UNEDF EDFs and their uncertainty propagation

Bridging nuclear ab-initio and energy-density-functional theories, Orsay 2-6 Oct., 2017

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Nuclear DFT

- The nuclear DFT is the only microscopic theory which can be applied throughout the entire nuclear chart
- Within the superfluid nuclear DFT, one needs to solve the Hartree-Fock-Bogoliubov (HFB) equation:

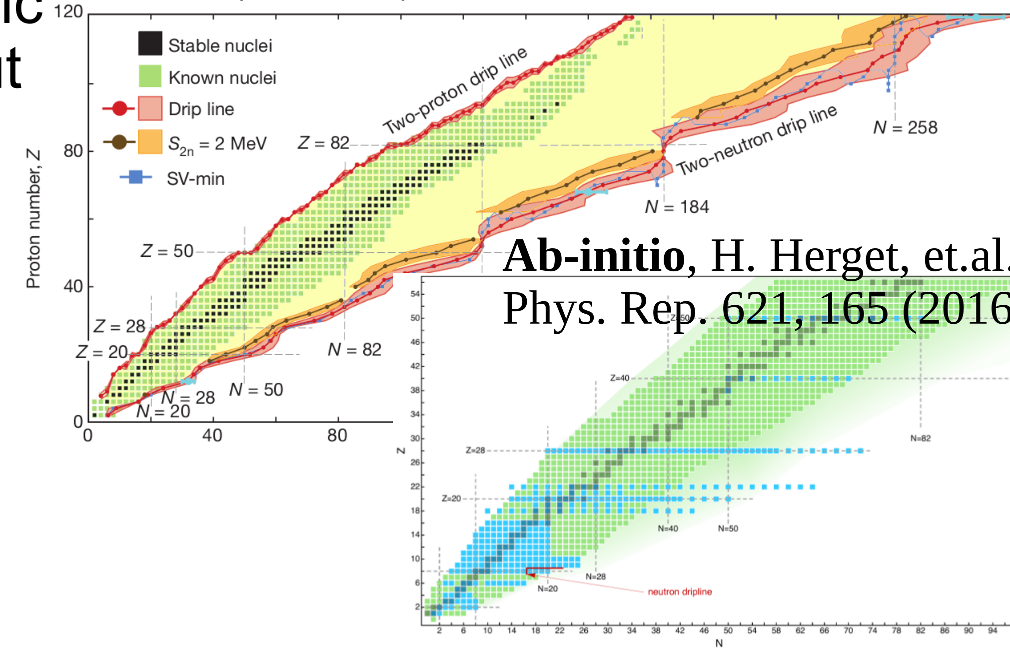
$$\begin{pmatrix} h-\lambda & \Delta \\ -\Delta^{*} & -h^{*}+\lambda \end{pmatrix}\begin{pmatrix} U_n \\ V_n \end{pmatrix} = E_n \begin{pmatrix} U_n \\ V_n \end{pmatrix}$$

- By solving this equation, we obtain the quasiparticle energies E_n and the matrices U and V which determine the generalized Bogoliubov quasiparticle transformation:

$$\hat{b}_{\alpha}^{\dagger} = \sum_{\beta} \left(U_{\beta\alpha} \hat{c}_{\beta}^{\dagger} + V_{\beta\alpha} \hat{c}_{\beta} \right)$$

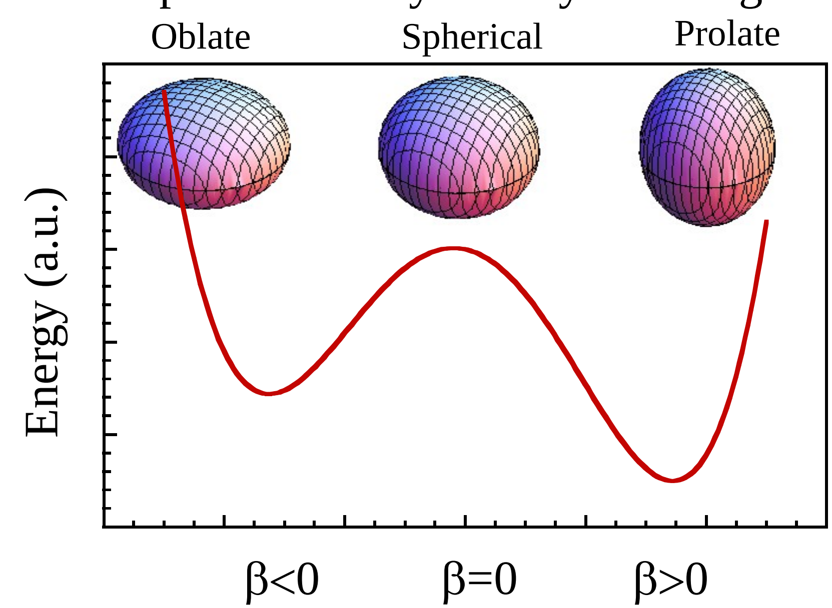
- Introduction correlations effectively via spontaneous symmetry breaking

DFT, J. Erler, et.al 2012



Ab-initio, H. Herget, et.al., Phys. Rep. 621, 165 (2016)

Spontaneous symmetry breaking



Skyrme EDF

- The key ingredient of the nuclear DFT is the nuclear energy density functional (EDF)
- The EDF incorporates complex many-body correlations within the energy density constructed from the nucleon densities and currents
- Currently there are three major EDF variants in the market: Skyrme, Gogny and relativistic mean-field models. All of these contain a set of parameters which needs to be adjusted to empirical input
- Time-even and time-odd parts of the Skyrme EDF reads as

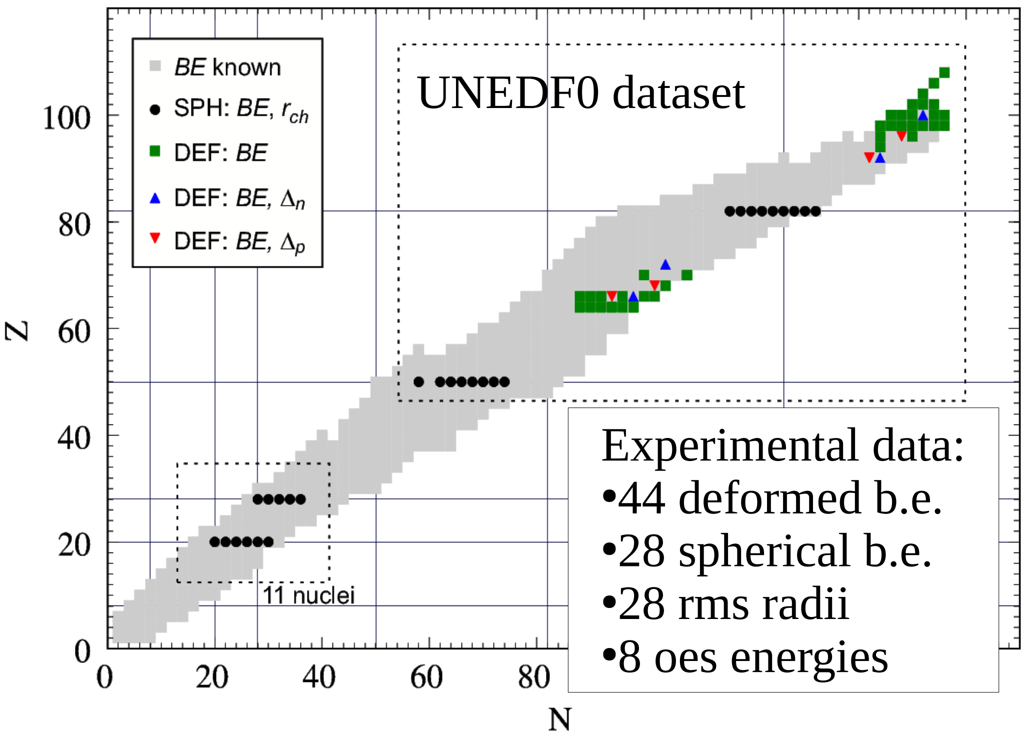
$$E_t^{even}(\boldsymbol{r}) = C_t^{\rho}\rho_t^2 + C_t^{\tau}\rho_t\tau_t + C_t^{\Delta\rho}\rho_t\Delta\rho_t + C_t^{\nabla J}\rho_t\nabla\cdot\boldsymbol{J}_t + C_t^{J}J_t^2$$

$$E_t^{odd}(\boldsymbol{r}) = C_t^{s}\boldsymbol{s}_t^2 + C_t^{j}\boldsymbol{j}_t^2 + C_t^{\Delta s}\boldsymbol{s}_t\cdot\Delta\boldsymbol{s}_t + C^{\nabla j}\boldsymbol{s}_t\cdot\nabla\times\boldsymbol{j}_t + C^{T}\boldsymbol{s}_t\cdot\boldsymbol{T}_t$$

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

- Skyrme EDF is constructed from local densities ($\rho,\tau,\boldsymbol{J},\boldsymbol{s},\boldsymbol{j},\boldsymbol{T}$) (and their derivatives), and coupling constants multiplying each term
- For the HFB ground state of even-even nucleus, only time-even part contributes. For excited states, both parts are active

Energy density optimization: UNEDF0 and UNEDF1



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

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

•UNEDF0 input data consisted of masses of deformed and spherical nuclei, charge radii, and pairing gaps

