Uncertainty estimation

From the era of the standard Skyrme EDFs to novel approaches

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ECT* Doctoral Training Programme, June 2017

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How many of you have used a model which includes fitted parameters?

How many of you have calculated the errors of the results?

You should. Fitting causes uncertainty, so your results will always have some uncertainty.

What's next?

- UNEDF models and their parameters
- Uncertainty estimation: what and why
- What did we learn from the uncertainties?

Theoretical models and degrees of freedom

Nuclear energy density functionals (EDFs) describe the system by using nucleonic densities and currents

Density functional theory (DFT) based methods can be used through the whole nuclear chart (mass tables, predictions)

The UNEDF models are “state-of-the-art” Skyrme-EDFs: created with computer scientists and mathematicians (optimization, uncertainties)

(Skyrme-) HFB

Two-body Hamiltonian can be expressed as

$$H = \sum_{n_1 n_2} e_{n_1 n_2} c_{n_1}^\dagger c_{n_2} + \frac{1}{4} \sum_{n_1 n_2 n_3 n_4} \bar{v}_{n_1 n_2 n_3 n_4} c_{n_1}^\dagger c_{n_2}^\dagger c_{n_4} c_{n_3}$$

(Bogolyubov transformation, expectation value)

Expectation value can be expressed with density and pairing density as energy density functional:

$$E[\rho, \tilde{\rho}]$$

Variation of energy with respect to density and pairing density

(Skyrme) HFB -equations

- **depend on the solution itself: must be solved iteratively**

In this work, the program **HFBTHO** was used.

Skyrme-EDF

- In this approach, the total energy is given by

$$E = E_{\text{kin}} + \int d^3r\,\mathcal{E}_{\text{Sk}} + E_{\text{Coul}} + E_{\text{pair}} - E_{\text{corr}}$$

kinetic term

Skyrme energy density (now only time-even)

Coulomb term

pairing

additional corrections

- Time-even Skyrme energy density reads $\mathcal{E}_{\text{Sk}} = \sum_{T=0,1} (\mathcal{E}_T^{\text{even}} + \mathcal{E}_T^{\text{odd}})$ where

$$\mathcal{E}_T^{\text{even}} = C_T^{\rho}\rho_T^2 + C_T^{\Delta\rho}\rho_T\Delta\rho_T + C_T^{\tau}\rho_T\tau_T + C_T^{J}\mathbb{J}_T^2 + C_T^{\nabla J}\rho_T\nabla\cdot\mathbf{J}_T$$

T=0 isoscalar
T=1 isovector

density

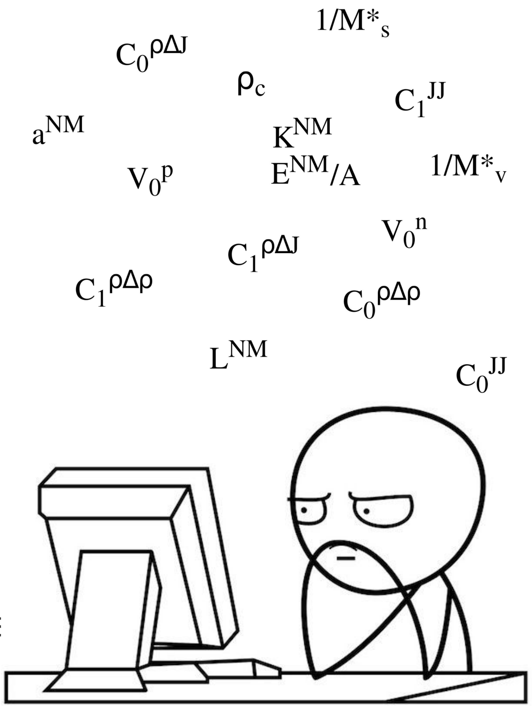
kinetic density
$=\nabla\nabla'\boldsymbol{\rho}(r,r')$

spin-current
$\sim(\nabla'-\nabla)\times\mathbf{s}(r,r')$

current (approximated with spin-current)

Skyrme-EDF

- Some of these constants C can be related to nuclear matter properties and variables which have some physical scale
  - some of the “C-parameters” can be replaced by more physical parameters (figure)
- Still, all the constants must be determined by adjusting the model to experimental data
  - different data -> different parameterizations, e.g. UNEDF0, UNEDF1, UNEDF2 - they have also other differences
- Adjusting, and underlying optimization process, causes statistical uncertainty



