Is the USDB interaction unique?

Towards shell model interactions with credible uncertainties

Nuclear Structure I, APS Global Physics Summit, Anaheim, CA

Tuesday March 18, 1:54 pm – 2:06 pm

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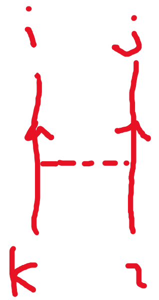
Nuclear shell model (no core)

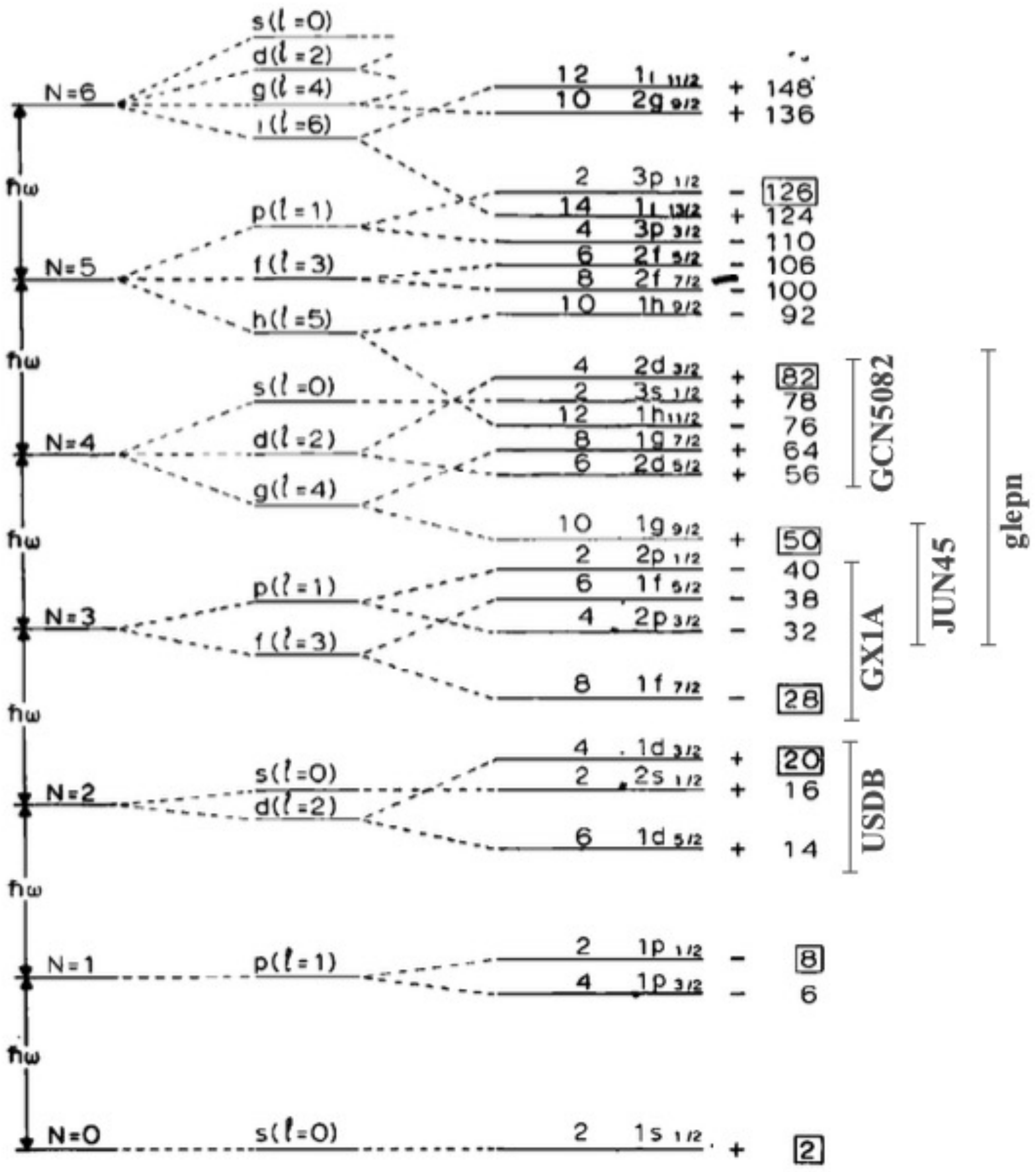
of particles in these orbits:
Mean-field energy

$$\hat{H}(\mathbf{c}) = \sum_i \epsilon_i \hat{n}_i + \sum_{i\le j,k\le l;JT} V_{ijkl;JT}\hat{T}_{ijkl;JT}$$