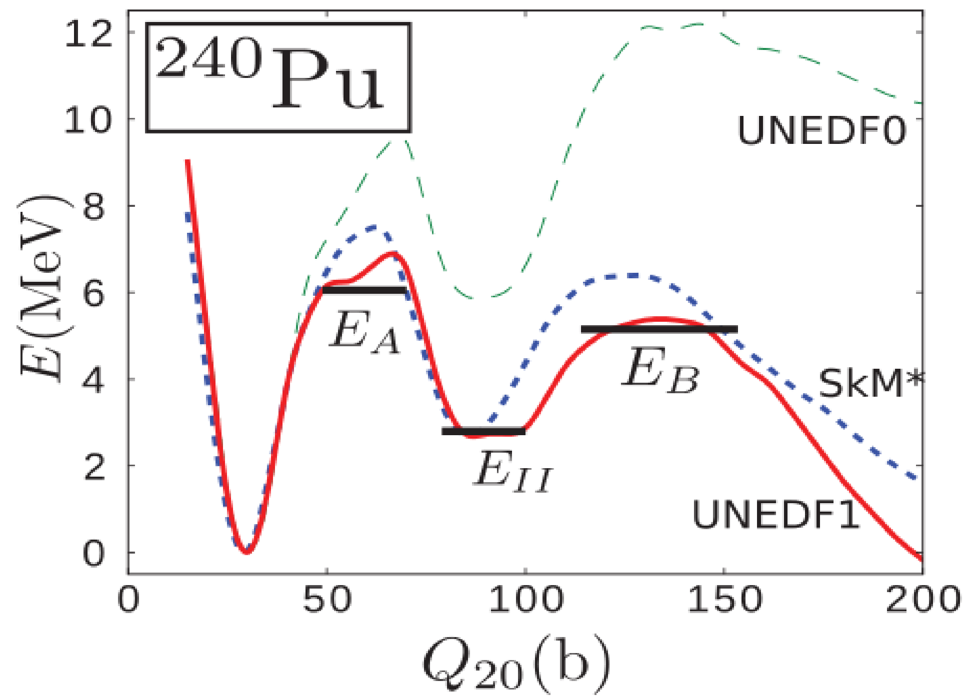
•Only time-even part of the EDF was adjusted for all UNEDF's

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)

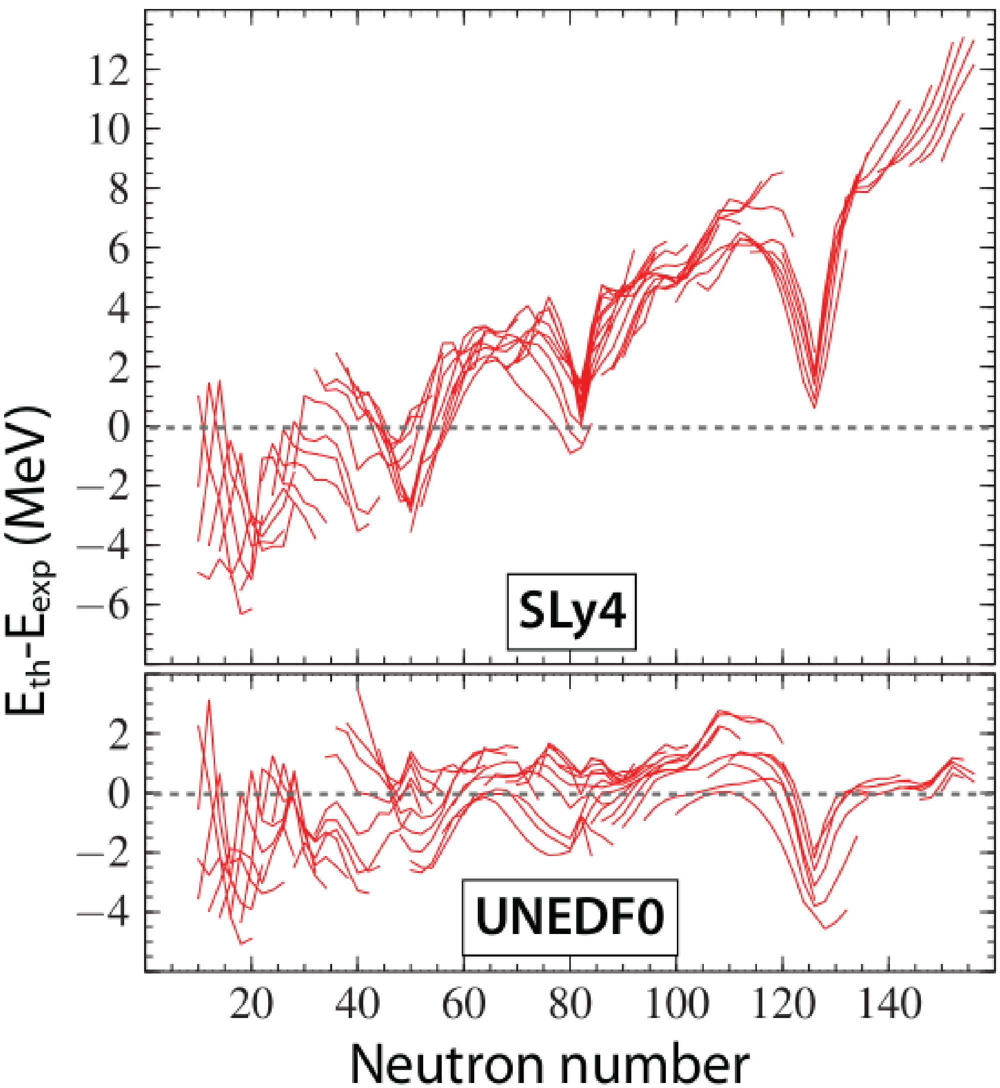
•UNEDF1 was the first parameterization which was systematically optimized at the deformed HFB level for fission studies

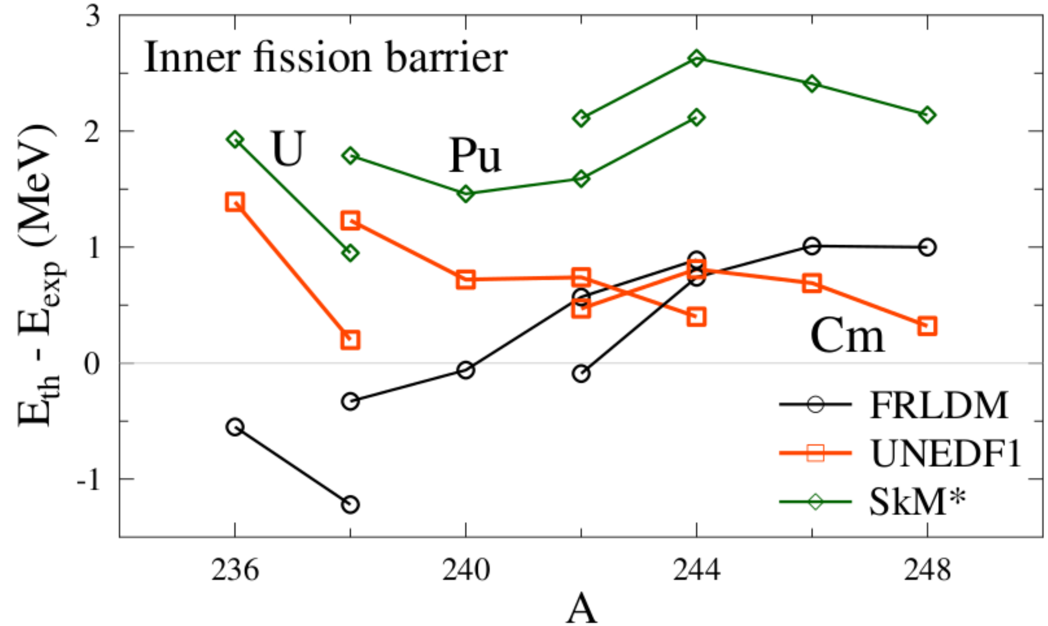
•UNEDF1 included data on 4 fission isomers states (^{226}U, ^{238}U, ^{240}Pu, ^{242}Cm), in addition to UNEDF0 data set

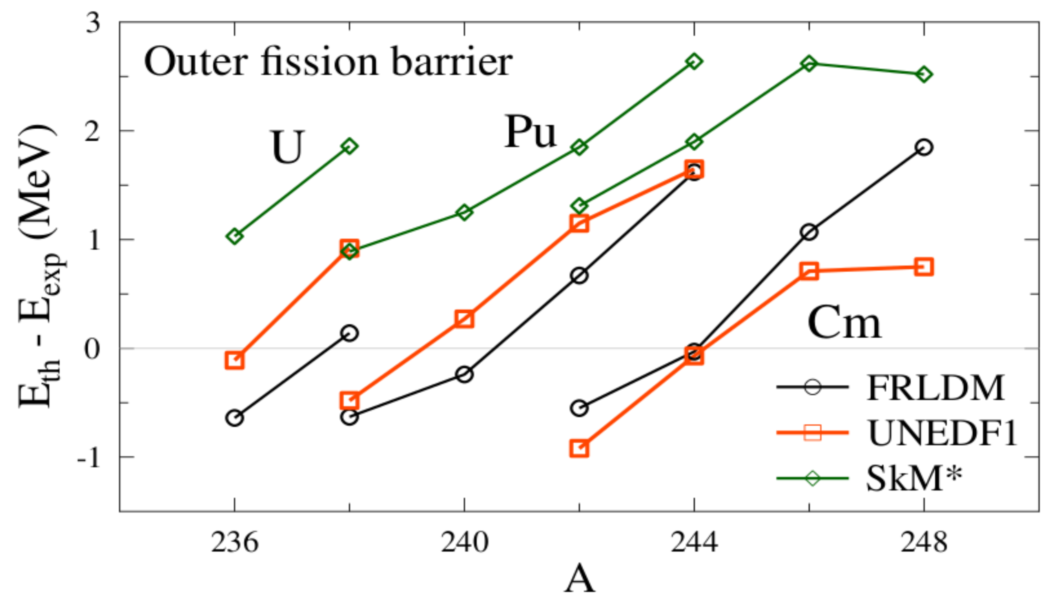


Energy density optimization: UNEDF0 and UNEDF1

- UNEDF0 reproduces masses at level of rmsd 1.4 MeV (UNEDF1: 1.9 MeV)
- UNEDF1 reproduces actinide fission barriers better than SkM*