Parameters in UNEDF models

saturation density

E per nucleon at equilibrium

nuclear matter incompressibility

symmetry energy coeff. and its slope

isoscalar and isovector effective mass

pairing strengths

EDF	ρ_c	$\frac{E^{\mathrm{NM}}}{A}$	K^{NM}	$a_{\mathrm{sym}}^{\mathrm{NM}}$	$L_{\mathrm{sym}}^{\mathrm{NM}}$	$1/M_s^*$	$1/M_v^*$	$C_t^{\rho\Delta\rho}$	$V_0^{\mathrm{n,p}}$	$C_t^{\rho\nabla J}$	C_t^{JJ}
UNEDF0	x	x		x	x		–	x	x	x	–
UNEDF1	x			x	x	x	–	x	x	x	–
UNEDF2	x		x	x		x	–	x	x	x	x

x = included in sensitivity analysis
\- = fixed
empty = boundary value

Optimization: least squares

Different data types

Number of points of a datatype

Output of calculation

Experimental value of an observable

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

Total number of data points

Number of parameters

Weight (make difference dimensionless, balances)

Data

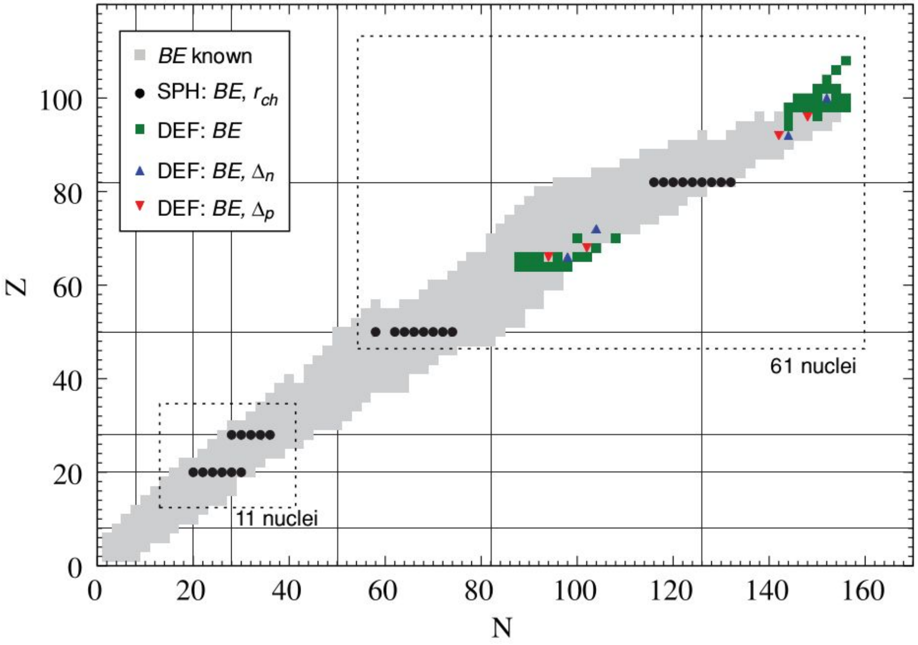
Spherical and deformed nuclei: (UNEDF0)

- binding energies
- charge radii
- pairing gaps

(UNEDF1: +excitation energies of fission isomers)

(UNEDF2: +single particle splittings)

Figure from Kortelainen et al. Phys. Rev. C 82 (2010) 024313

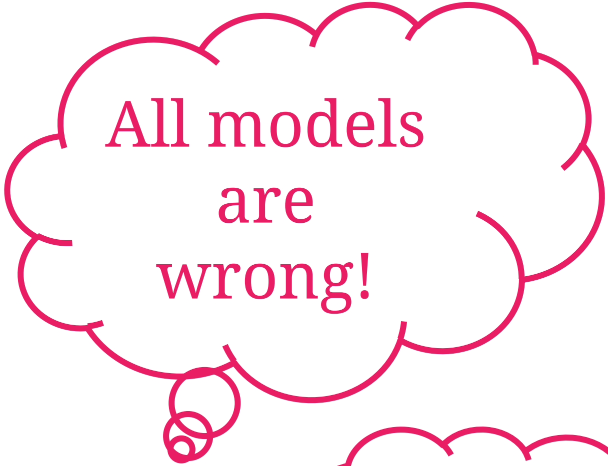


(UNEDF0 data)

Why are uncertainty estimates important?