Matrix elements:
Residual 2-body interaction

Get these from effective field theory



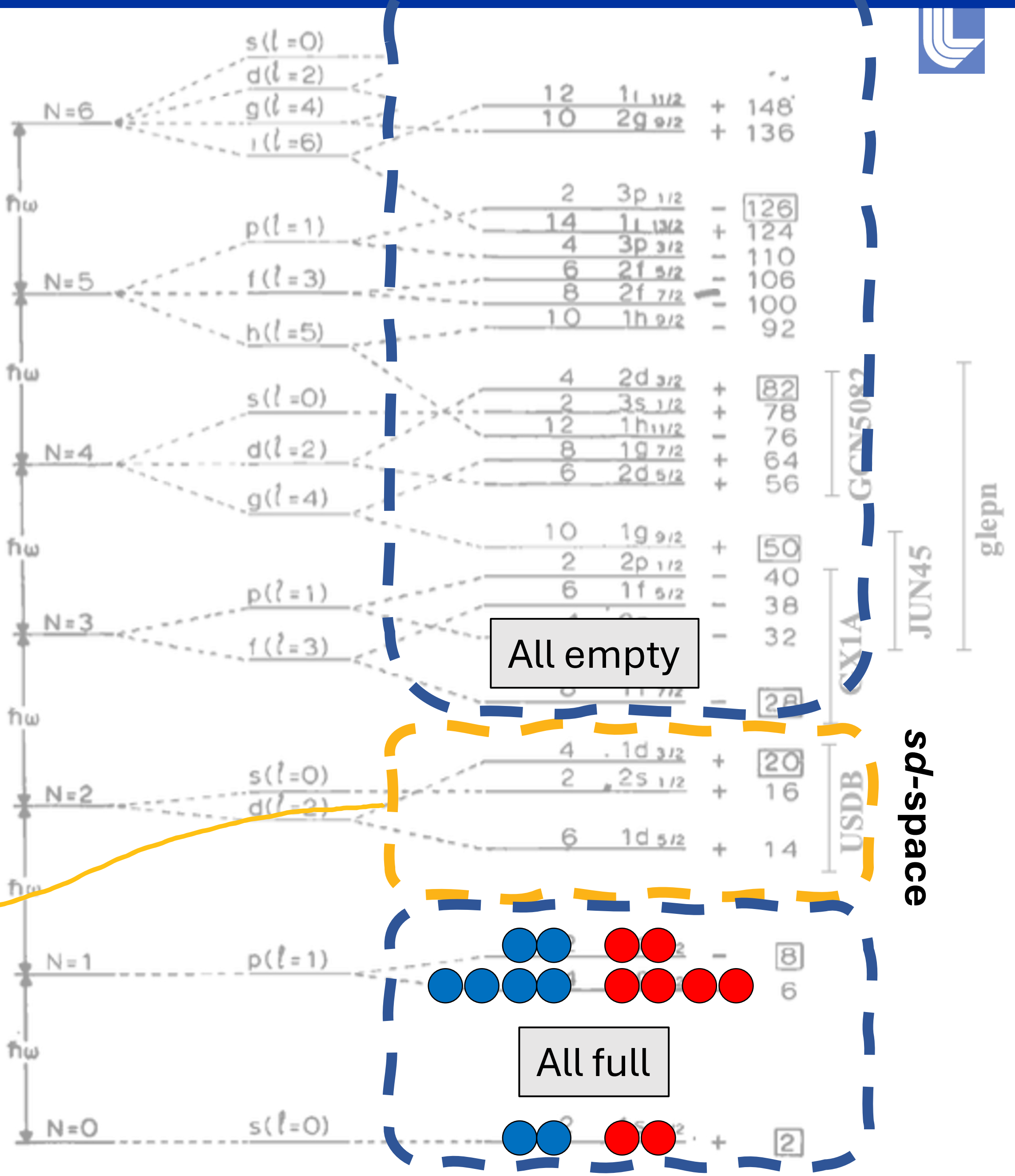


Nuclear shell model (with core)

$$\hat{H}(\mathbf{c}) = \sum_i \epsilon_i \hat{n}_i + \sum_{i \le j, k \le l; JT} V_{ijkl;JT} \hat{T}_{ijkl;JT}$$

Renormalized "effective interaction"

$$\hat{H}(\mathbf{c}) = \sum_i \epsilon_i \hat{n}_i + \sum_{i \le j, k \le l; JT} V_{ijkl;JT} \hat{T}_{ijkl;JT}$$



USDB: the most famous renormalized-interaction

B. A. Brown *et al.*, PRC 74, 034315 (2006)

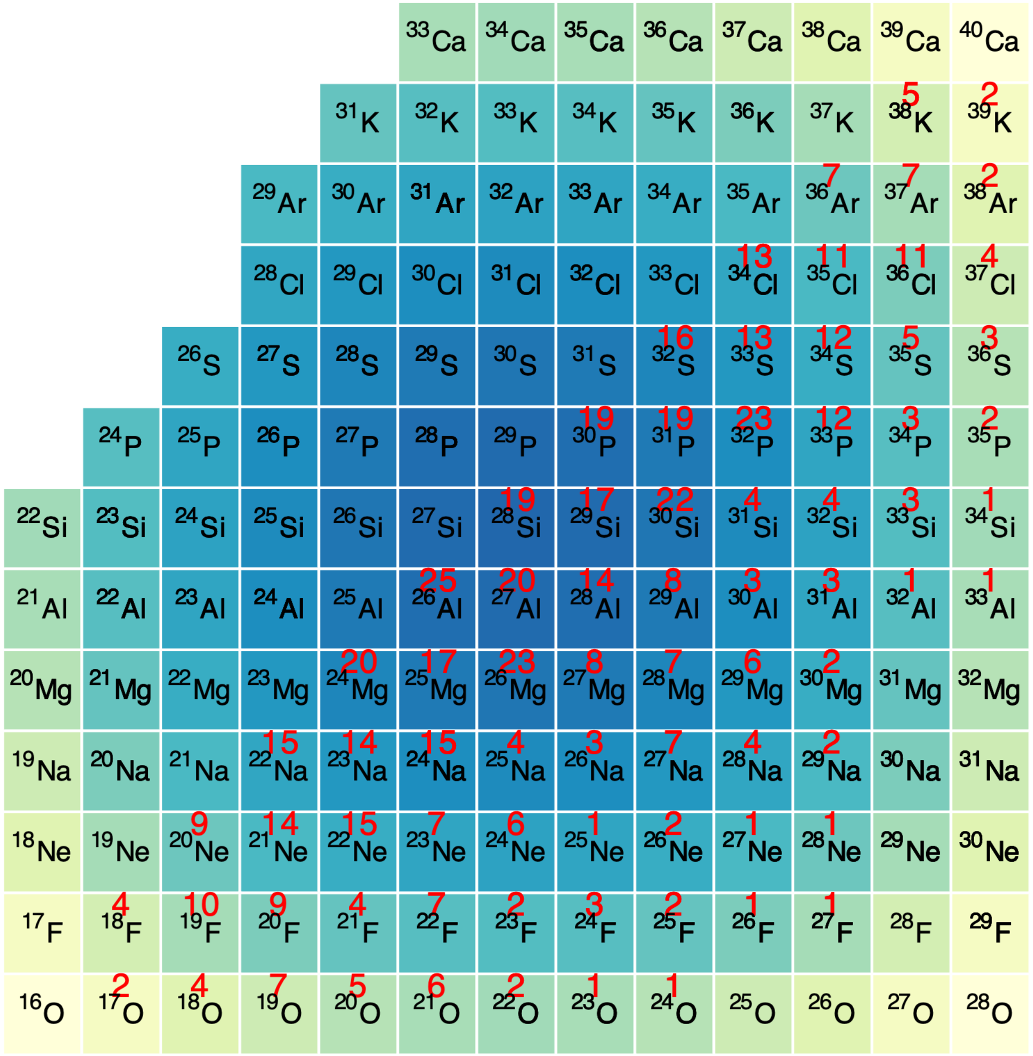
- 3 single-particle energies
- 66 residual two-body matrix elements
- Fit to data:

$$\min_c \chi^2 = \min_c \sum_{i=1}^{608} \left(\frac{SM_i(c) - E_i}{\sigma_i} \right)^2$$

$$\sigma_i^2 = \sigma_i^2(Experiment) + \sigma_i^2(Theory)$$

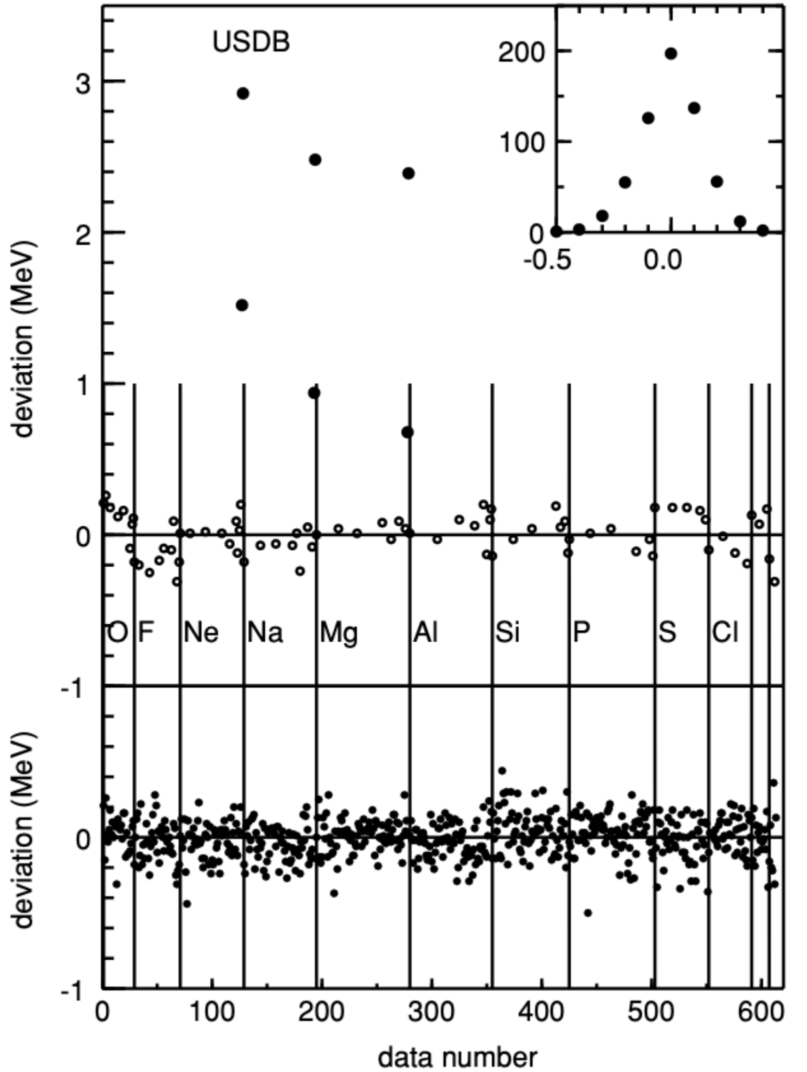
a few keV << 150 keV

- 608 energy levels
  - 77 binding energies
  - 531 excitation energies



USDB: 130 keV is the uncertainty of the shell model

B.A.Brown et al., PRC 74, 034315 (2006)



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608 energy levels
- 77 binding energies
- 531 excitation energies

χ^2-minimization UQ analysis:
- Uncertainty set by parameter-of-fit: $\sigma(theory)$
- Analysis assumes linear approximation
- Assumes multivariate normal distribution of parameters

See:
J.Fox *et al.*, PRC 101, 054308 (2020)
J.Fox *et al.*, PRC 108, 054310 (2023)

Overall distribution of errors: standard deviation of 130 keV

What I set out to do: refit USDB with a fast emulator and better statistics

Wishlist:

1. Future: fit new interactions in very large model spaces

   Train an emulator for shell model calculations (eigenvector continuation)

   Inspired by: S. Yoshida *et al.*, Prog. Theor. Exp. Phys. 2022 053D02

2. Credible uncertainty estimation

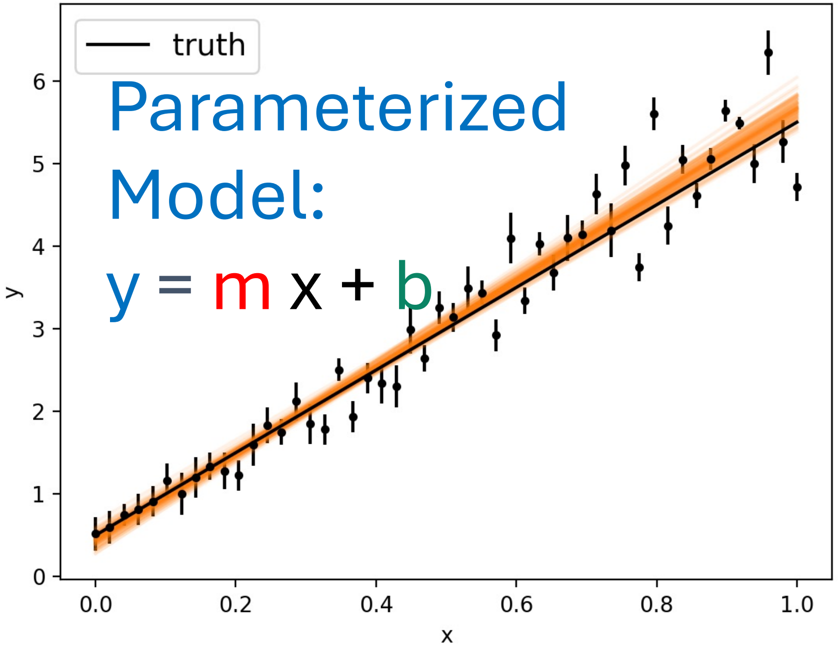
   Fit using robust statistical tools: MCMC