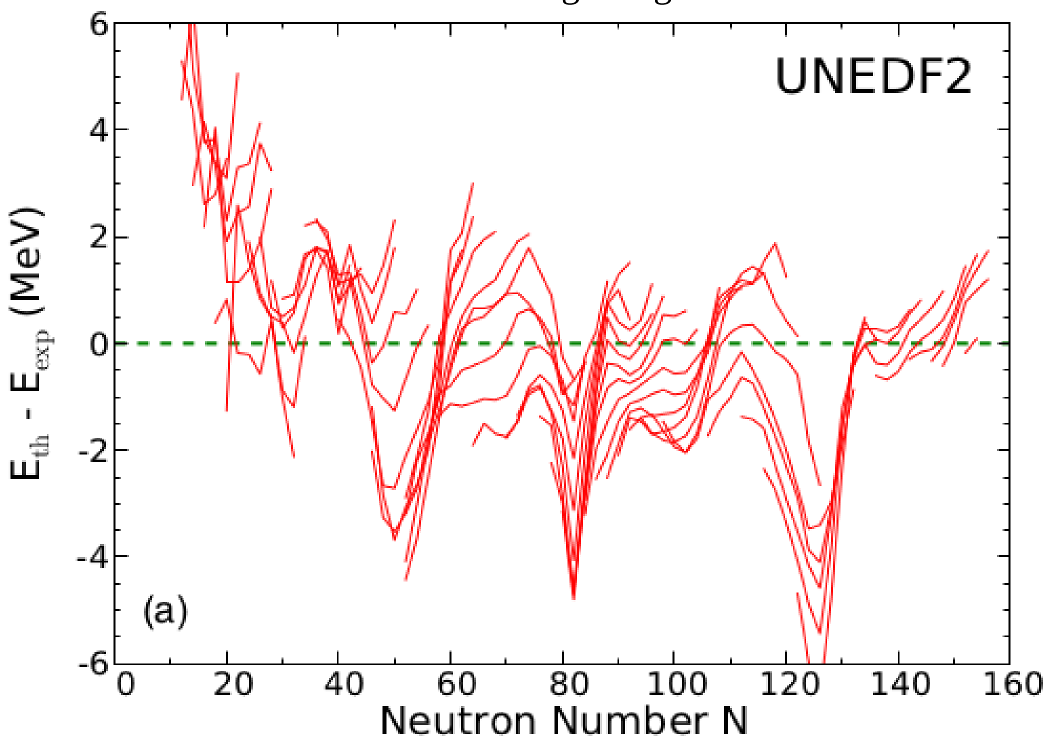
Energy density optimization: UNEDF2

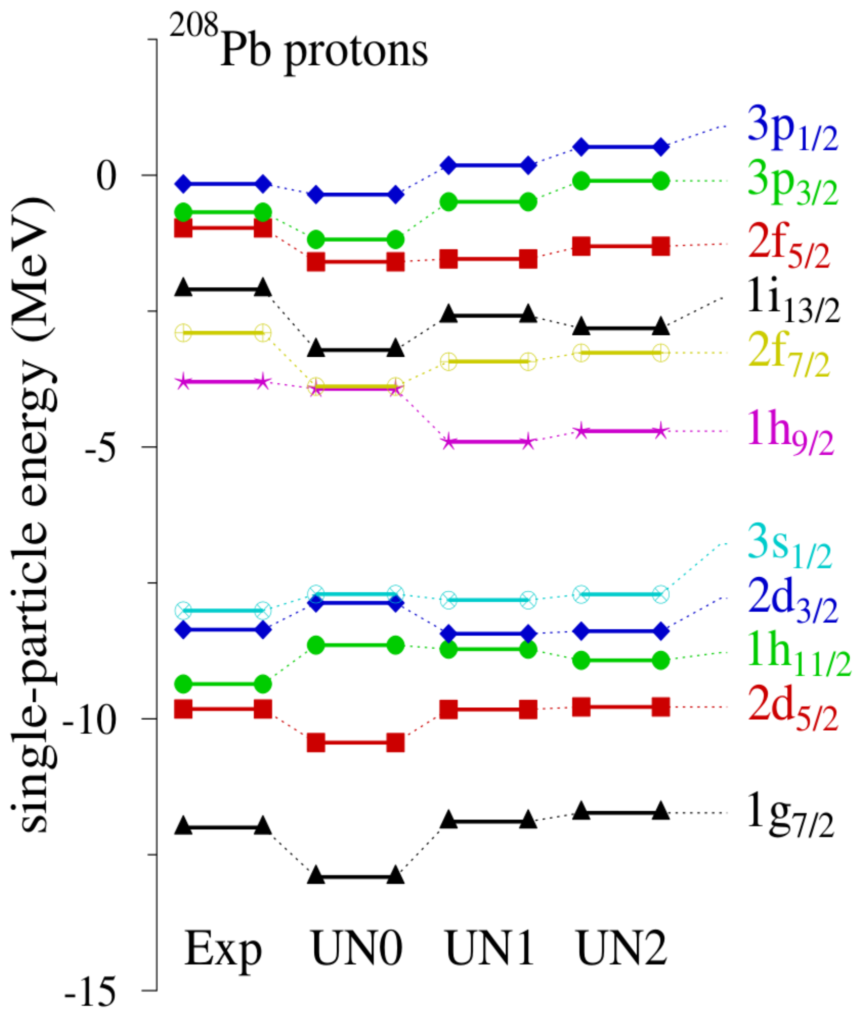
- Optimization of Skyrme-like ED with respect of 14 parameters at deformed HFB level: Tensor terms now included

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

- Focus on shell structure: Single particle energies included in the optimization. These are handled with blocked HFB calculations

UNEDF2 binding energies





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)

Performance of UNEDF EDFs

RMS deviations of various observables (in units of MeV or fm)

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

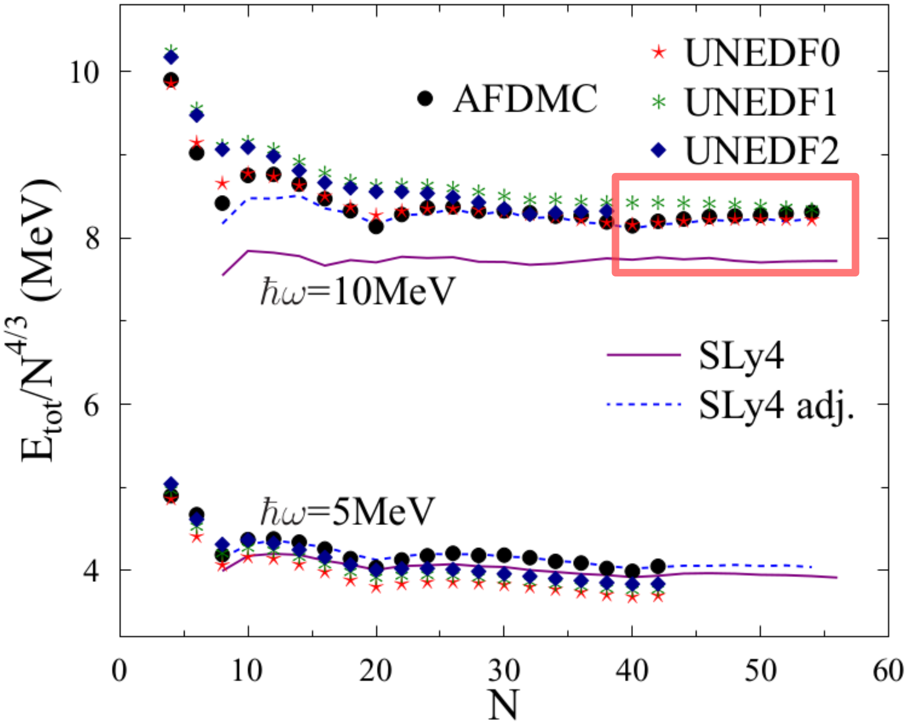
RMS deviations of single particle energies (in MeV)

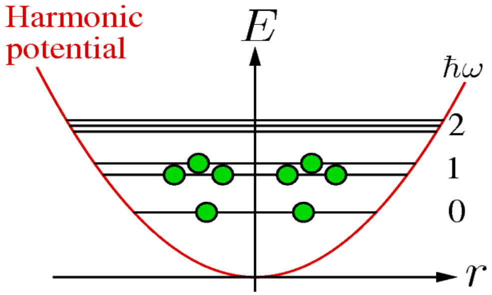
Nuclei	UNEDF0	UNEDF1	UNEDF2
All	1.42	1.38	1.38
Light	1.80	1.72	1.74
Heavy	0.94	0.97	0.95

(best attainable RMS deviation for Skyrme s.p. energies is around 1.1-1.2 MeV)

- Generally, UNEDF2 gives no or only marginal improvement over to UNEDF1
  $\Rightarrow$ Novel EDF developments required to improve precision