- Theoretical models are used for extrapolations: we should know how accurate and precise our predictions are
- Uncertainties give valuable information about the theory

One way to find out statistical errors is to apply the knowledge of model parameter uncertainties



Calculating standard deviation:

$$\sigma^2(y) = \sum_{i,j=1}^{n} \mathrm{Cov}(x_i, x_j) \left[\frac{\partial y}{\partial x_i}\right] \left[\frac{\partial y}{\partial x_j}\right]$$

The standard deviation of an observable y squared is...

...a sum of...

..the covariance matrix elements multiplied by...

..the product of partial derivatives of y with respect to the parameters.

Calculating standard deviation:

$$\sigma^2(y) = \sum_{i,j=1}^{n} \underbrace{\mathrm{Cov}(x_i, x_j)} \underbrace{\left[\frac{\partial y}{\partial x_i}\right]\left[\frac{\partial y}{\partial x_j}\right]}$$

Covariance matrix elements were calculated already earlier.
Basically, Cov(x_i,x_j) tells you how two variables change together.

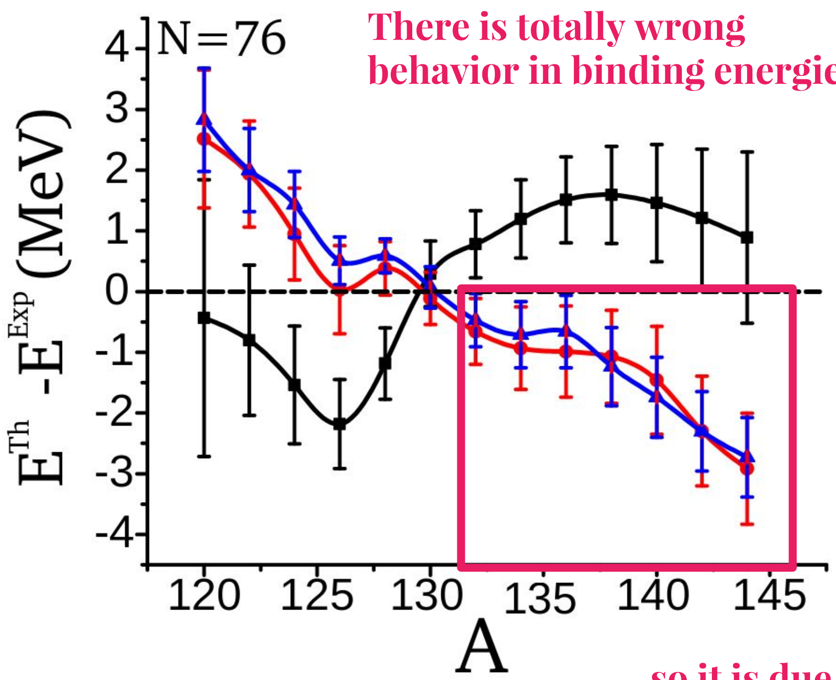
Partial derivatives can be approximated by finite differences:

$$\frac{\partial y}{\partial x_i} \approx \frac{y(x_1, x_2, \ldots, x_i + \Delta x_i, \ldots, x_n) - y(\mathbf{x})}{\Delta x_i}$$