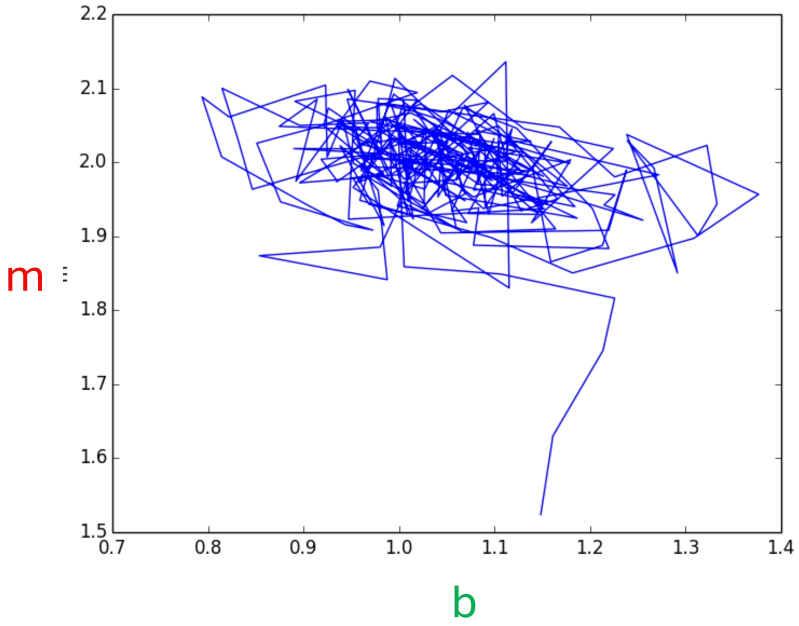
   Inspired by: C. Pruitt *et al.*, PRC 107, 014602 (2023)

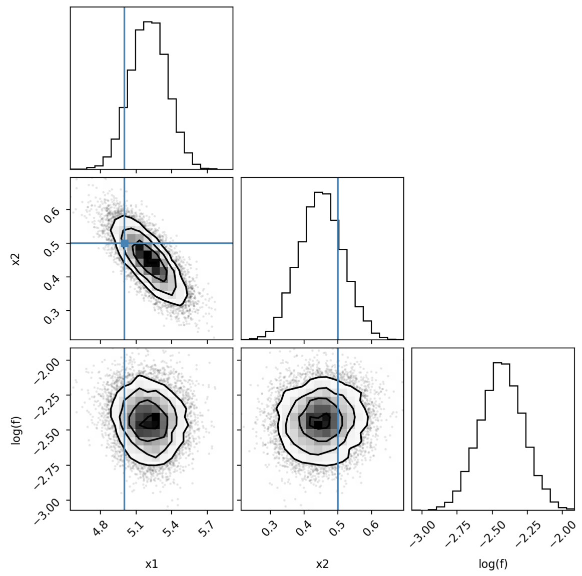
Ready for Markov Chain Monte Carlo (MCMC)

χ^2-minimization UQ analysis:
- Uncertainty set by parameter-of-fit: $\sigma(theory)$
- Analysis assumes linear approximation
- Assumes multivariate normal distribution of parameters

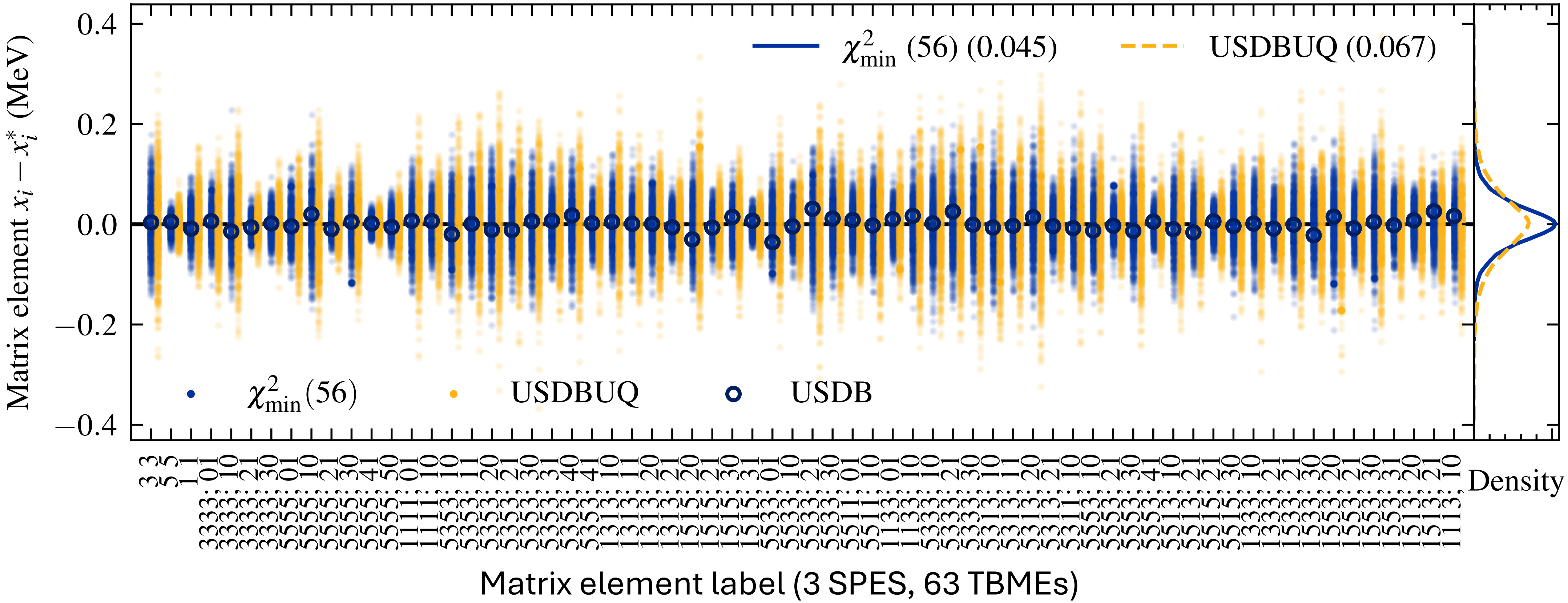
MCMC UQ analysis:
- Uncertainty set by parameter-of-fit: $\sigma(theory)$
- ~~Analysis assumes linear approximation~~
- ~~Assumes multivariate normal distribution of parameters~~







