t^{\tau}\rho_t\tau_t + C_t^{\Delta\rho}\rho_t\Delta\rho_t + C_t^{\nabla J}\rho_t\nabla\cdot\boldsymbol{J}_t + C_t^{J}\mathrm{J}_t^2$$

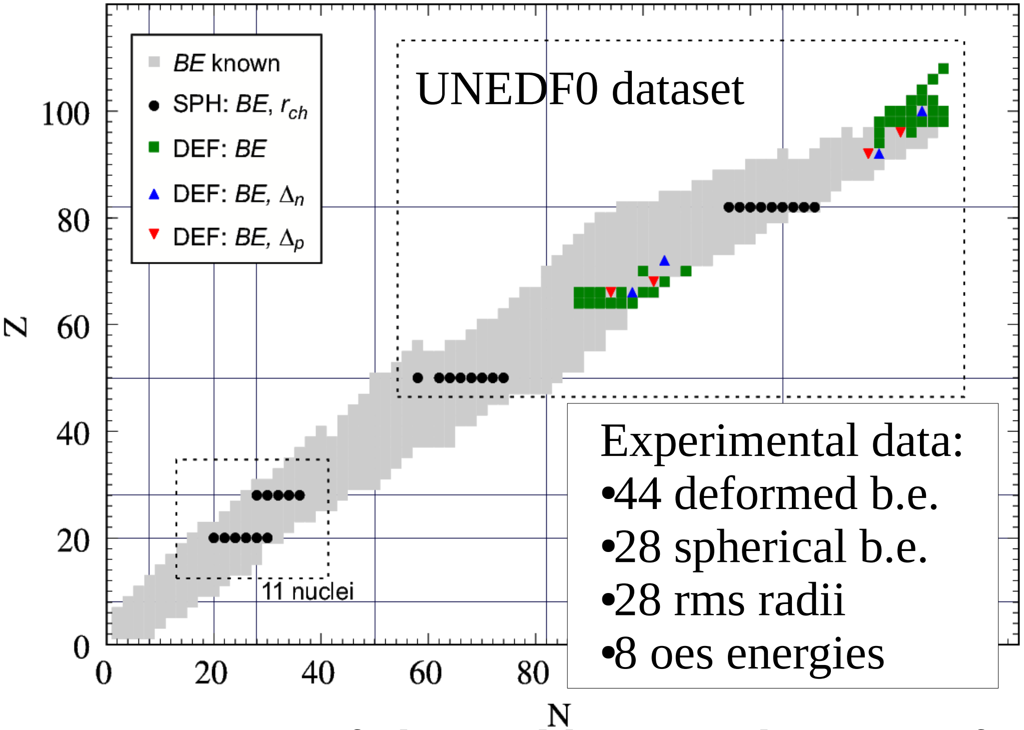
$$C_t^{\rho} = C_{t0}^{\rho} + C_{tD}^{\rho}\rho_0^{\gamma} \quad , \quad t=0,1$$

- Skyrme EDF is constructed from bilinear terms of density matrices and their derivatives up to the 2nd order
- Each term multiplied by a constant coupling constant (except density dependent C^{ρ})
- Volume part of the ED can be parameterized with infinite nuclear matter parameters
- Coupling constants adjusted to experimental input