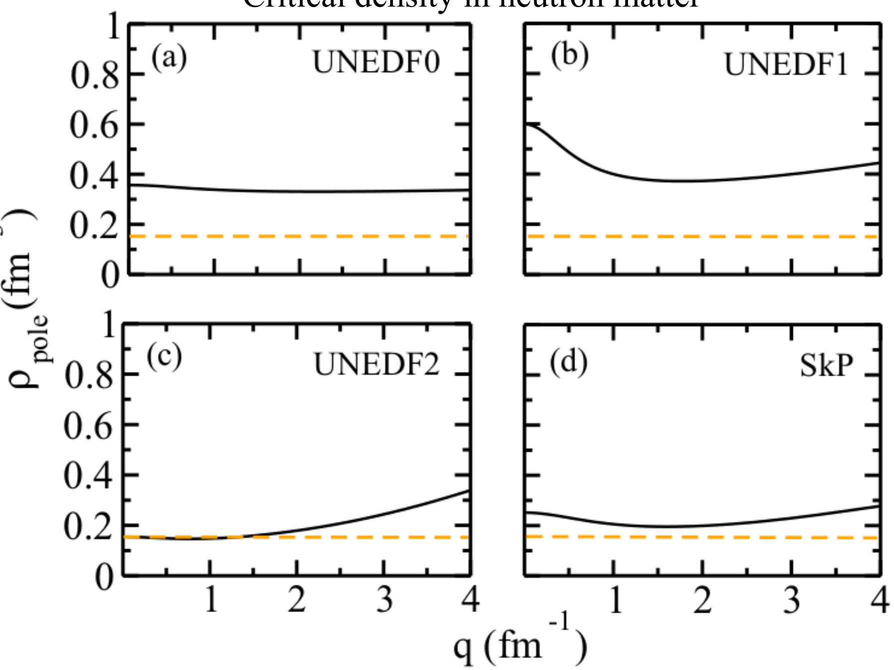
Neutron droplets



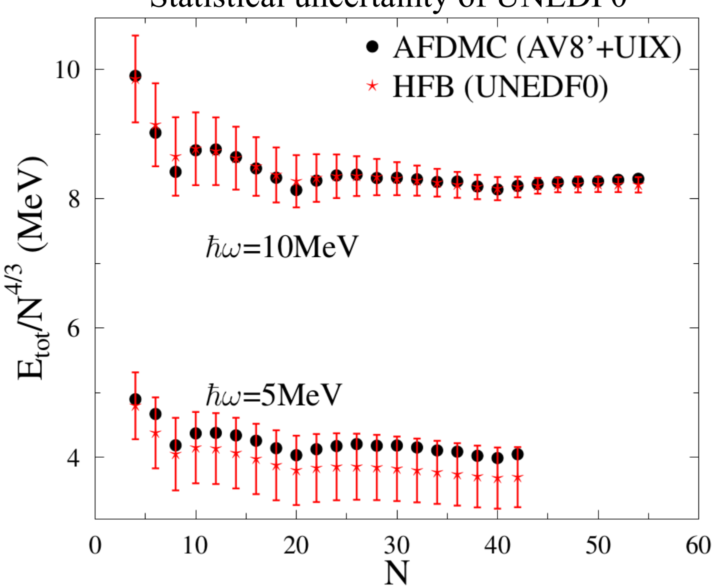


- Neutron droplets offer an ideal test environment to test EDF properties in inhomogeneous neutron matter
- UNEDF0,1,2 results follow quite closely earlier AFDMC results (S. Gandolfi et.al., PRL106, 012501 (2011))
- With UNEDF2 neutron matter instability around density of 0.16 fm^{-3} shows up with higher particle number. This prevents HFB calculation
- Instability diagnostics important in novel EDF development

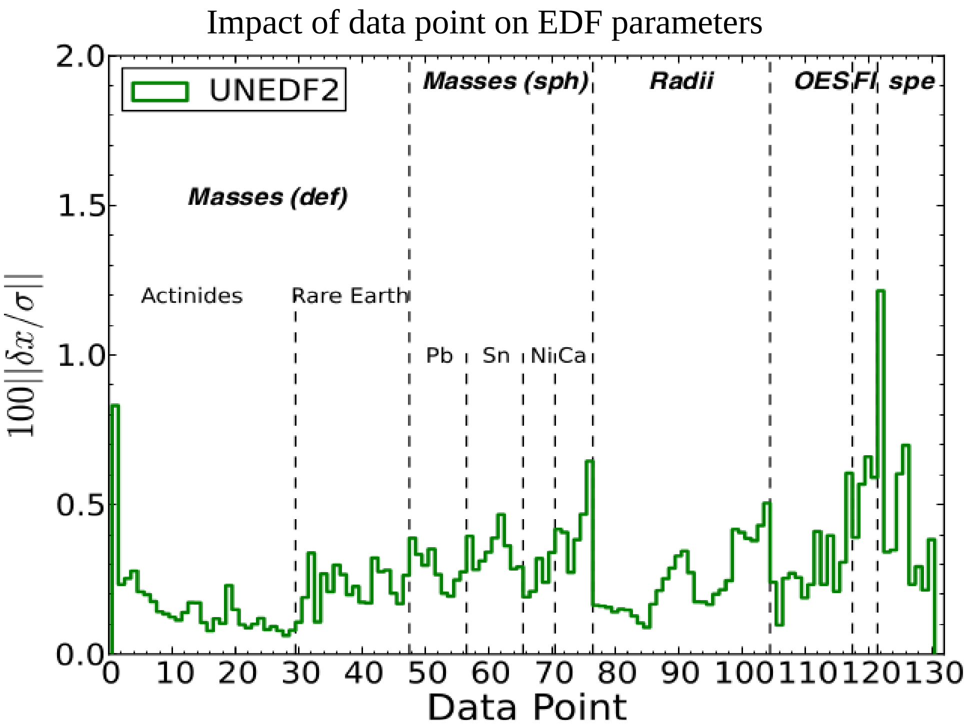
Critical density in neutron matter

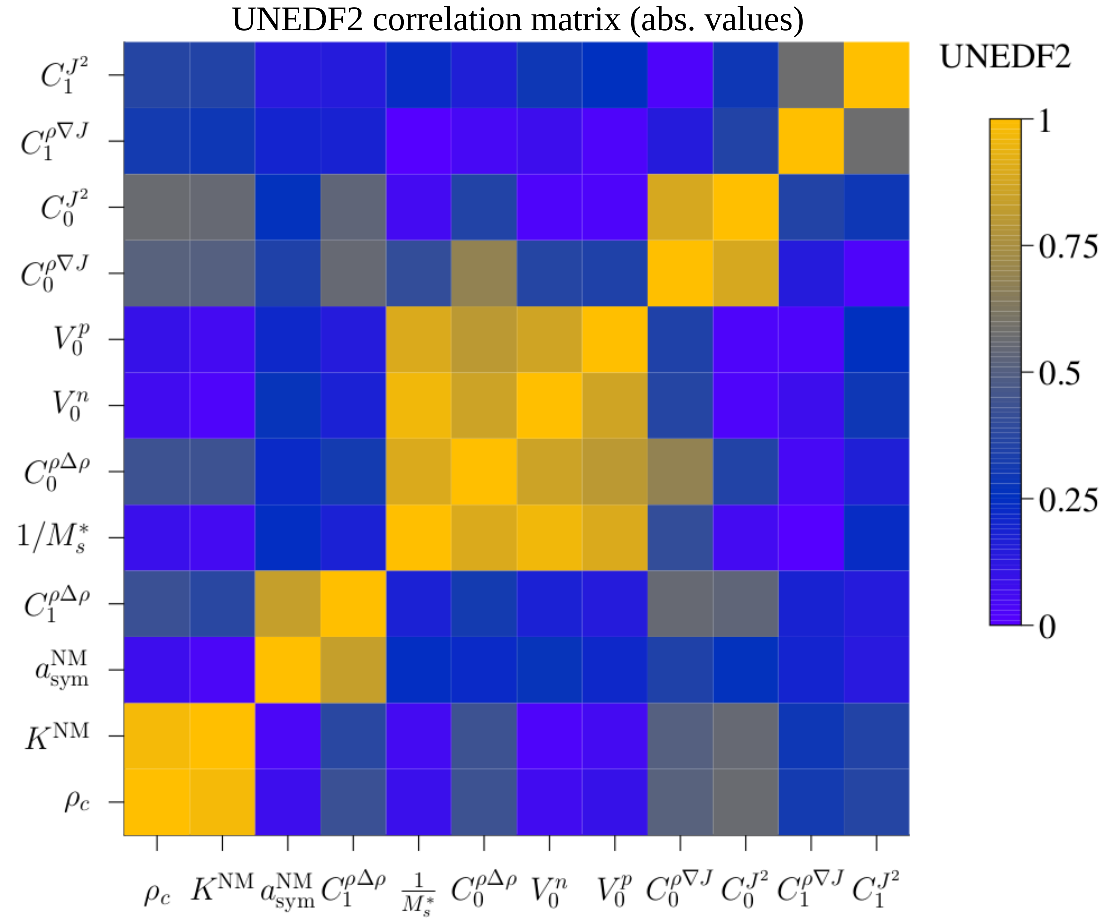


Statistical uncertainty of UNEDF0



Sensitivity analysis





- With UNEDF0,1 and 2, a complete sensitivity analysis was done for the obtained χ^2 minimum, providing standard deviations and correlations of the model parameters
- Sensitivity analysis can also tell what is the impact of given data point to the position of minimum
- During UNEDF EDF optimization, parameters had certain boundary values
- If model parameter must stay within some bounds, and these bounds do not include χ^2 minimum, sensitivity analysis can not be done for this parameter
- May have impact when computing error propagation for various observables