Introducing USDB with UQ, “USDBUQ”

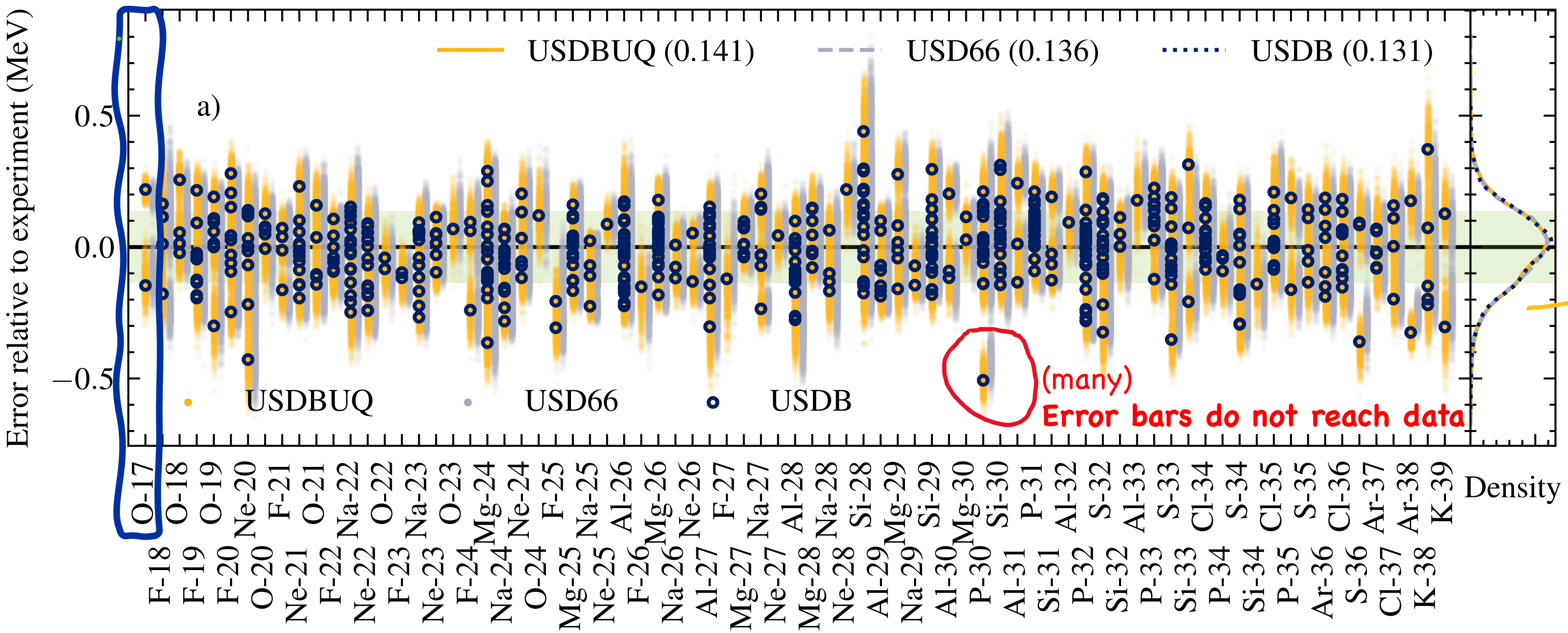


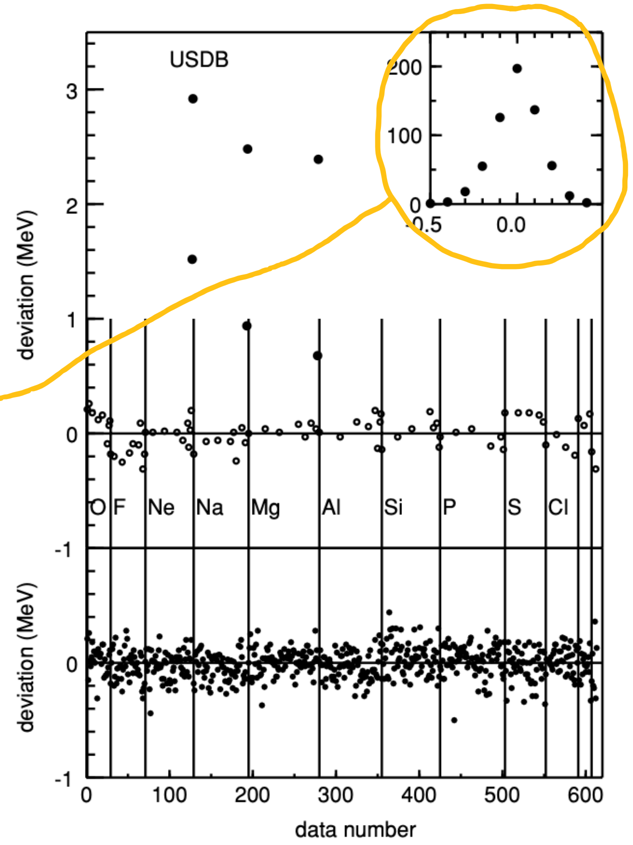
USDB is unique*, but it is shallow.

The end!

USDBUQ: USDB with error bars. Are they credible?

