MSU Faculty of Physics
Skobeltsyn Institute of Nuclear Physics

NEW MASS EVALUATION AND ITS IMPLICATION FOR THE NEUTRON-RICH NUCLEOSYNTHESIS PRODUCT YIELD

JINR

St Petersburg University

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Nuclear physics and elementary particle physics
Nuclear physics technologies

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Objectives

1. Binding energies predictions

local mass relations – math formulas, including few binding energies

- 1969: First applied (Garvey and Kelson)
- 1969: Formula describing the np-pairing Δ_{np} (Kravtsov)
- 1974: Estimation the binding energy with Δ_{np} (Janecke)
...
- 2012: Estimation the binding energy with Δ_{np} on AME 2012 (Jiang)

- *understanding of different mass relations improved*
- *experimental database significantly increased*

- Our previous works: estimate the binding energy with Δ_{np} based on AME 2016 for heavy nuclei with new approximations
- This work: application of new approximation approaches, estimate the binding energy with Δ_{np} for SHE and drip lines area

2. R-process nucleosynthesis calculations using numeric model based on the SkyNet library to obtain final mass distributions of r-process products at the temperature of 1.2 GK

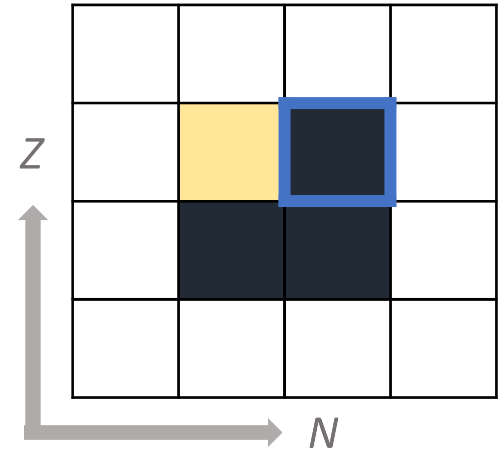
- Calculations were performed using different mass models including Δ_{np} calculations

Residual *np*-interaction and mass predictions

Mass relations for *np*-correlations:

$$\Delta_{np}(Z,N) = \left[S_p(Z,N) - S_p(Z,N-1)\right] =$$
$$= [B(Z,N) - B(Z,N-1)] - [B(Z-1,N) - B(Z-1,N-1)]$$

[Kravtsov V.A. Sov. Phys. JETP. 1959]

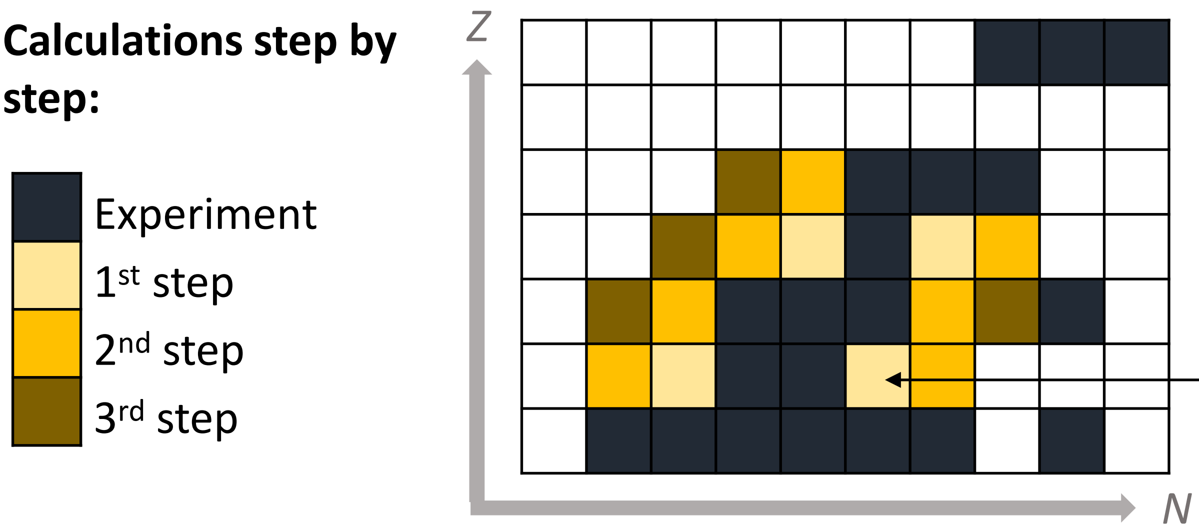


Predicted binding energy (1 of 4 possible formulas):

$$B_{pred}(Z,N-1) =$$
$$= B(Z,N) - B(Z-1,N) + B(Z-1,N-1) - \Delta_{np}^{cal}(Z,N)$$

[J. Janecke, H. Behrens // Phys. Rev. C 1974]

Calculations step by step:



The binding energy of such nucleus can be expressed from 2 Δ_{np} => their averaging is used