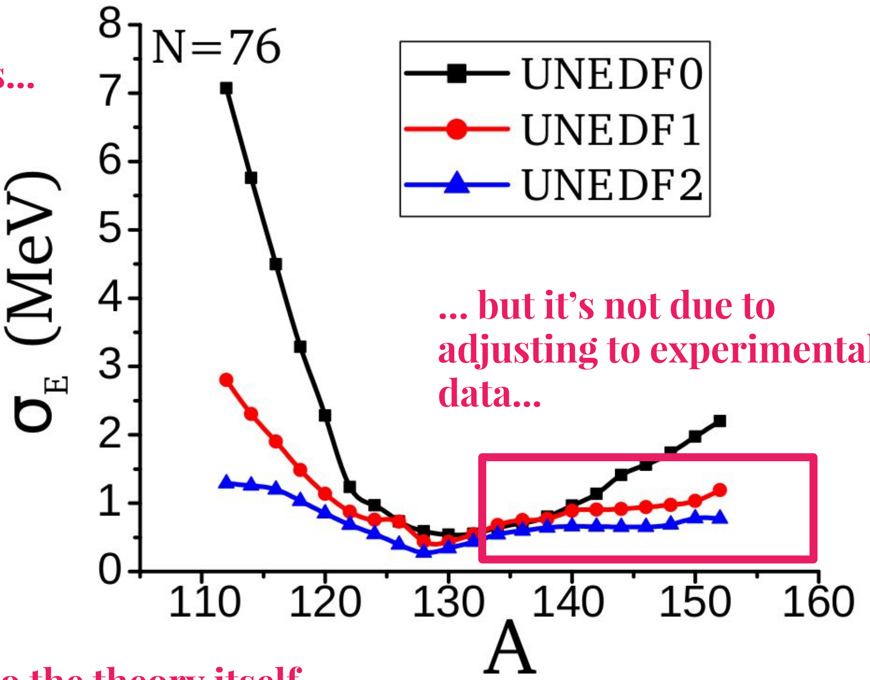
Fitting causes uncertainty.
What do we gain from uncertainty estimation?

Uncertainties can reveal missing theory:

There is totally wrong behavior in binding energies…



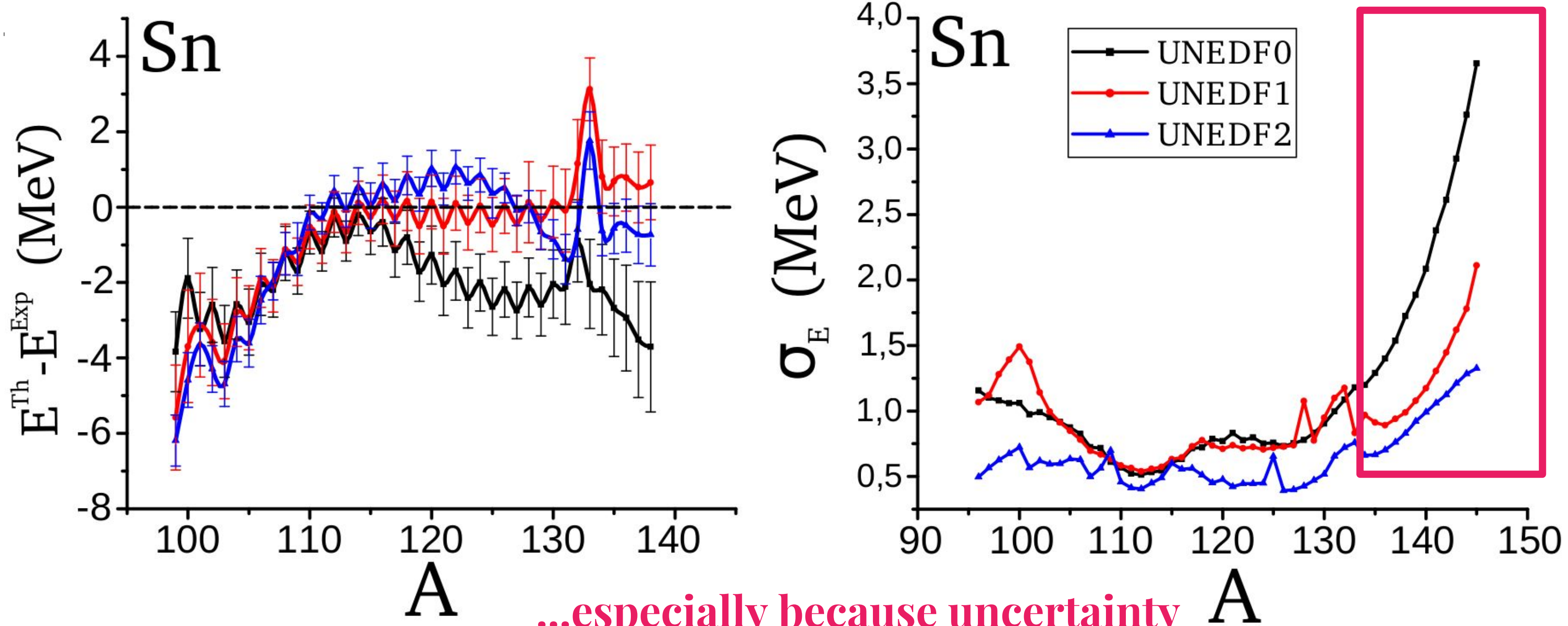
… but it's not due to adjusting to experimental data…



… so it is due to the theory itself - we are missing some theory!