Just like USDB classic, the standard error is ~130-140 keV

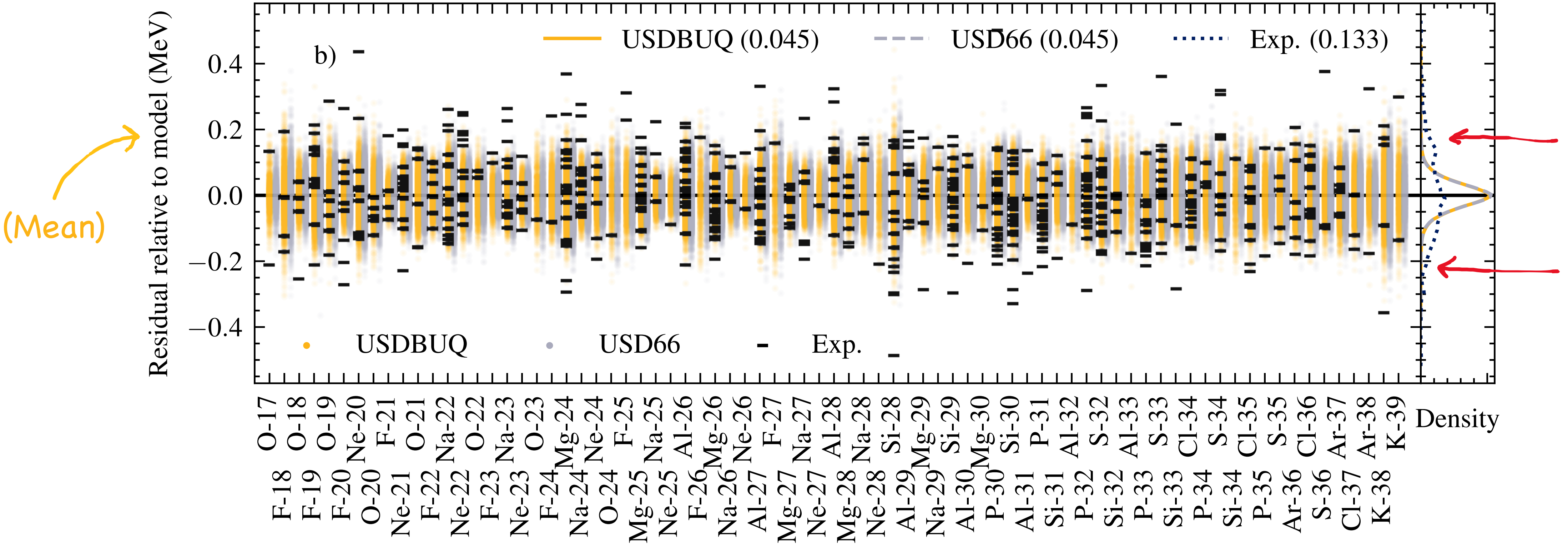




But wait, the error bars do not seem to cover the data!

Let's center the errors on the model:

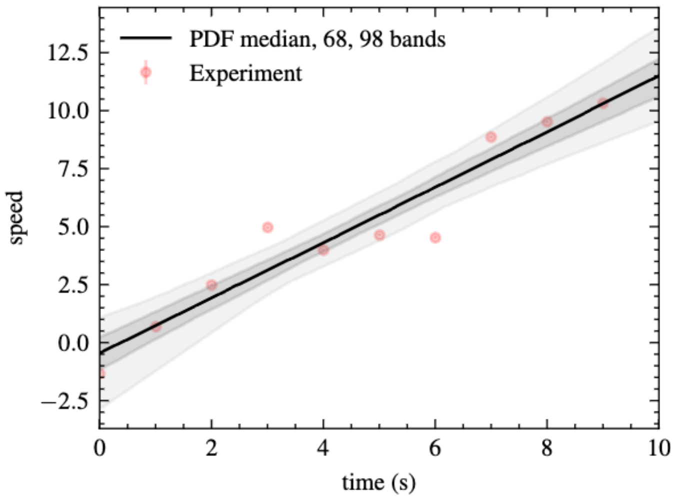
99% **confidence interval** covers only **40%** of the data



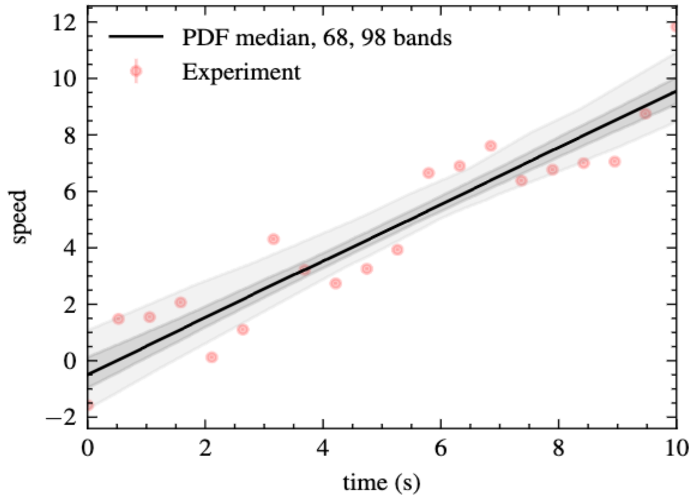
USDBUQ (and previous fits) may be overconfident

With uncorrelated noisy measurements, **confidence intervals shrink** with number of data