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

Energy density optimization: UNEDF0 and UNEDF1

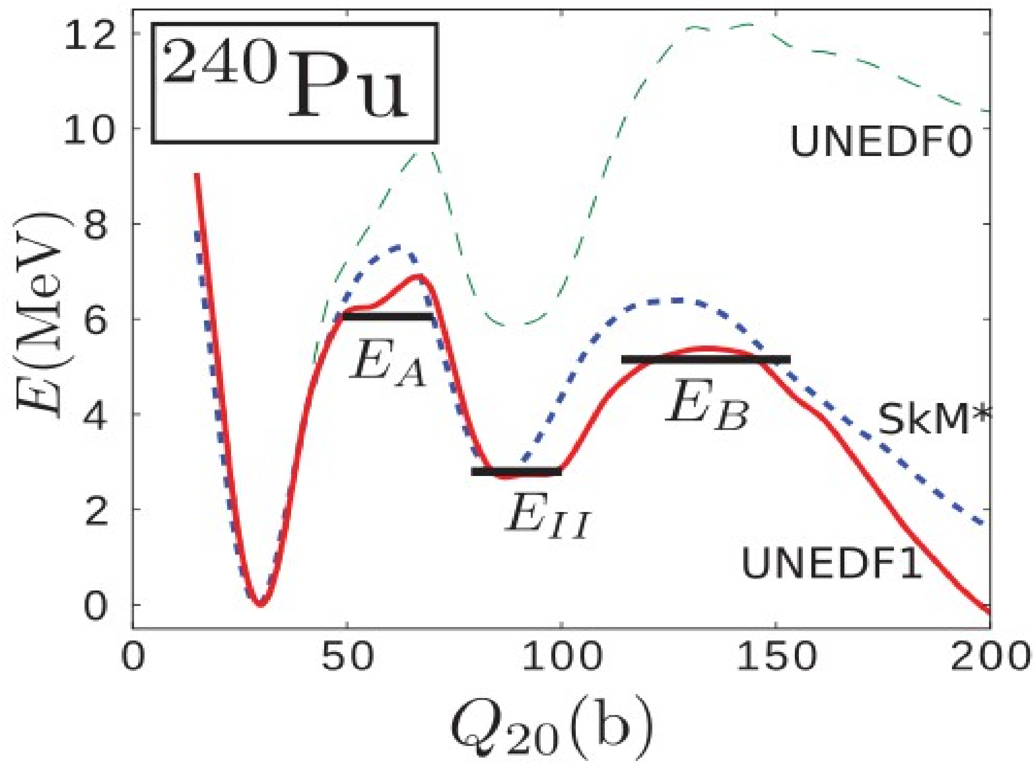


UNEDF0: M. K., T. Lesinski, J. Moré, W. Nazarewicz, J. Sarich, N. Schunck, M. V. Stoitsov, S. Wild, PRC 82, 024313 (2010)

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 deformed HFB level

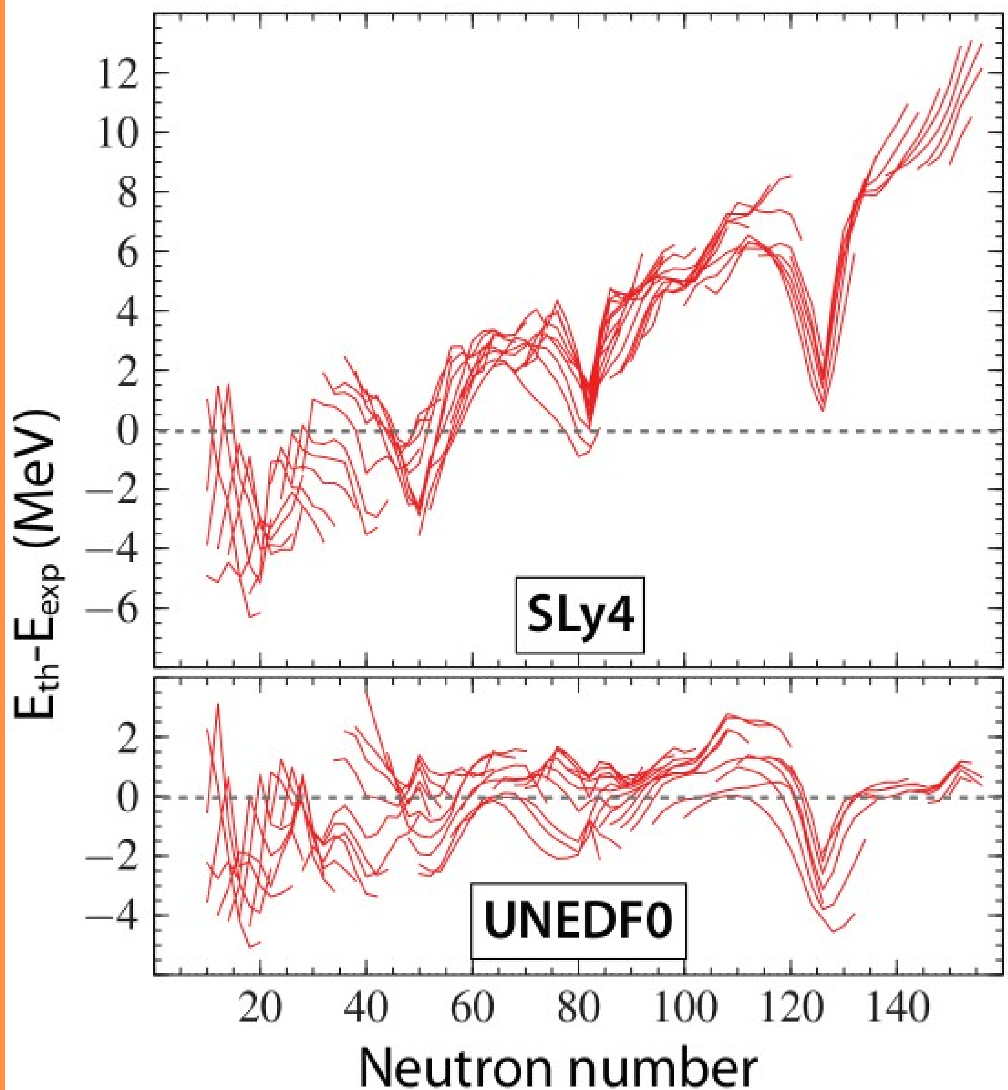
$$\rho_c, E^{NM}/A, K^{NM}, a^{NM}_{sym}, L^{NM}_{sym}, M_s^{-1}$$
$$C_0^{\rho\Delta\rho}, C_1^{\rho\Delta\rho}, V_0^n, V_0^p, C_0^{\rho\nabla J}, C_1^{\rho\nabla J}$$