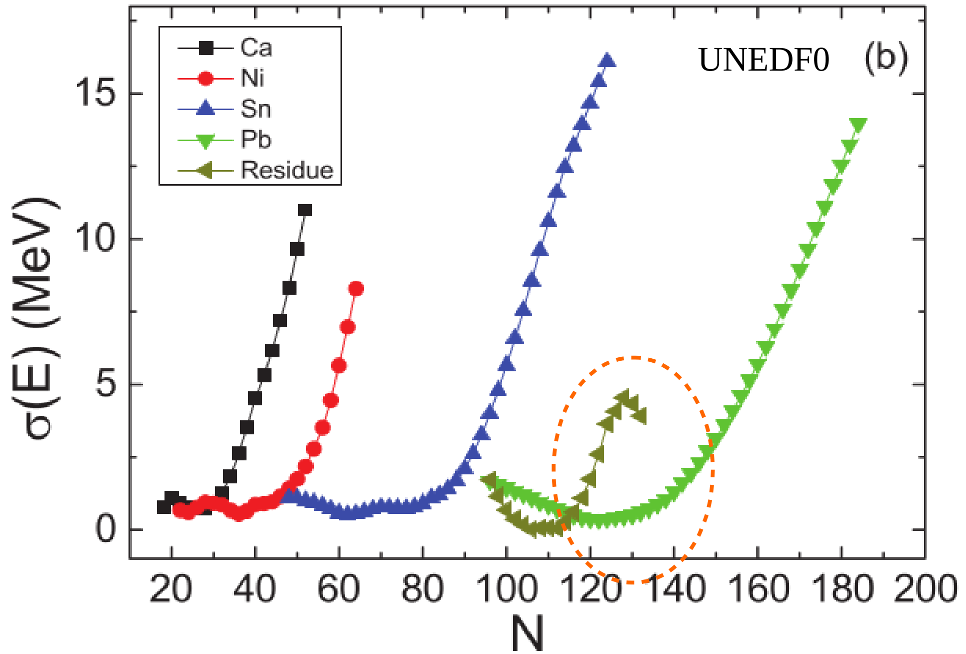
Uncertainty quantification

- Uncertainty quantification allows to assess predictive power of the model, i.e. how much can we trust predicted quantities
- Statistical error of some observable *y* can be calculated by using the covariance matrix of the model

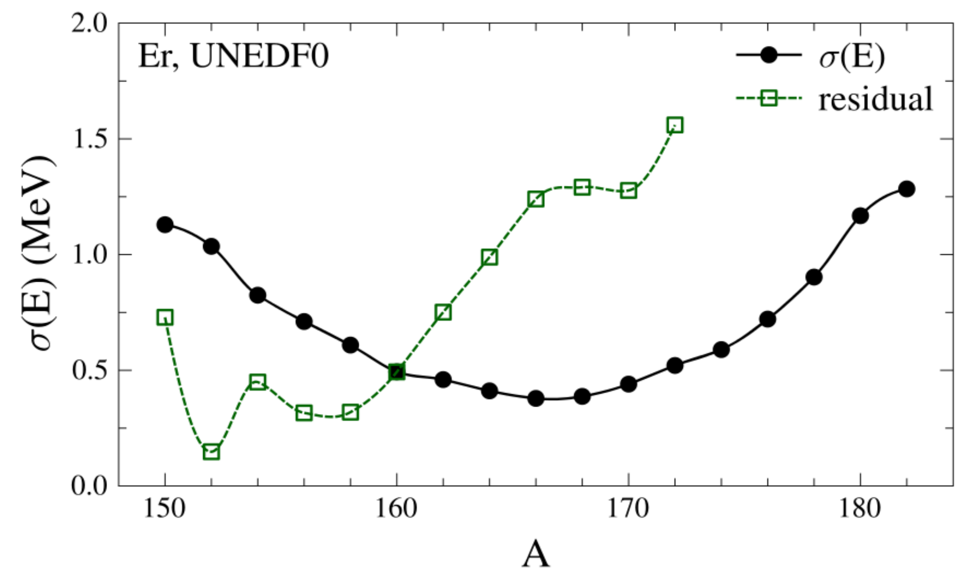
$$\sigma_y^2 = \sum_{i,j} \mathrm{Cov}(x_i, x_j) \left[\frac{\partial y}{\partial x_i} \frac{\partial y}{\partial x_j} \right]$$

- For some of the binding energies, statistical error is significantly smaller compared to residue from experimental data
  - Indication of deficiency of the model
  - "Model is blind to its own shortcomings"
- General trend is that propagated error increases sharply towards neutron rich nuclei: Badly constrained isovector part of the EDF
- Another uncertainty component is the systematic error. Much harder to quantify

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

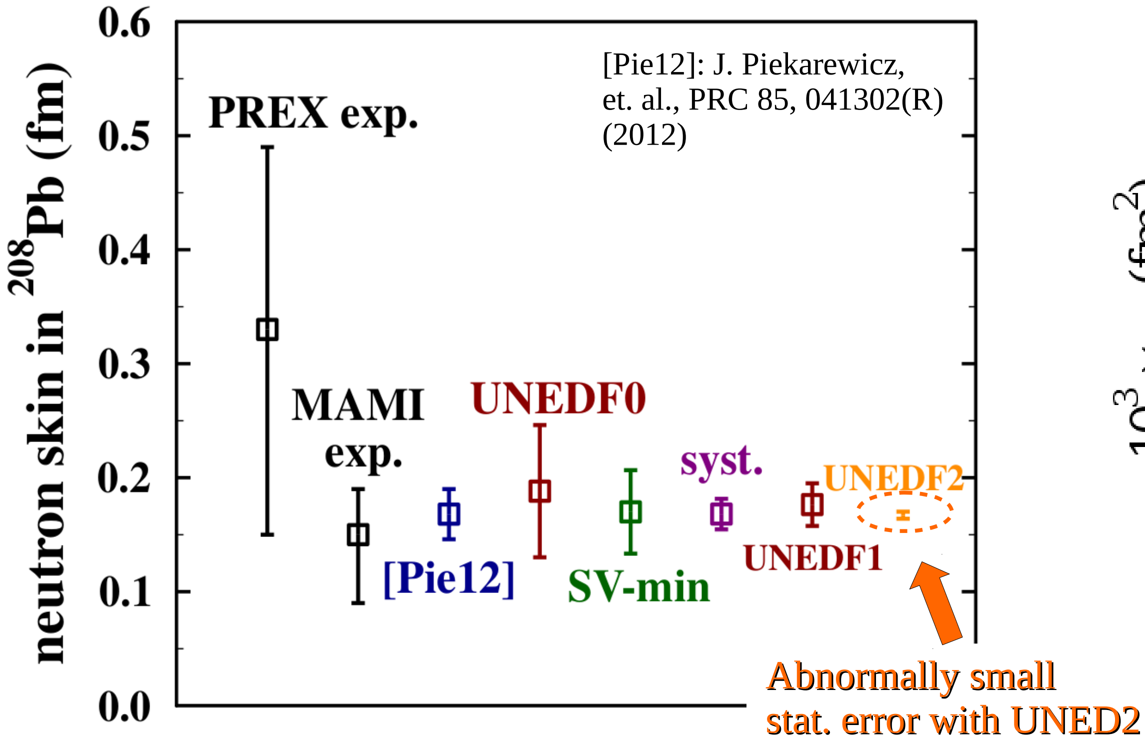


M. K., J. Phys. G 42, 034021 (2015)

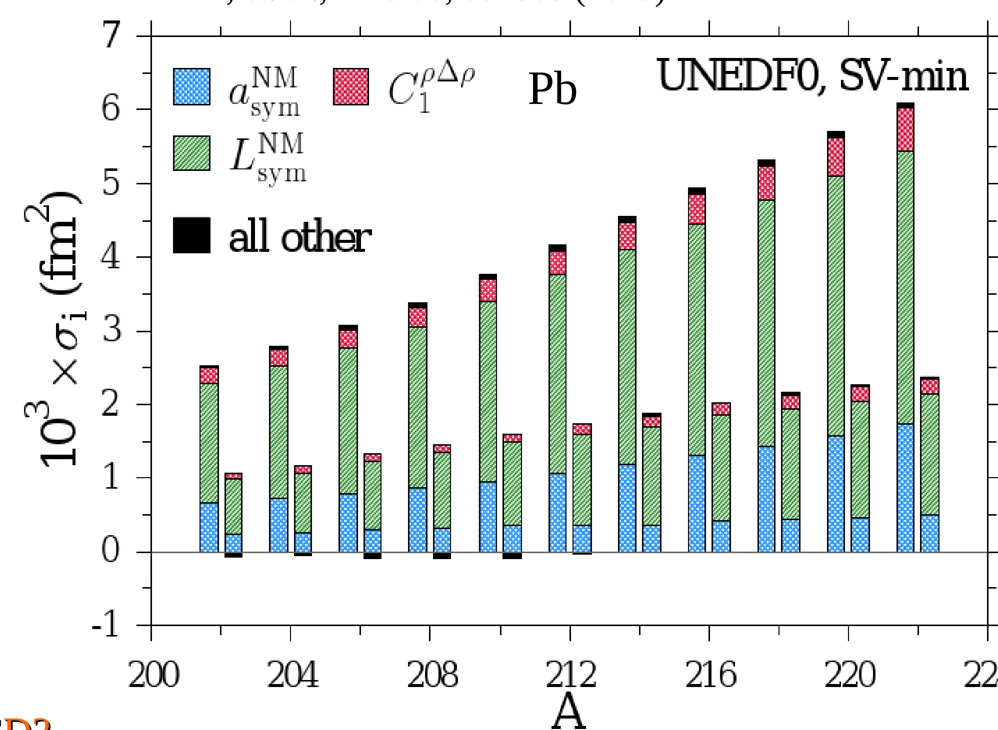


Neutron skin thickness

- Neutron skin thickness in ^{208}Pb was recently measured in P-REX and MAMI experiments. This gives valuable information about the neutron matter equations of the state
- P-REX experimental error bar larger than model uncertainties, MAMI error bar similar in magnitude compared to statistical model error
- Statistical uncertainty comes mostly from the uncertainty related to the density dependence of the symmetry energy. This reflects to uncertainty of the neutron matter density.
- With UNEDF2 L_{sym} was excluded from sensitivity analysis, since it hit the boundary value during optimization process. ⇒ Abnormally small statistical error for neutron skin thickness.

