Nuclear mass table based on Bayesian estimation of binding energy difference expressions

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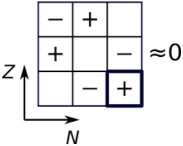
Local mass relations

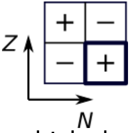
Introduction

Nuclear mass tables based on local mass relations are solutions of partial difference equations $\hat{O}^n W(N,Z) = \tau(N,Z)$. Example: transverse Garvey–Kelson mass equation (homogeneous PDE)



$$M(N+2, Z-2) - M(N,Z) + M(N+1,Z) -$$
$$-M(N+2, Z-1) + M(N, Z-1) - M(N+1, Z-2) \approx 0$$

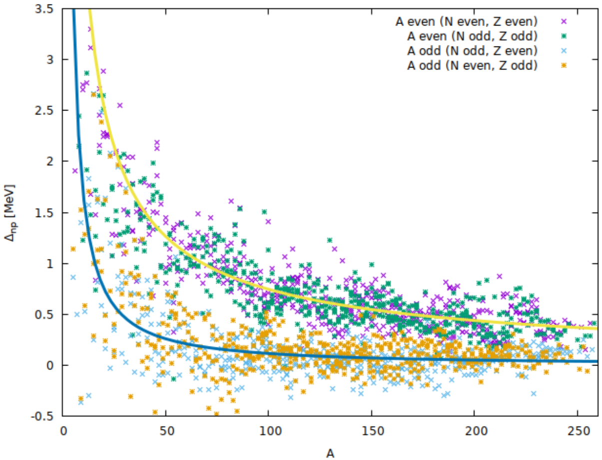
This work as continuation of [Vladimirova et al., AIP Conf. 2377, 070003 (2021)] uses the residual *pn*-interaction energy



$$\Delta_{np}(N,Z) = B_d(N,Z) - B_n(N,Z-1) - B_p(N-1,Z),$$

which determines an inhomogenous PDE.

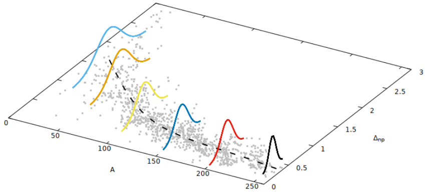
Behaviour of $\Delta_{np}(A)$ for medium and heavy nuclei



(Data from AME2020)

As a function of the mass number Δ_{np} separates into 2 branches for odd and even A and shows little dependence on shell effects or pairing.

Estimation of $\Delta_{np}(A)$ using the Bayes theorem



$$P_{\text{post}}(\theta|x) = \frac{L(x|\theta)P_{\text{prior}}(\theta)}{P(x)}$$

$P_{\text{posterior}}(\theta|x)$ — posterior distribution of θ, x — observed data, $L(x|\theta)$ — likelihood function, $P_{\text{prior}}(\theta)$ — prior distribution of θ, $P(x)$ — marginal distribution.

"Prior knowledge" + "data" $\rightarrow$ "posterior knowledge"

Treat experimental Δ_{np}^{exp} at each point as random values with normal distribution $\Delta_{np}(A) \sim N(\mu_A, \sigma_A^2)$.

$$\ln L(\{\Delta_{np}^{\text{exp}}\}|\{\mu\},\{\sigma^2\}) = \sum_{A=A_{\min}}^{A_{\max}} \sum_{\substack{\Delta_{np,i}^{\text{exp}} \\ \text{for this } A}} \ln N(\Delta_{np,i}^{\text{exp}}|\mu_A, \sigma_A^2)$$