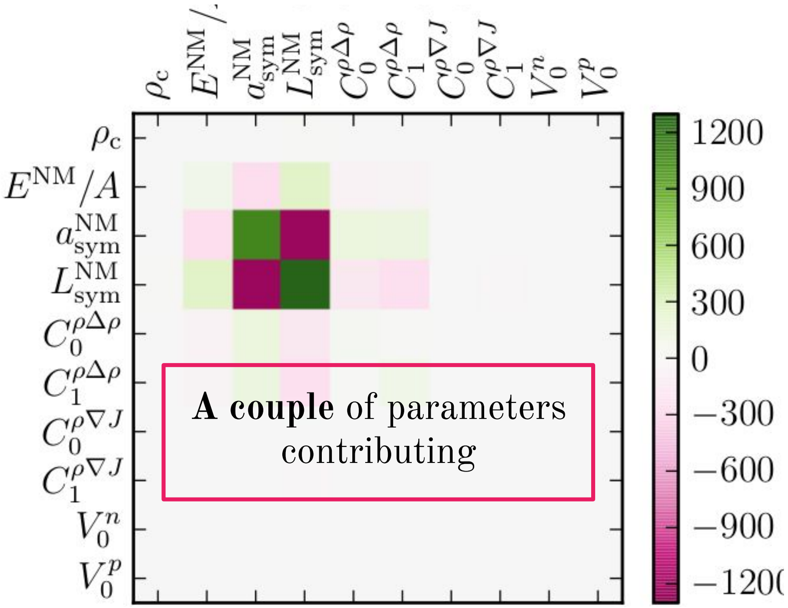
A “nice” fact: no odd-even staggering in the uncertainties!

We need uncertainties when we give predictions

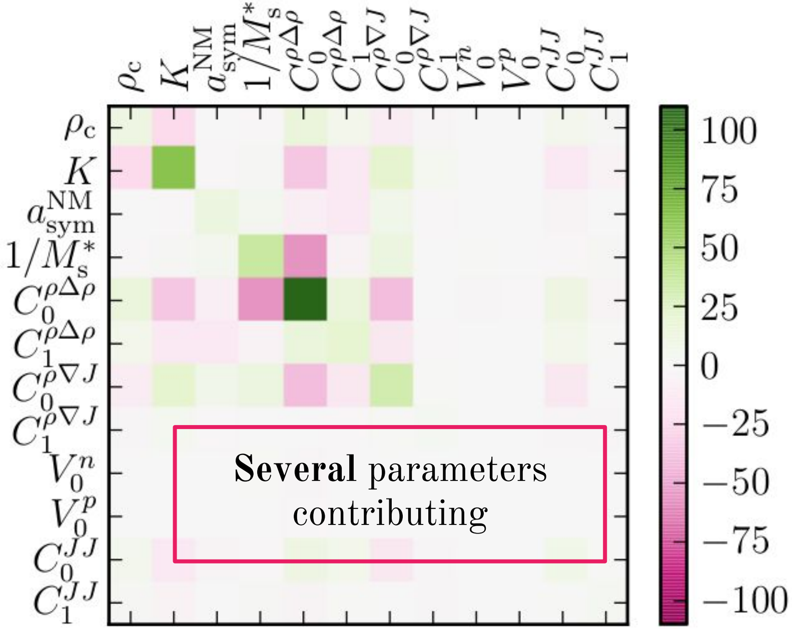


...especially because uncertainty increases when going towards neutron rich nuclei!

Where does the main contribution to the errors come from?