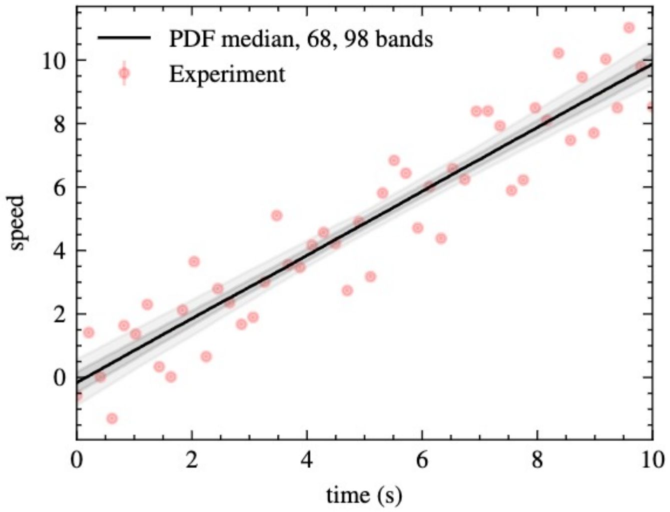
10 data points



20 data points

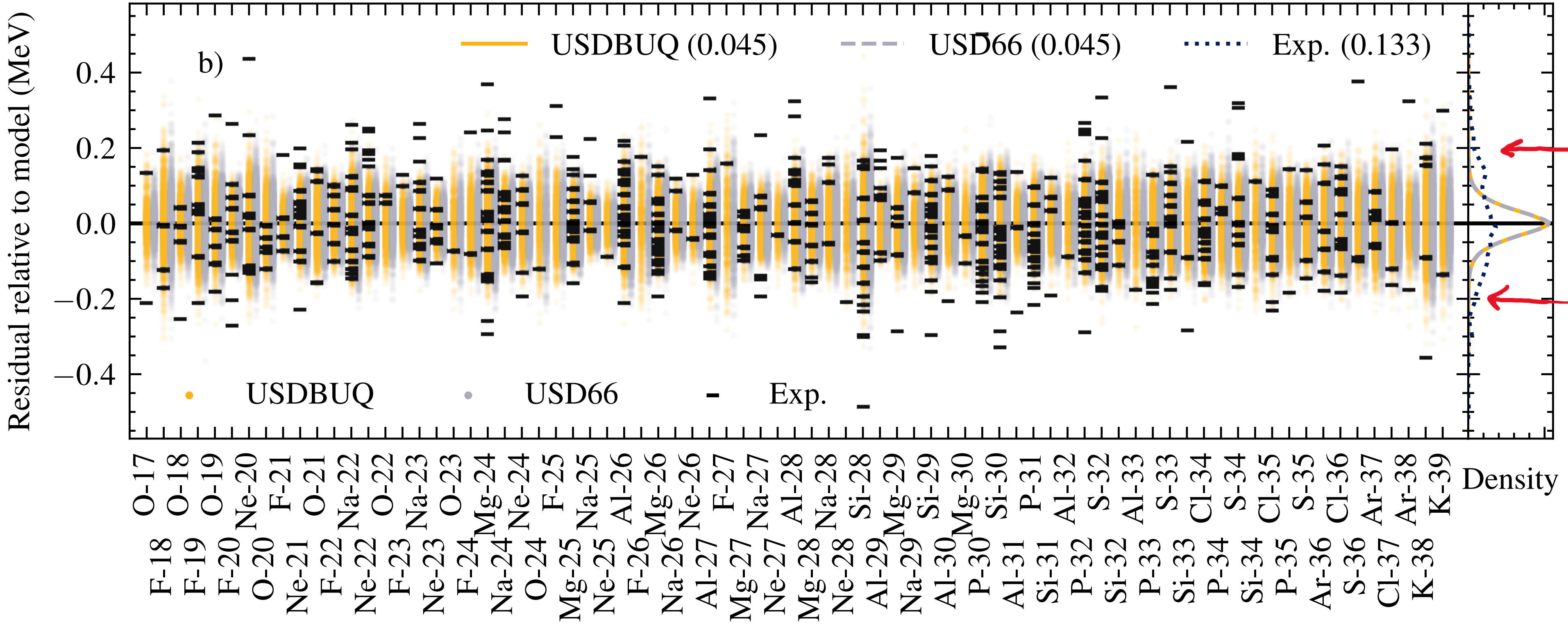


50 data points



"Noise from flawed measurements are washed out"

Residual is dominated by *systematic* and *correlated* model defect, NOT noisy measurement!



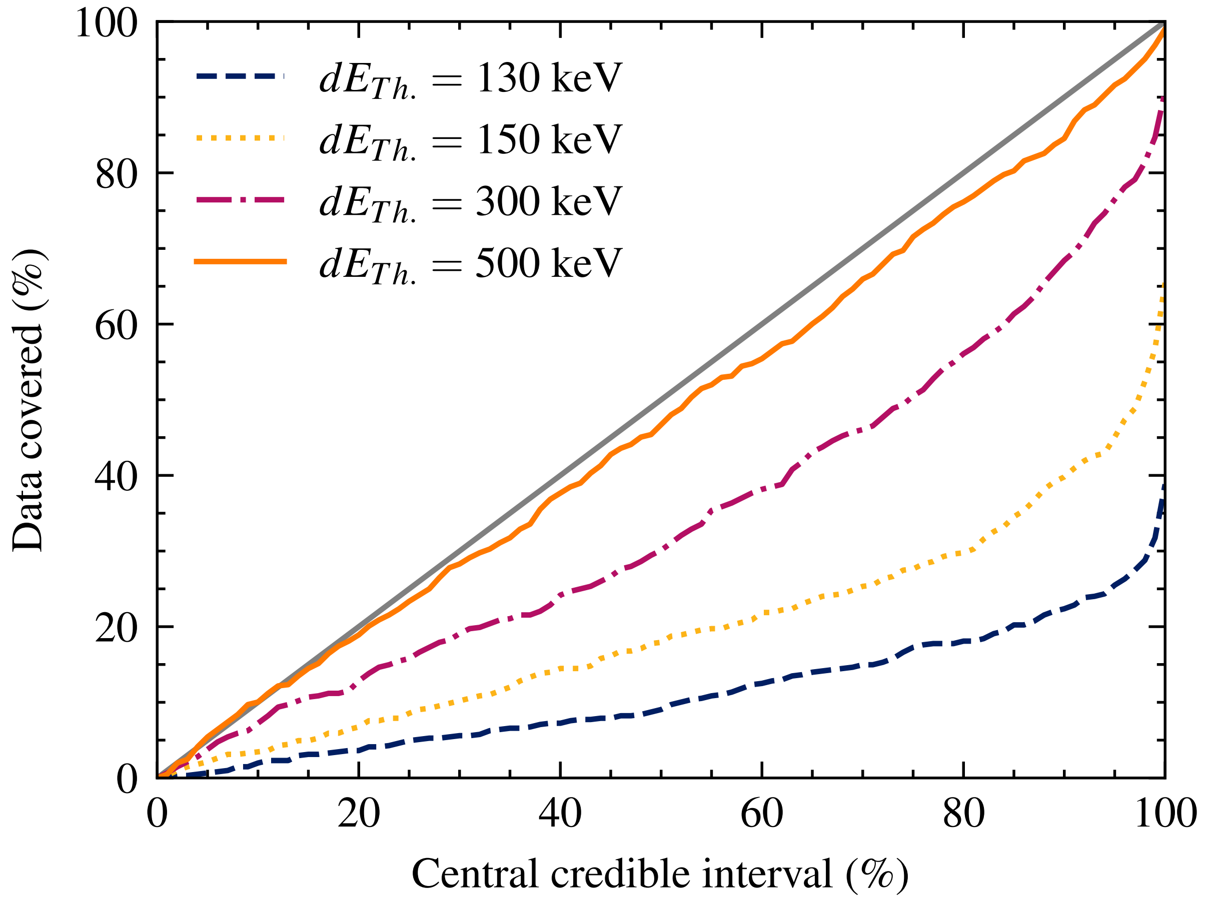
$$\sigma_i^2 = \sigma_i^2(Experiment) + \sigma_i^2(Theory)$$