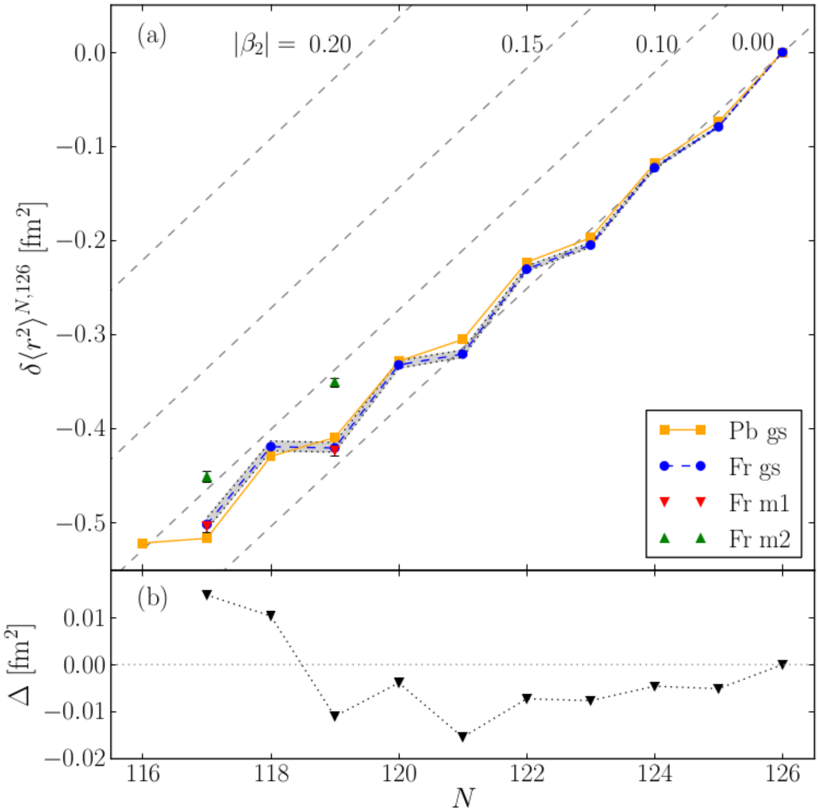


MK, et. al., PRC 88, 031305 (2013)



Charge radii of light Fr isotopes

A. Voss, et.al, Phys. Rev. C **91**, 044307 (2015)



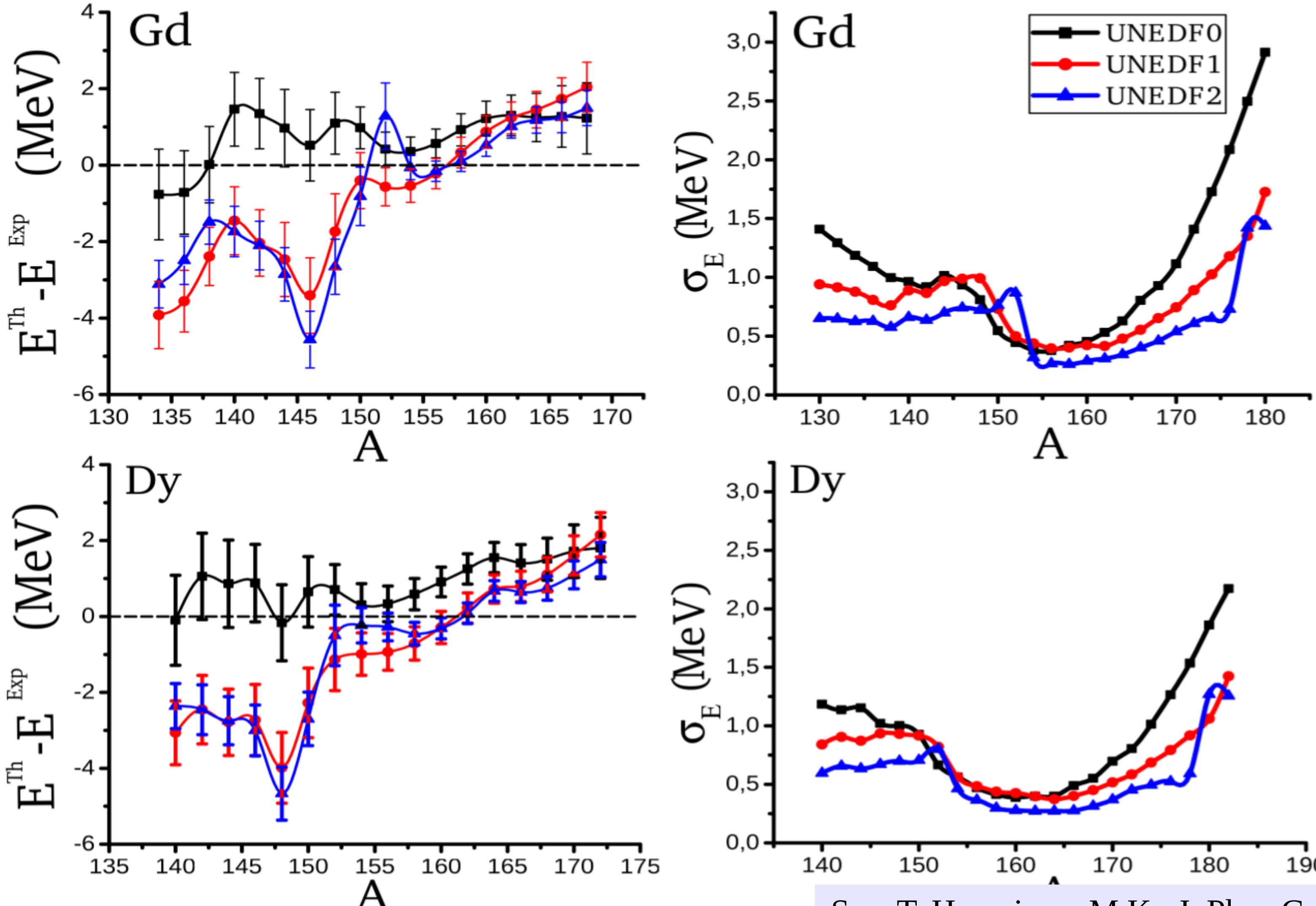
Charge radii and binding energies of Fr isotopes

A	$\langle r_{ch}\rangle$ (fm)		B (GeV)	
	EDF	Expt.	EDF	Expt.
213	5.576(6)	5.577	−1.65714(49)	−1.65468(1)
212	5.573(6)	5.570	−1.64825(52)	−1.64657(1)
211	5.567(6)	5.566	−1.64046(57)	−1.63912(1)
210	5.563(5)	5.559	−1.63109(63)	−1.63024(1)
209	5.561(5)	5.556	−1.62270(73)	−1.62261(1)
208	5.560(5)	5.548	−1.61336(76)	−1.61344(1)
207	5.557(5)	5.547	−1.60483(79)	−1.60554(2)
206	5.556(5)	5.539	−1.59535(81)	−1.59587(3)
205	5.554(5)	5.539	−1.58686(87)	−1.58787(1)
204	5.551(5)	5.532	−1.57721(91)	−1.57788(2)

- Charge radii of light Fr isotopes were recently measured at TRIUMF. This allowed to test predictive power of the UNEDF0 model
- Comparison to UNEDF0 prediction shows that even though binding energies can be reproduced well, charge radii of the lightest Fr isotopes could not be reproduced so well

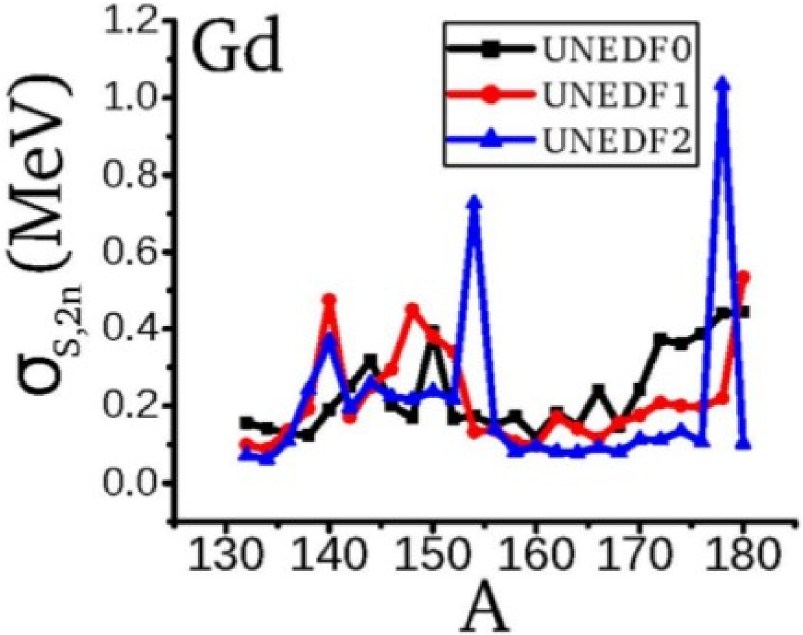
Uncertainty propagation in deformed rare earth nuclei, binding energy