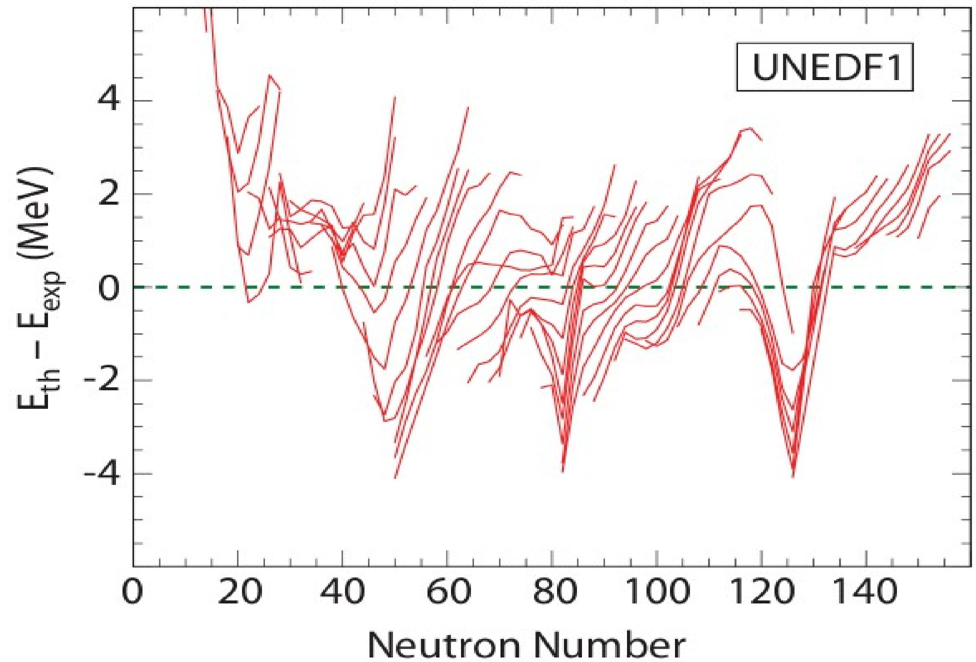


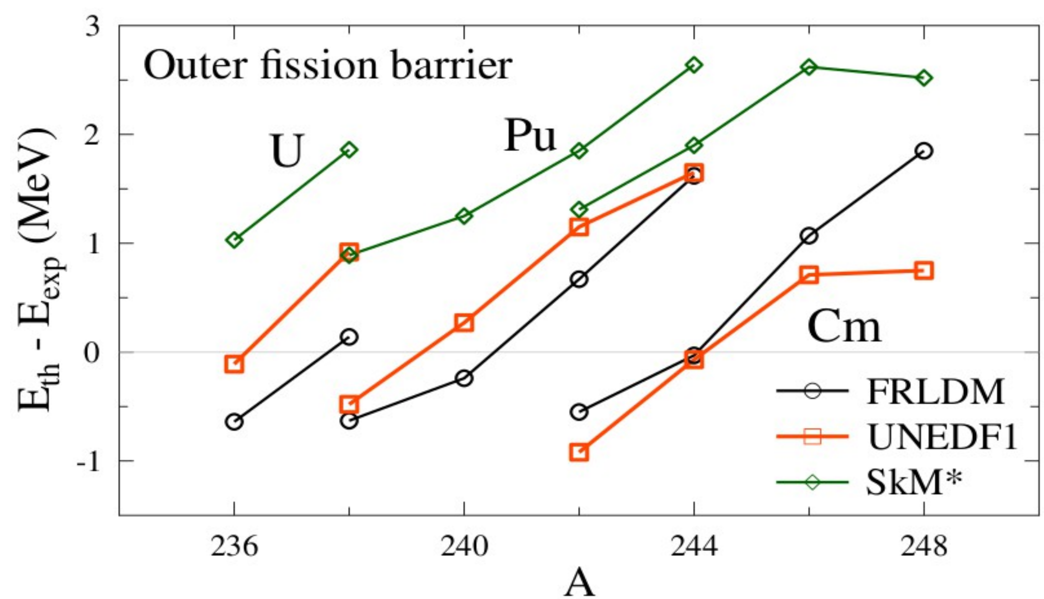
•UNEDF1 was the first parameterization which was systematically optimized at the deformed HFB level for fission studies

•UNEDF1 included data on 4 fission isomers states (^{226}U, ^{238}U, ^{240}Pu, ^{242}Cm)