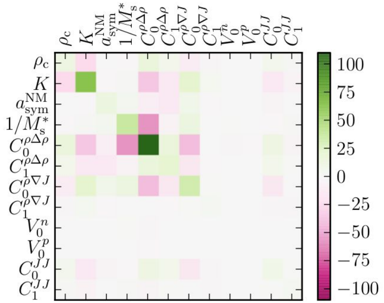


UNEDF0

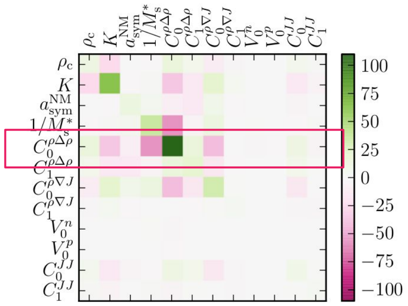


UNEDF2

BE of Gd180

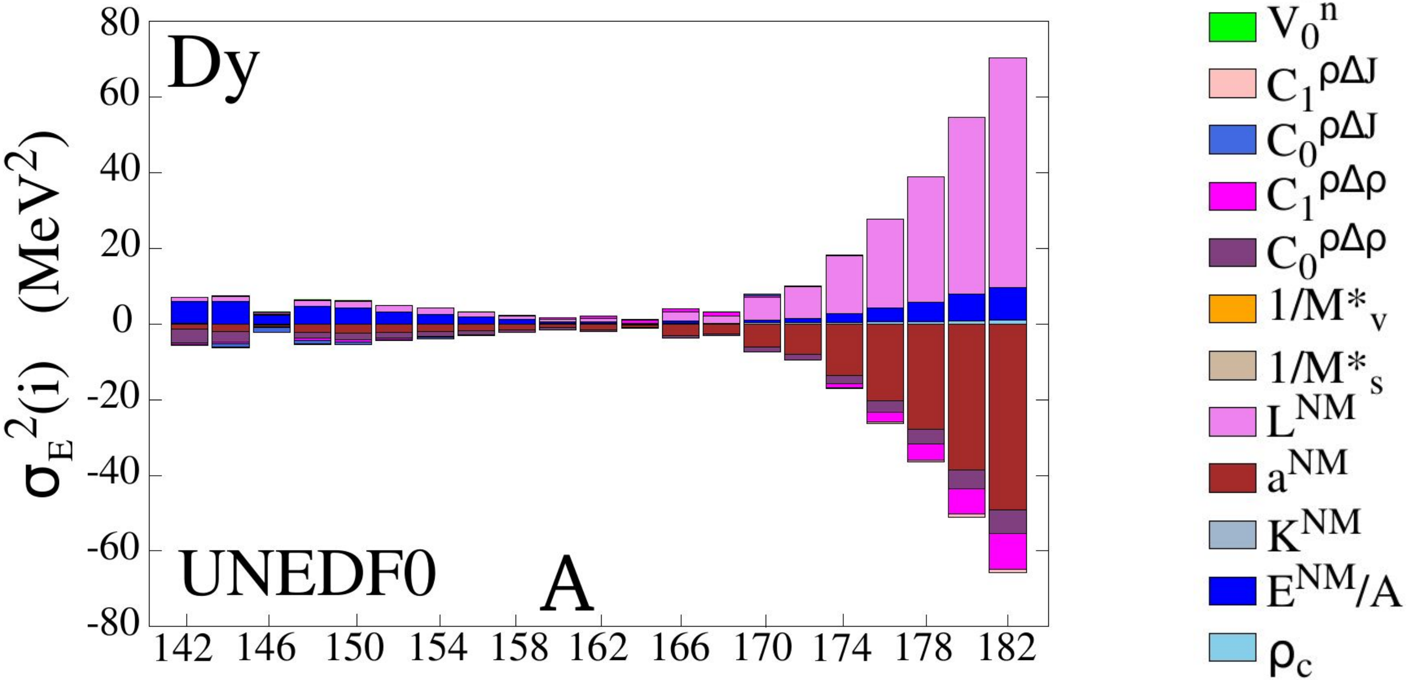


A color matrix is not very efficient when you want to show overall behavior: sum once over parameters



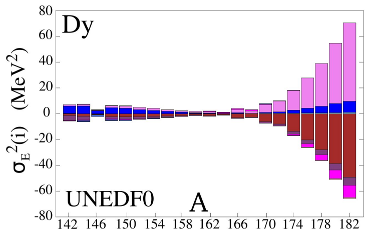
Overall behavior in isotopic chains

The uncertainty of UNEDF0 depends mainly on a couple of parameters...