- Propagated statistical uncertainties for rare earth binding energies follow similar patter to those in semi magic nuclei: Nuclei far from stability have larger theoretical uncertainties
- The latter the UNEDF model, the smaller are the uncertainties. However, best correspondence with experimental values is with UNEDF0

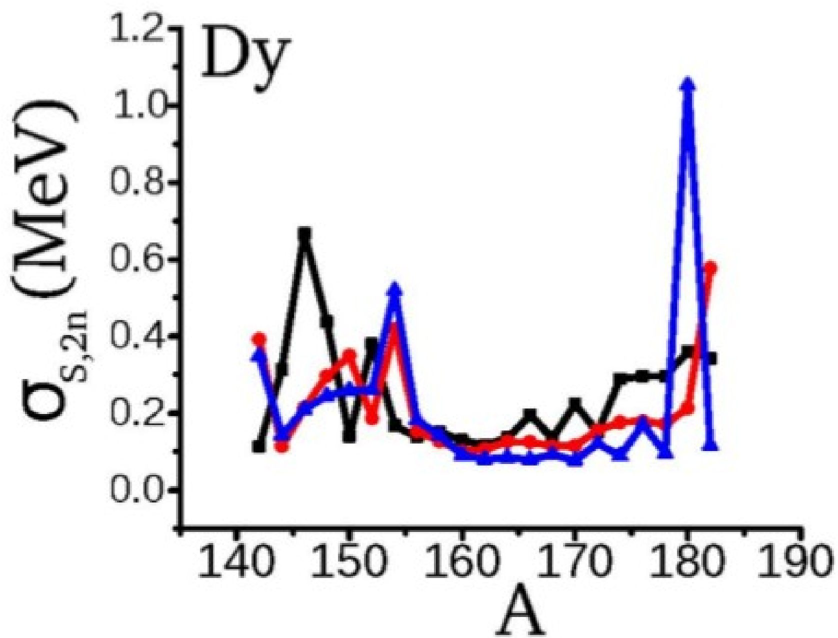


See: T. Haverinen, M.K., J. Phys G 44 044008 (2017)

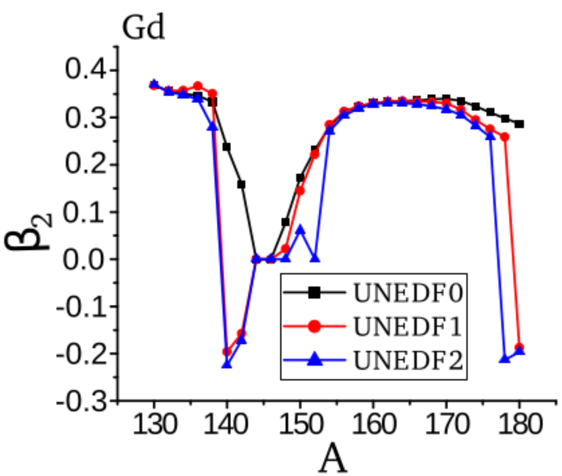
Uncertainty propagation in deformed rare earth nuclei, S_{2n} value



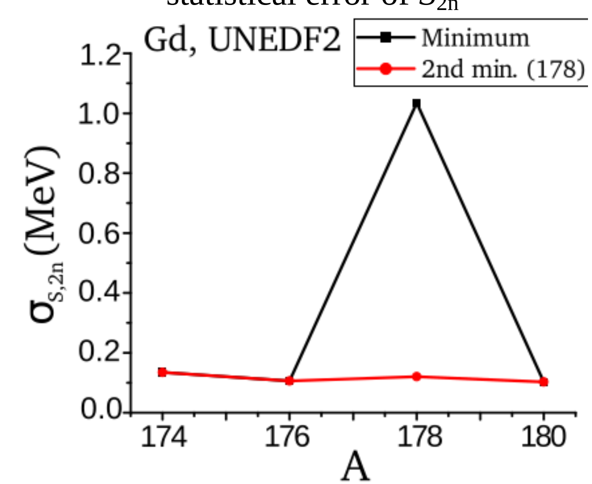
- Generally, with two-neutron separation energies, the statistical uncertainty is smaller compared to binding energies. Some of the uncertainties with isovector part are canceled out
- Statistical uncertainty has some sudden large values with some particular isotopes
- These are connected to a sudden change of deformation
- For example, deformation has a sudden change at A=178 with UNEDF2
- By using the secondary minimum of this nucleus, the deformation change is small and propagated error is similar to neighboring nuclei