UNEDF0 and UNEDF1: Performance







Energy density optimization: UNEDF2

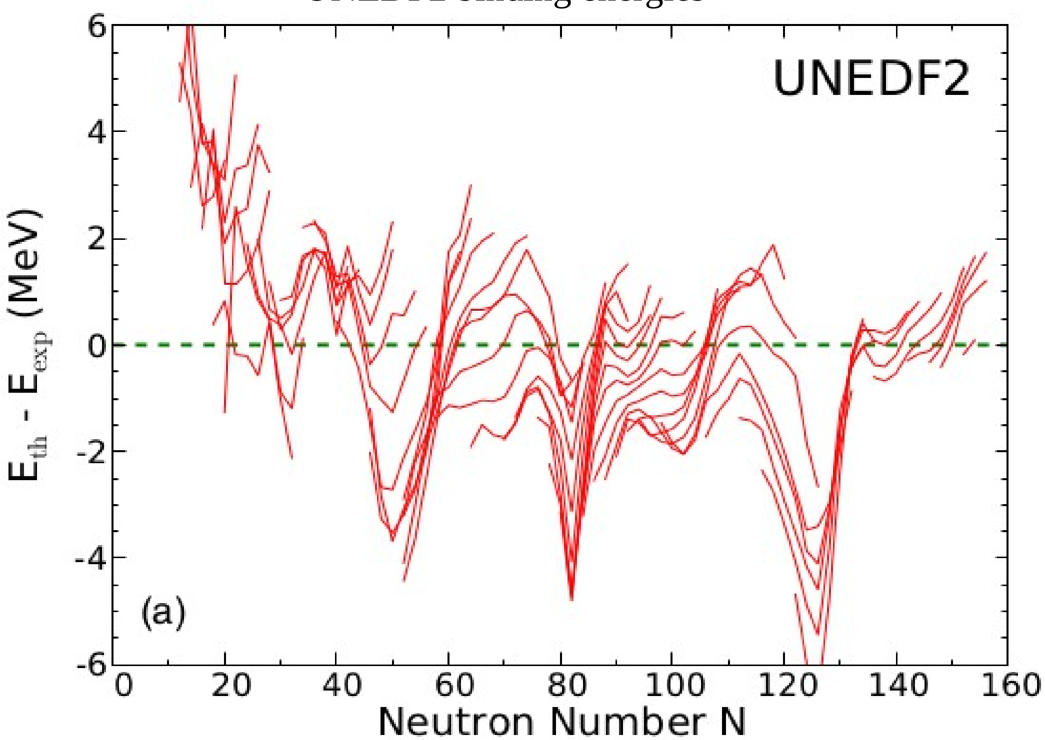
- Optimization of Skyrme-like ED with respect of 14 parameters at deformed HFB level: Tensor terms now included