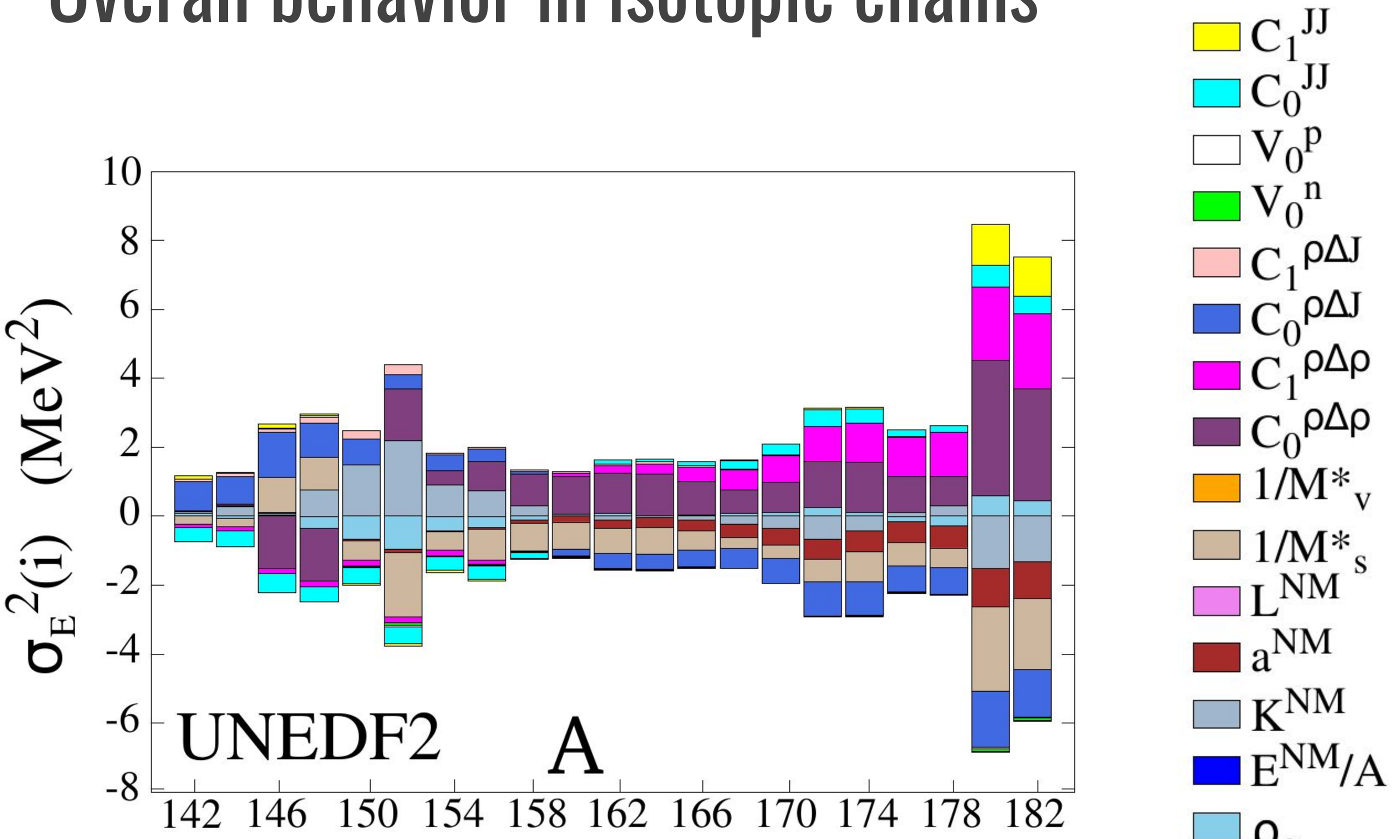


(Row sum)

Overall behavior in isotopic chains



... but the situation has changed in later parameterizations.