Intrinsic deformation

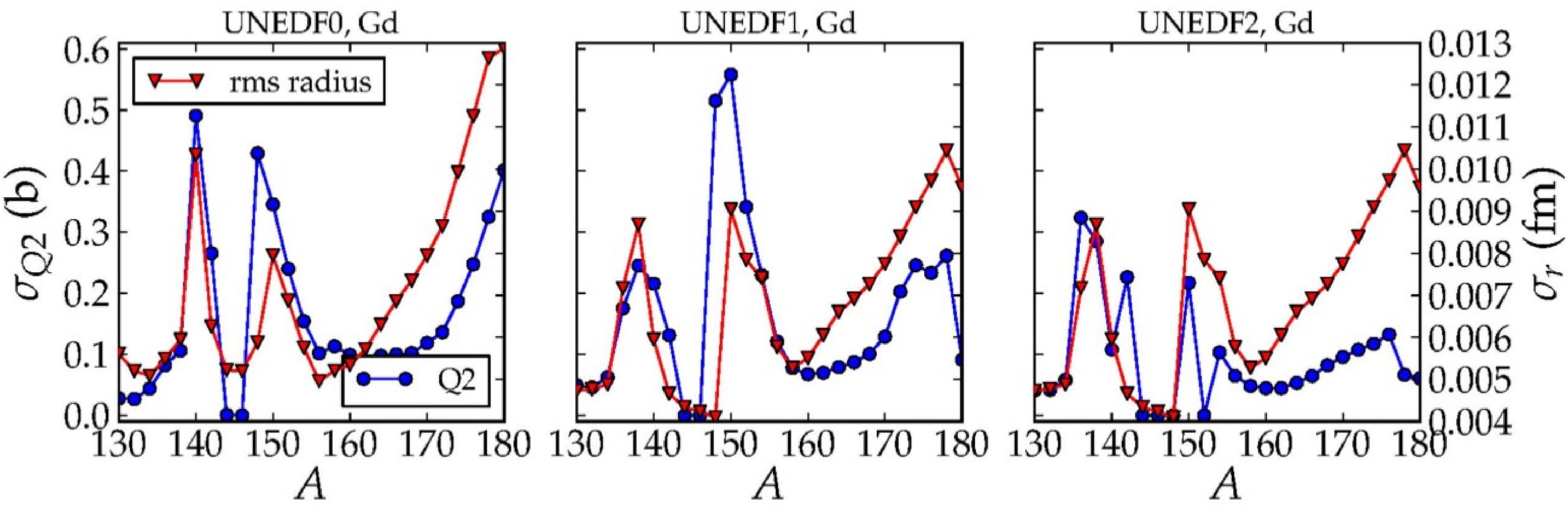


statistical error of S_{2n}

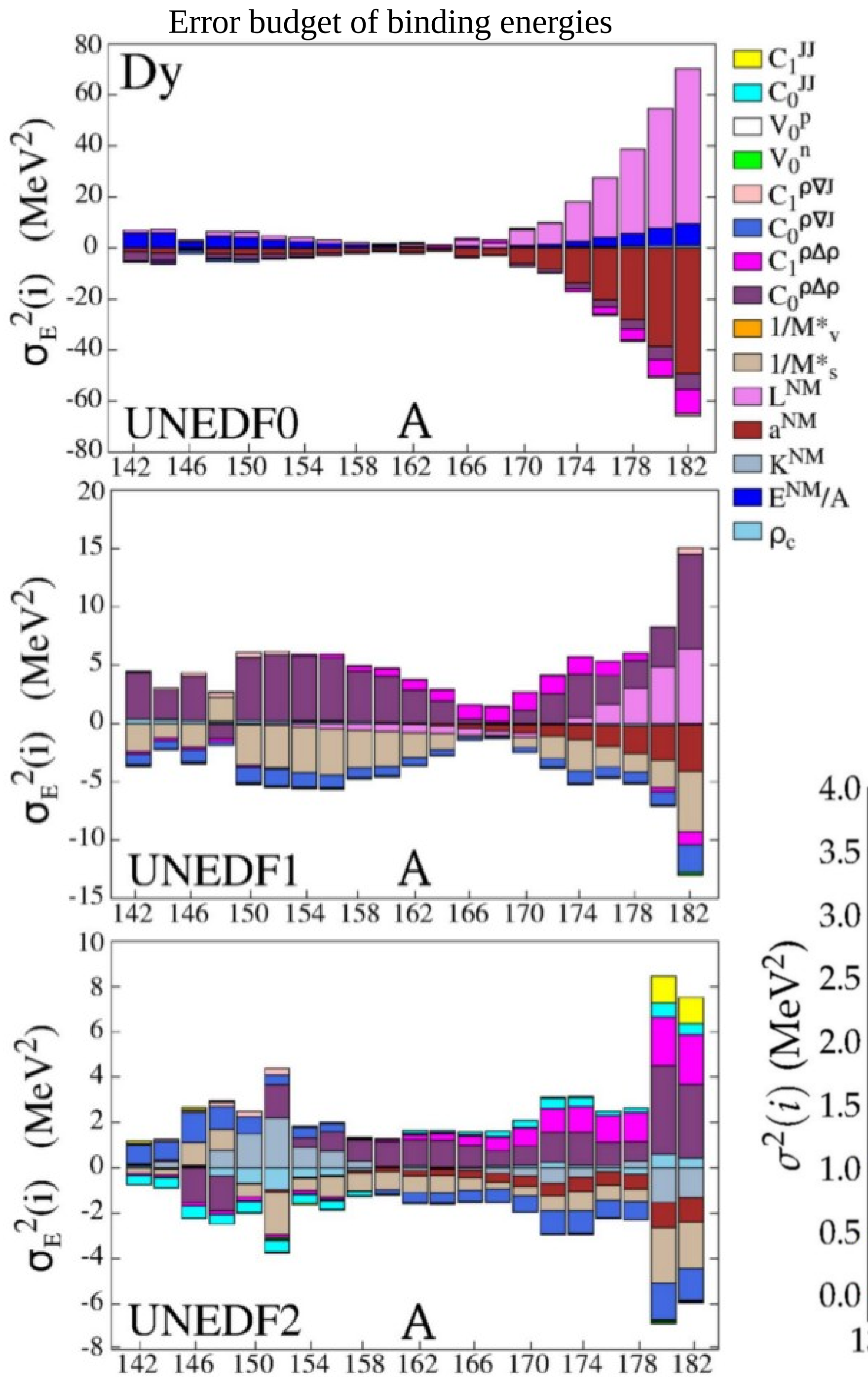


Uncertainty propagation in deformed rare earth nuclei, rms radius

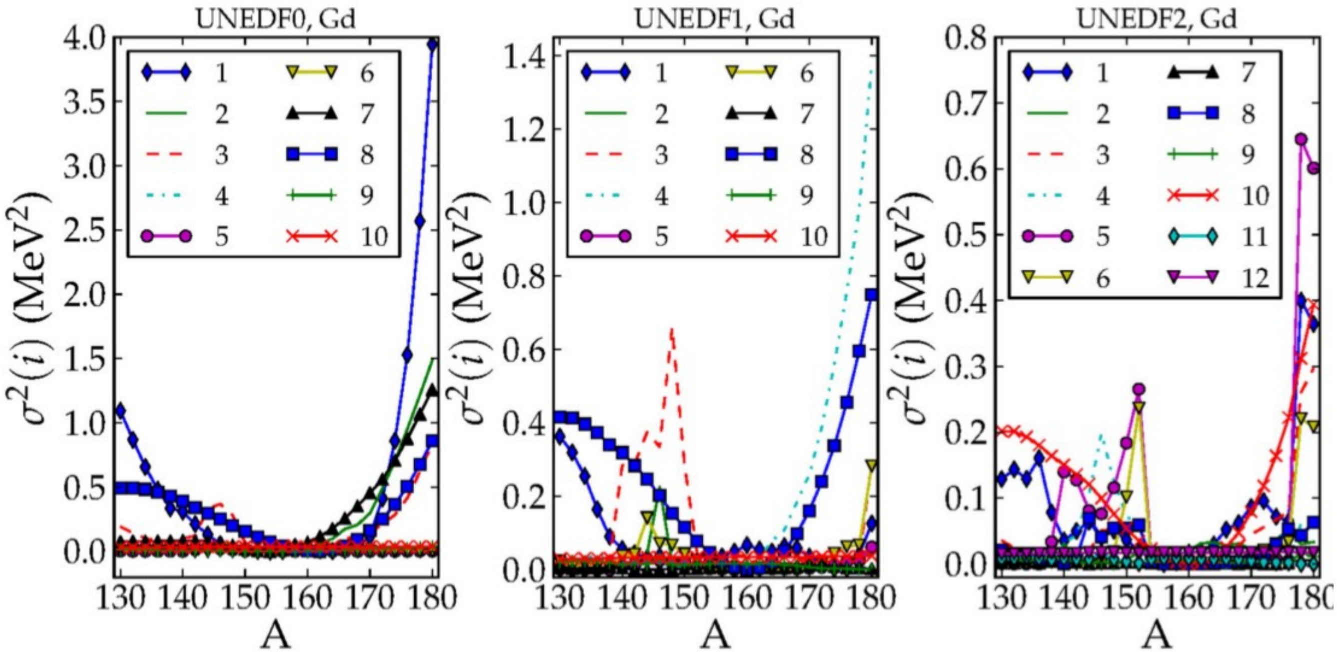
- Systematic error of radii and intrinsic quadrupole moment are strongly connected, as expected, since the presence of deformation increases radius
- Some of the nuclei close to semi-magicity are spherical, and thus the deformation uncertainty vanishes
- High values of uncertainty next to spherical nuclei are due to soft deformation energy landscape with respect of quadrupole deformation.



Uncertainty propagation in deformed rare earth nuclei, error budget

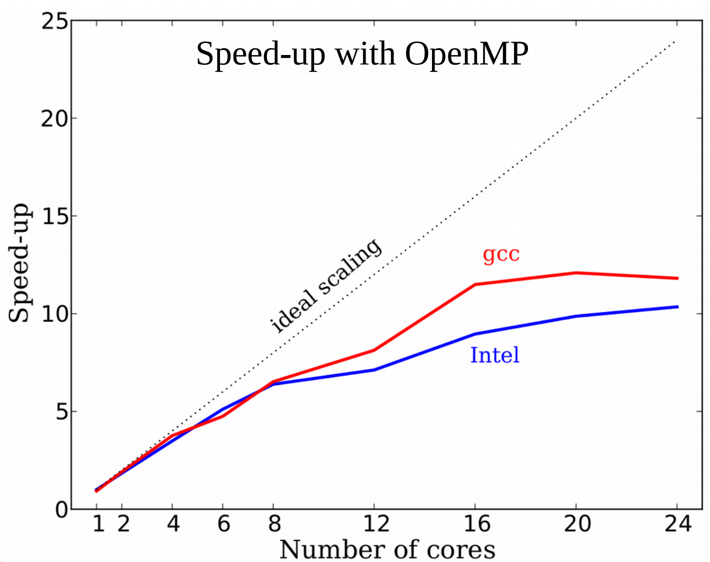


- By looking at the error budget, one can see which of the parameters contribute most on the statistical error
- With UNEDF0 only few parameters seems to be important ones, when looking at uncertainty of the binding energy.
- The eigenmode formalism also shows that only a few parameters contribute significantly. Most important eigenvectors mostly consists of those parameters which were found important in error budget
- With UNEDF1 and 2 more parameters become important



Towards novel EDF

- Many results point out that the limits of current EDFs have been reached and novel approaches are required
- One approach is finite range pseudopotential, suitable for beyond mean-field calculations (Jyväskylä, Lyon & York collaboration)
- Current status looks promising (see Karim's talk). Parameter optimization presently at spherical HFB level
- In future we plan to adjust parameters at axially deformed HFB level
- A new HFB solver, `HFBtemp`, has been developed to calculate deformed nuclei



`HFBtemp`

- A modular HFB solver, in which one could freely combine various basis (axial, 3D Cartesian, ...) with various EDFs (Skyrme, finite range, ...), and later with other components (FAM-QRPA, PNP, AMP, …)
- Coding is done with c++ (2011 standard). Many external libraries used (Eigen, boost, yaml-cpp)
- Uses a lot of template programming structures
- Current implementation includes axial and 3D Cartesian harmonic oscillator bases, Skyrme EDF and finite range EDF for axial case
- OpenMP parallelization for a single HFB calculation, MPI parallelization available for multiple HFB calculations
- Good scaling with OpenMP

Conclusions and outlook

- UNEDF0, 1 and 2 presents a optimization scheme of Skyrme-like EDF, which includes progressively more experimental data.
- Many UNEDF2 properties slightly worse than with more specialized UNEDF0 or UNEDF1. UNEDF2 is the best all-around Skyrme EDF from UNEDF family
- 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.

- Error propagation can be computed with the covariance matrix
- Biding energies show that isovector parameters are not yet well enough constrained
- With deformed nuclei, deformation effects and uncertainties seems to have nontrivial impact on statistical error of two-neutron separation effect
- Usually only a few parameters (or eigenmodes) contribute on statistical error of binding energy

Future:

- Novel EDFs should be developed, to improve accuracy and to avoid some other problems present with the Skyrme. Sensitivity analysis essential

Open questions

Towards novel EDFs, what do we want?

- Limits of current EDFs have been reached and novel approaches are needed
- What do we want to improve? (Answer "everything" is ideal, but not a practical one)
- How can we achieve this improvement?

- One important choice is whether to continue at single-reference level, or develop EDF intended for multi-reference calculations

Single-reference	Multi-reference
+ computationally cheap, parameter adjustment easily doable - no good quantum numbers due to symmetry breaking	+ access to good quantum numbers and to spectroscopy - computationally heavy, parameter adjustment presently doable only at single reference level

- With EDFs intended for multi-reference level, in the light of the current situation, no density dependence allowed
- What kind of mathematical form (or terms) the EDF suitable for multi-reference calculations should have? Any guidance from ab-initio side what terms are important ones?

Towards novel EDFs, data and parameter adjustment

- EDF parameters needs to be adjusted to experimental input
- Typically masses, radii, pairing gaps, etc. has been used
- At the single-reference levels we have experience how different kind of data types can constrain EDF parameter space and how well various observables are usually reproduced
- What about parameter adjustment for EDFs intended for multi-reference calculations?
- How can we improve spectroscopic quality of a novel multi-reference EDF? What kind of data is required for such task?
    - Level scheme? (odd/even N,Z, rotational bands, vibrational states, open/closed shell)
    - EM transitions?
    - Beta transitions?
- Presently parameter adjustment is computationally practical only at the single-reference level. What kind of observables can be used at SR level to improve spectroscopic quality at MR level?
- How much can approximate symmetry restoration schemes help?
- Can ab-initio results constrain those parameters which are usually poorly constrained?