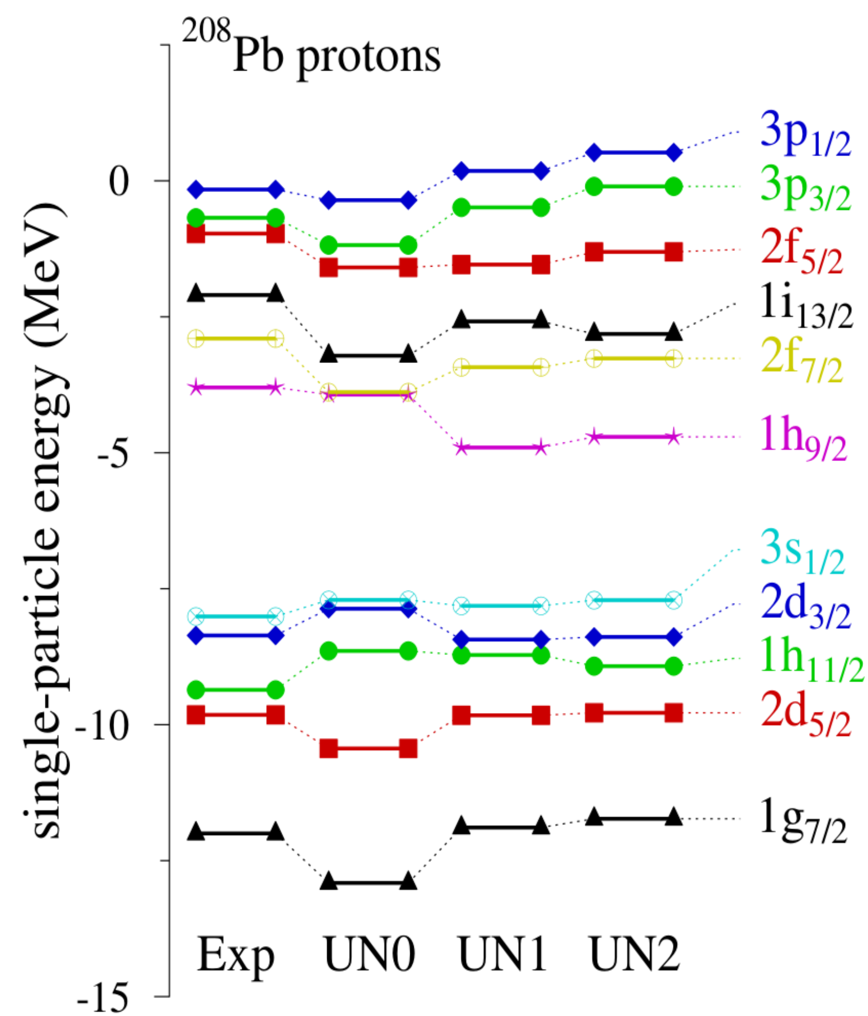
$$\rho_c, E^{NM}/A, K^{NM}, a_{sym}^{NM}, L_{sym}^{NM}, M_s^{-1}$$
$$C_0^{\rho\Delta\rho}, C_1^{\rho\Delta\rho}, V_0^n, V_0^p, C_0^{\rho\nabla J}, C_1^{\rho\nabla J}, \boxed{C_0^J, C_1^J}$$