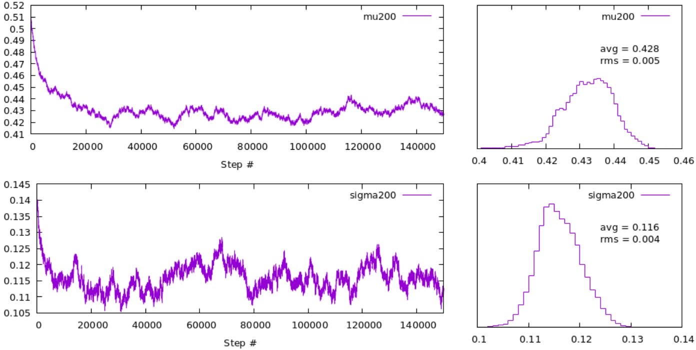
Regularization condition

- Smoothness of $\Delta_{np}(A)$ results from Tikhonov's regularization condition on $\mu(A)$ and $\sigma(A)$ and can be interpreted as prior knowledge.
- Originally, Tikhonov's regularization was formulated for the least squares method: $\chi^2_{\text{reg}} = \chi^2 + \tau||\theta||^2$, where τ is the regularization parameter. Penalty on high amplitude of θ.
- Expressed as prior distribution:
  $\ln P_{\text{prior}}(\theta) = -\tau||\theta||^2 = -\tau(\sum \mu_A^2 + \sum \sigma_A^2)$.
- Derivative: $\ln P_{\text{prior}}(\theta) = -\tau(\sum(\mu_{A+1} - \mu_A)^2 + \sum(\sigma_{A+1} - \sigma_A)^2)$.
- 2nd derivative:
  $\ln P_{\text{prior}}(\theta) = -\tau(\sum(2\mu_{A+1} - \mu_A - \mu_{A+2})^2 + \sum(2\sigma_{A+1} - \sigma_A - \sigma_{A+2})^2)$.

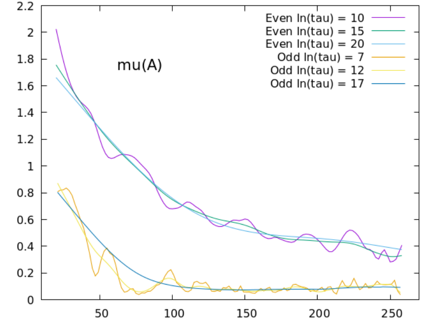
MCMC method

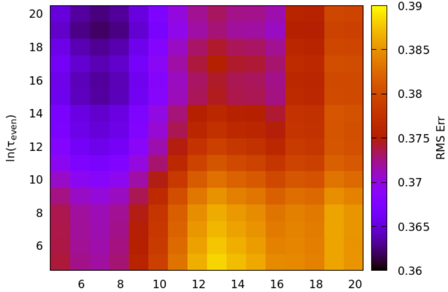
Bayesian estimates of $\{\mu\}$ and $\{\sigma\}$ are obtained by sampling from the posterior distribution with the MH algorithm of random walk:

1. Randomly generate new $\{\mu, \sigma^2\}_{t+1}$.
2. Calculate $\alpha = \frac{L(\{\Delta_{np}^{\text{exp}}\}|\{\mu,\sigma^2\}_{t+1})P_{\text{prior}}(\{\mu,\sigma^2\}_{t+1})}{L(\{\Delta_{np}^{\text{exp}}\}|\{\mu,\sigma^2\}_{t})P_{\text{prior}}(\{\mu,\sigma^2\}_{t})}$.
3. Accept $\{\mu, \sigma^2\}_{t+1}$ with probability α, otherwise accept $\{\mu, \sigma^2\}_{t}$.
4. Go to step 1.



Choice of regularization parameters



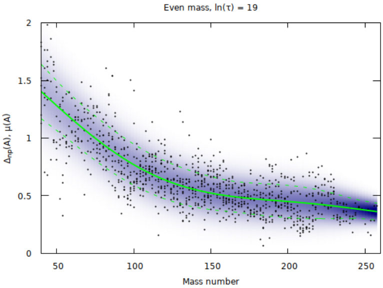


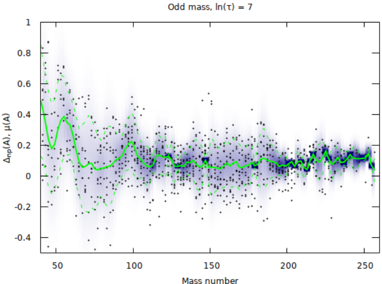
For each $\tau_{\text{odd,even}}$: use AME2016 to predict masses of 65 new nuclei in AME2020, calculate RMS error of prediction. Best $\ln \tau_{\text{odd}} = 7$, $\ln \tau_{\text{even}} = 19$.

Model	RMS Err [keV]
MCMC	361.9
No MCMC (LMR)	376.5
FRMD2016	909.2
HFB-17	729.6
DZ10*	815.2
DZ10GP*	289.1

* No ^{46}Mn, ^{50}Co, ^{73}Rb, ^{211}Pa in DZ10(GP).