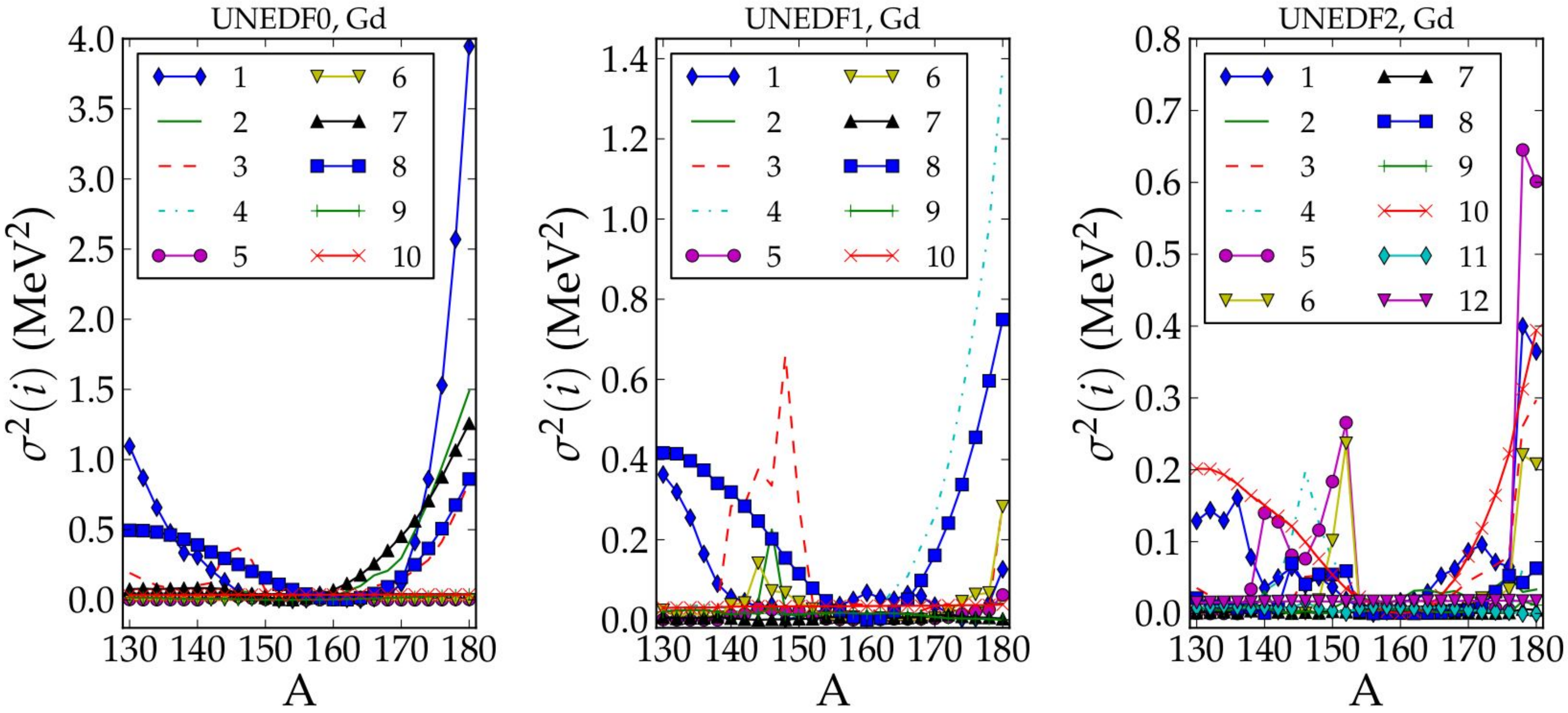
(Row sum)

Eigenvectors of covariance matrix

- By diagonalizing the covariance matrix one can represent the the statistical errors (eigenvalues) in **a condensed form**
- The biggest eigenvalues correspond to the most weakly constrained **directions** of the parameter space

Statistical errors represented in the eigenmode formalism

(for binding energy, the eigenvectors not shown here)



We have reduced the uncertainties quite a lot from UNEDF0 to UNEDF2...

...but still theoretical uncertainties are far away from experimental precision.

One of the most frequently asked questions:

I have used a Skyrme interaction in my calculations. Can I use your calculated uncertainties to approximate error bars?

No no no no and NO!
You have to calculate them yourself!

Uncertainty depends highly on the data used in fitting.

What we learned from the uncertainties?

- We are definitely missing some theory in UNEDFs models (and overall in Skyrme)
- Even the “state-of-the-art” EDFs give errors of the order of MeVs
- Uncertainties depend highly on the data used in fitting: uncertainties cannot be approximated by uncertainties of other EDFs

Systematic errors???

We have to move on: we need new theory and in order to go beyond mean field...

Thank you!

More fun here

Journal of Physics G: Nuclear and Particle Physics

PAPER

Uncertainty propagation within the UNEDF models

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Published 8 March 2017 • © 2017 IOP Publishing Ltd
Journal of Physics G: Nuclear and Particle Physics, Volume 44, Number 4
Focus on Enhancing the Interaction Between Nuclear Experiment and Theory Through Information and Statistics