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

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)

UNEDF2 binding energies

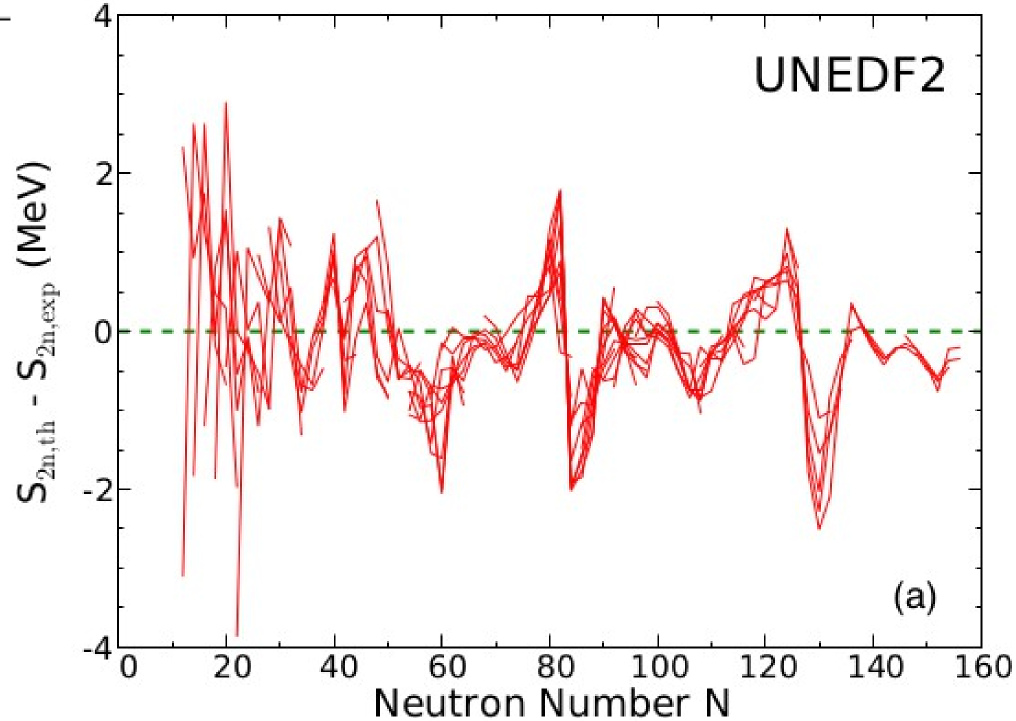




UNEDF2: Global properties

RMS deviations of various observables

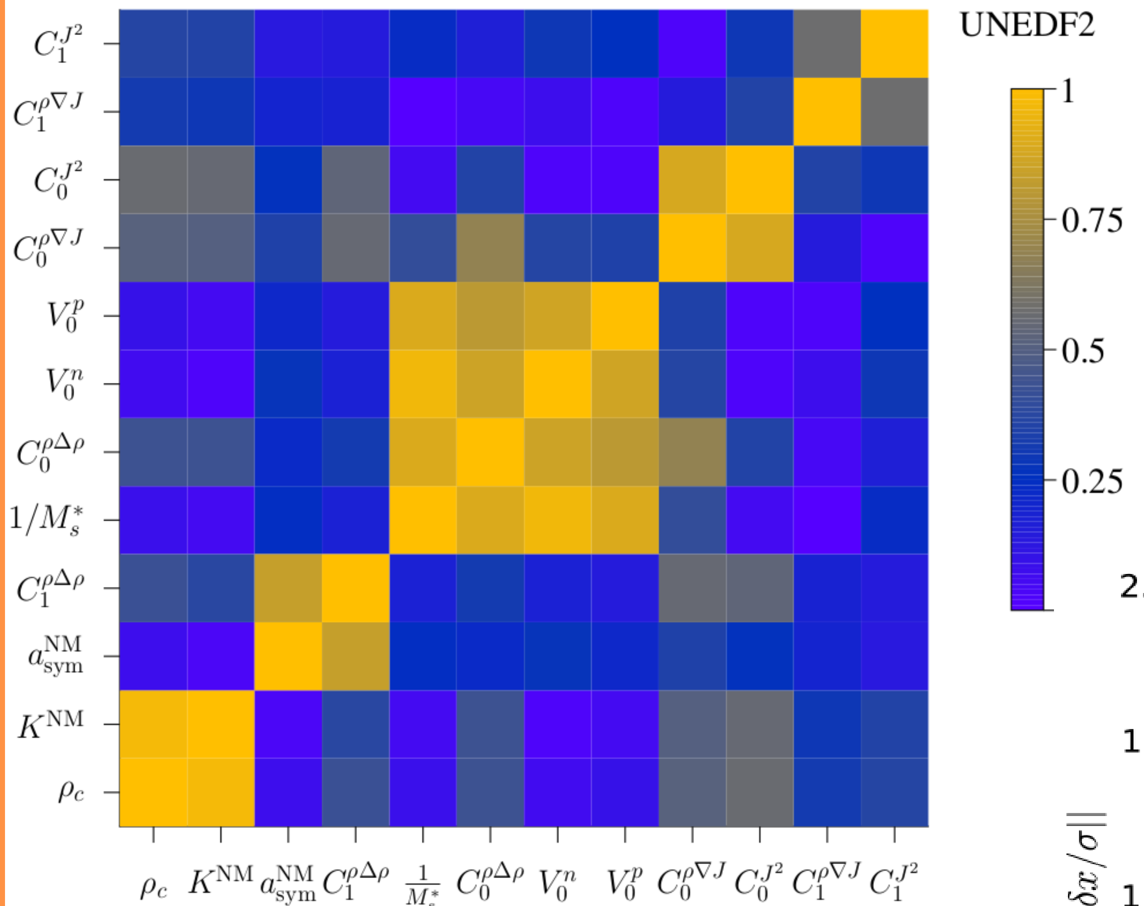
Observable	UNEDF0	UNEDF1	UNEDF2
E	1.428	1.912	1.950
E $(A < 80)$	2.092	2.566	2.475
E $(A \geqslant 80)$	1.200	1.705	1.792
S_{2n}	0.758	0.752	0.843
S_{2n} $(A < 80)$	1.447	1.161	1.243
S_{2n} $(A \geqslant 80)$	0.446	0.609	0.711
S_{2p}	0.862	0.791	0.778
S_{2p} $(A < 80)$	1.496	1.264	1.309
S_{2p} $(A \geqslant 80)$	0.605	0.618	0.572
$\tilde{\Delta}_n^{(3)}$	0.355	0.358	0.285
$\tilde{\Delta}_n^{(3)}$ $(A < 80)$	0.401	0.388	0.327
$\tilde{\Delta}_n^{(3)}$ $(A \geqslant 80)$	0.342	0.350	0.273
$\tilde{\Delta}_p^{(3)}$	0.258	0.261	0.276
$\tilde{\Delta}_p^{(3)}$ $(A < 80)$	0.346	0.304	0.472
$\tilde{\Delta}_p^{(3)}$ $(A \geqslant 80)$	0.229	0.248	0.194
R_p	0.017	0.017	0.018
R_p $(A < 80)$	0.022	0.019	0.020
R_p $(A \geqslant 80)$	0.013	0.015	0.017