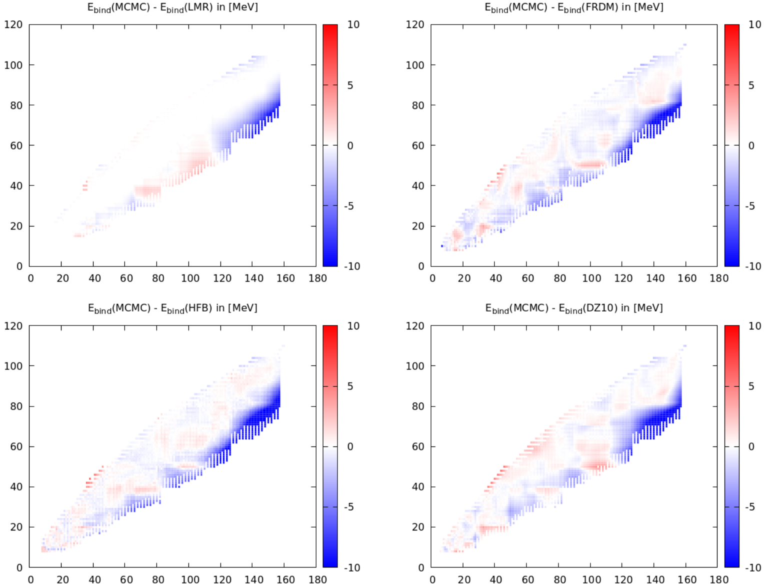
Obtained estimates of Δ_{np}



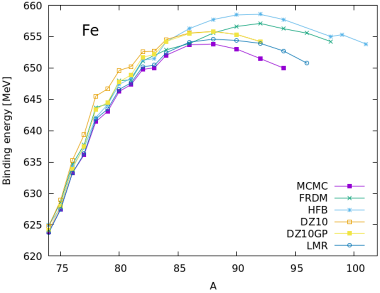


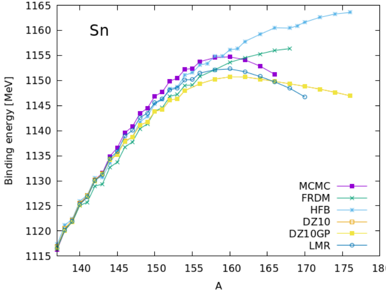
Comparison of predicted binding energies

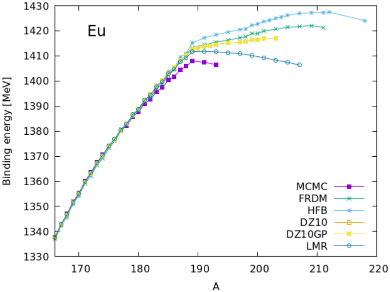
Use Δ_{np} estimates to extrapolate AME2016