a few keV << 130 keV

This sets the size of error bars

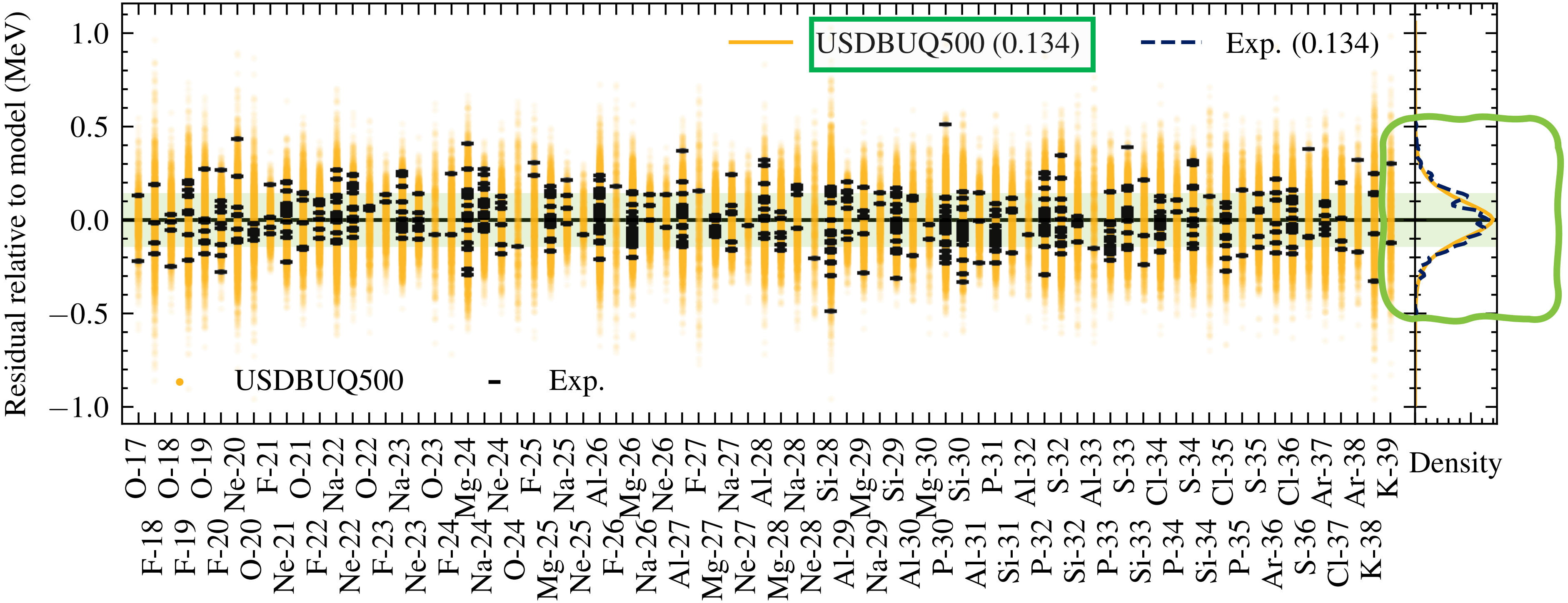
We do NOT want **confidence intervals** to decrease with # of data

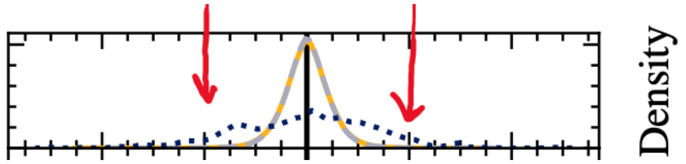
Working solution: empirical data coverage test

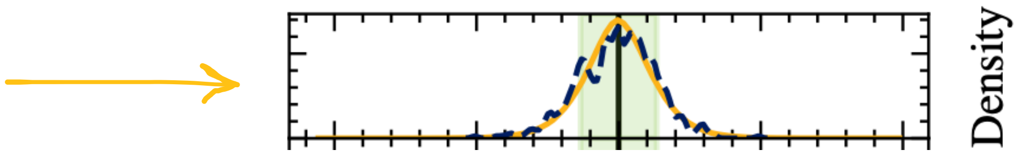


Does this mean the Shell model uncertainty is 500 keV instead of 130 keV?

Takeaway: be careful when applying “textbook” statistics to real problems







500 keV is not actual uncertainty

USDBUQ500 stat sheet

Standard error of **random prediction**:

- 190 keV (USDB is 130 keV)

Standard error of **averaged prediction:**

- 134 keV

Average half-width of **error bar**:

- 134 keV

Preprint available: arXiv 2503.11889