•Generally, UNEDF2 gives no or only marginal improvement over to UNEDF1

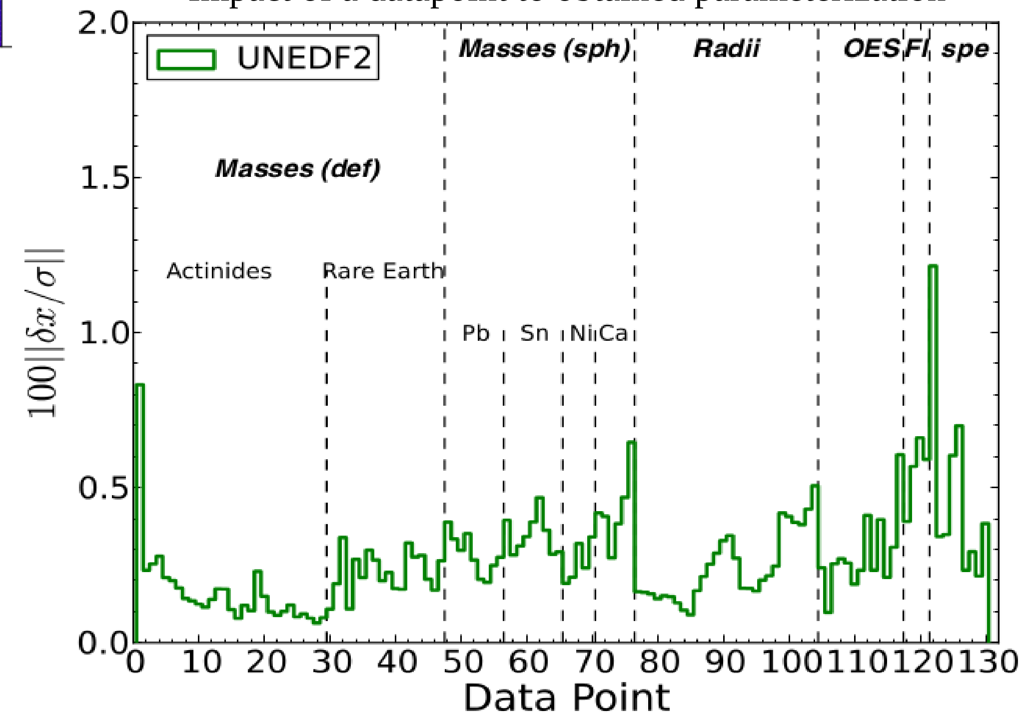
⇒ Novel EDF developments required to improve precision (see Jacek's talk)

Sensitivity analysis



- With UNEDF0,1 and 2, a complete sensitivity analysis was done for the obtained minimum
- Standard deviations and correlations of optimized EDF parameters
- Crucial information when addressing predictive power. E.g propagation of the error.

Impact of a datapoint to obtained parameterization



- Sensitivity analysis shows that UNEDF2 fully constrained with the data
  - $\Rightarrow$ Major improvements not possible in the Skyrme-EDF framework

Conclusions and outlook

- UNEDF0, 1 and 2 presents a optimization scheme of Skyrme-like EDF, which includes progressively more experimental data.
- Many UNEDF2 properties sligthly worse than with more specialiced UNEDF0 or UNEDF1. UNEDF2 is the best all-around Skyrme EDF
- Sensitivity analysis shows that further major improvements for UNEDF2 are unlikely
- Generally, limits of the Skyrme-like EDF models have been reached: Novel EDFs required to improve precision. This conclusion is also supported by several other studies.

- Possible future directions: EDFs with higher order derivatives, DME-based functionals, regularized higher-order functionals.
- Future EDF optimizations schemes should include sensitivity analysis to assess the predictive power of the model

Backup slides

UNEDF parameters

x	SLy4	UNEDF0	UNEDF1	UNEDF2
ρ_c	0.16000	0.16053	0.15871	0.15631
E/A	−15.972	−16.056	−15.8	−15.8
K	229.901	230.0	220.0	239.930
a_{sym}	32.004	30.543	28.987	29.131
L	45.962	45.080	40.005	40.0
$1/M_s^*$	1.439	0.9	0.992	1.074
$C_0^{\rho\Delta\rho}$	−76.996	−55.261	−45.135	−46.831
$C_1^{\rho\Delta\rho}$	+15.657	−55.623	−145.382	−113.164
V_0^n	−258.200	−170.374	−186.065	−208.889
V_0^p	−258.200	−199.202	−206.580	−230.330
$C_0^{\rho\nabla J}$	−92.250	−79.531	−74.026	−64.309
$C_1^{\rho\nabla J}$	−30.750	45.630	−35.658	−38.650
C_0^{JJ}	0.000	0.000	0.000	−54.433
C_1^{JJ}	0.000	0.000	0.000	−65.903

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]

UNEDF properties