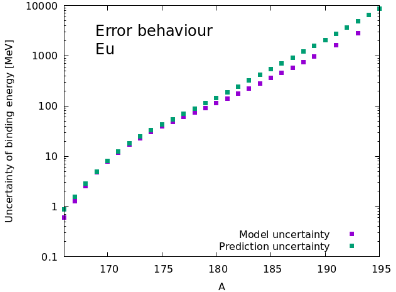


Comparison of predicted binding energies



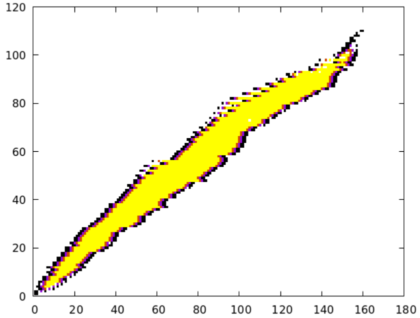


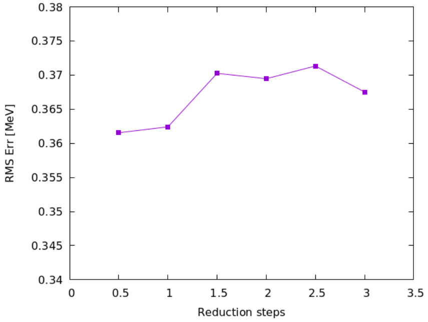




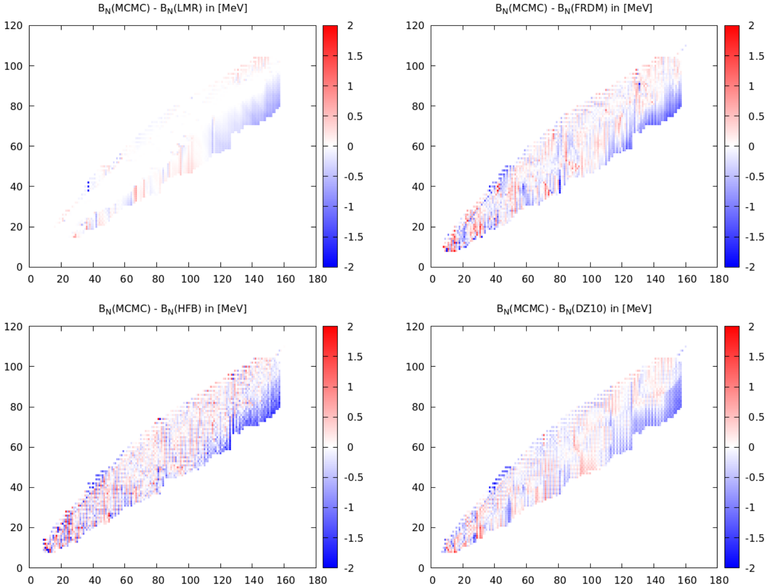
Stability of prediction

Reduce number of nuclei in AME2016 layer-by-layer, calculate RMS error.





Comparison of predicted neutron thresholds



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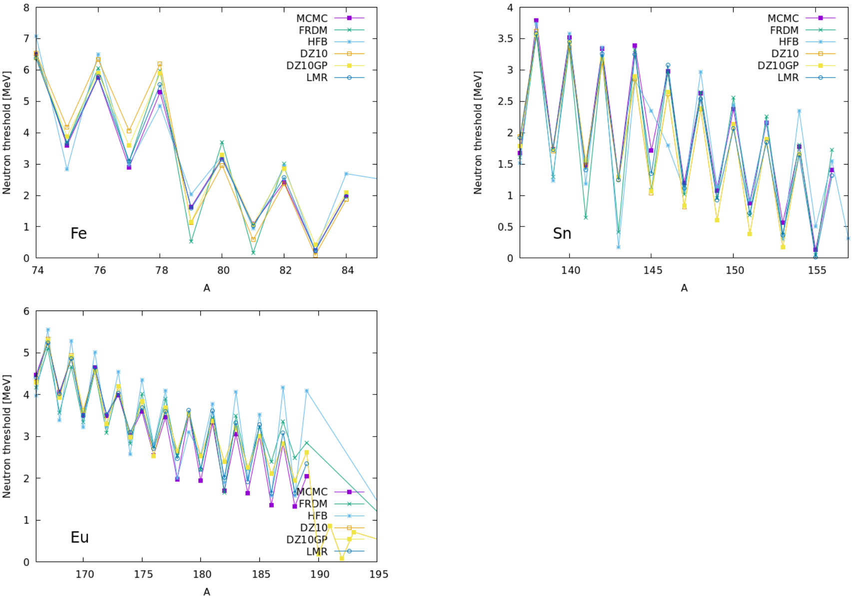
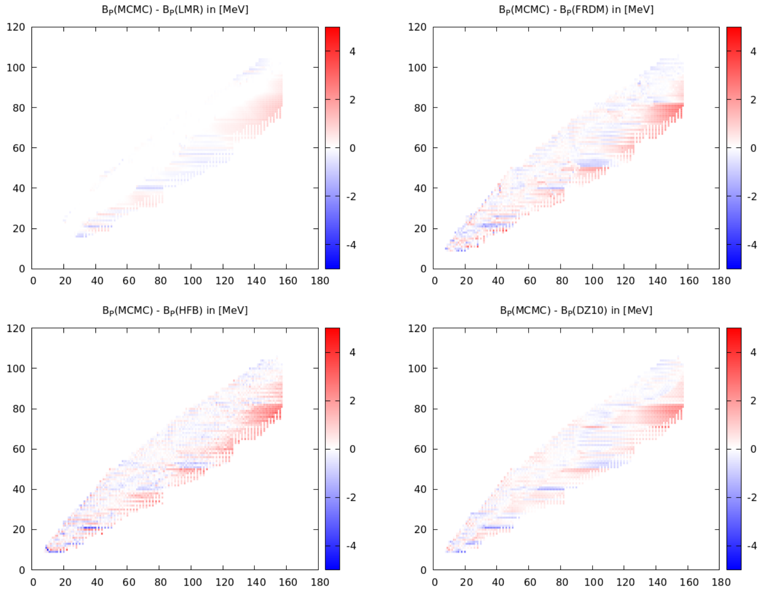


Comparison of predicted proton thresholds



Conclusions

- Nuclear mass model based on Bayesian estimation of Δ_{np} is described.
- Very simple Monte-Carlo computation method: no numeric minimization, root finding, etc.
- Obtained RMS error value of 0.36 MeV is an improvement in comparison to the older version.
- Error scales quadratically with number of steps.
- $\Delta_{np}(A)$ shows preference for non-smooth behaviour for odd-A nuclei.

Thank you!