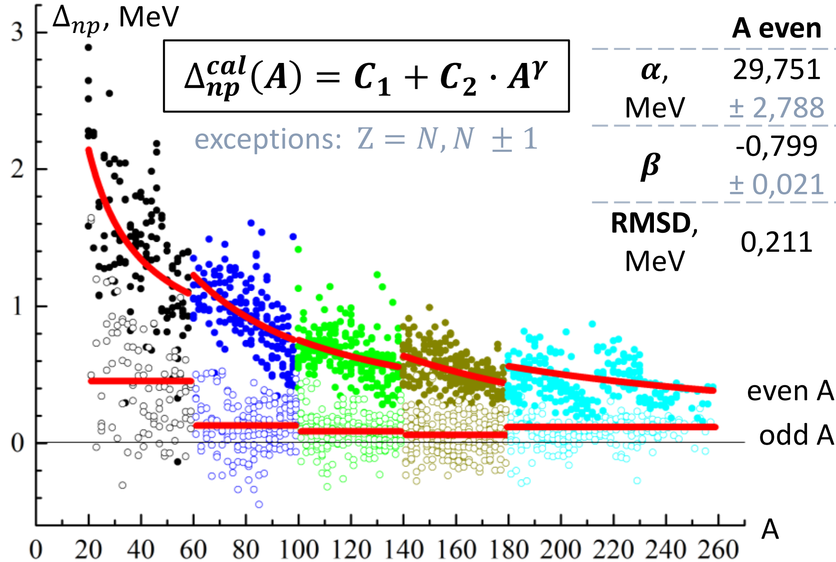
Method predictive power – accuracy of previous results

1. Predictions by Δ_{np}

$$\Delta_{np}^{cal}(A) = C_1 + C_2 \cdot A^{\gamma}$$

exceptions: $Z = N, N \pm 1$

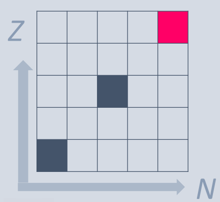
	A even	A odd
α, MeV	29,751 ± 2,788	44,251 ± 21,926
β	-0,799 ± 0,021	-1,294 ± 0,116
RMSD, MeV	0,211	0,182



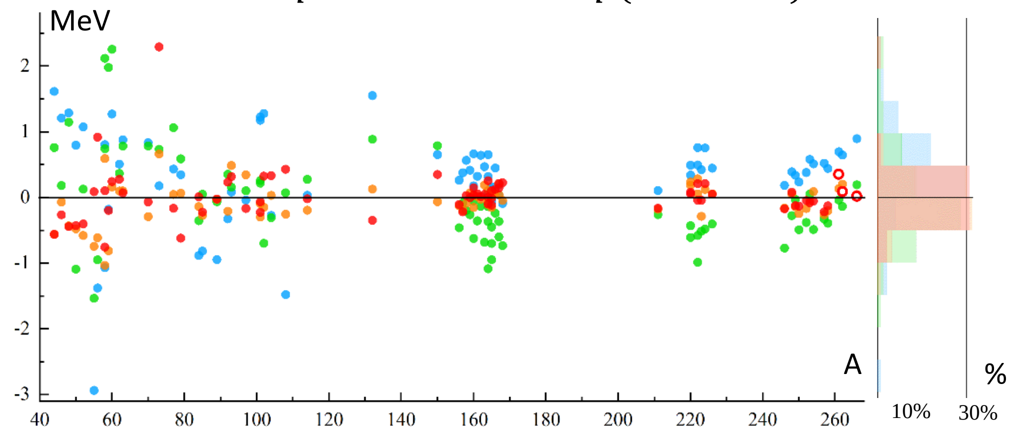
2. Prediction extension with machine learning

Preliminary results

- ✓ **SVR** (support vector regression) algorithm
- ✓ Energies of neighboring nuclei ate using as input parameters: **B/A(N, Z) prediction based on the B/A of nuclei (N–2, Z–2) and (N–4, Z–4)**
- ✓ **Input array of experimental data AME 2016 expanded with Δ_{np} estimates** (steps ⩽ 15)
- ✓ The result is stable for at least 2 iterations of the ML algorithm

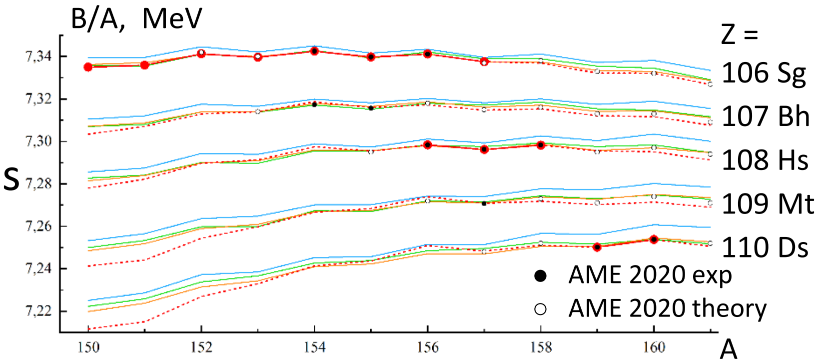


Difference $B_{predicted} - B_{exp(AME2020)}$

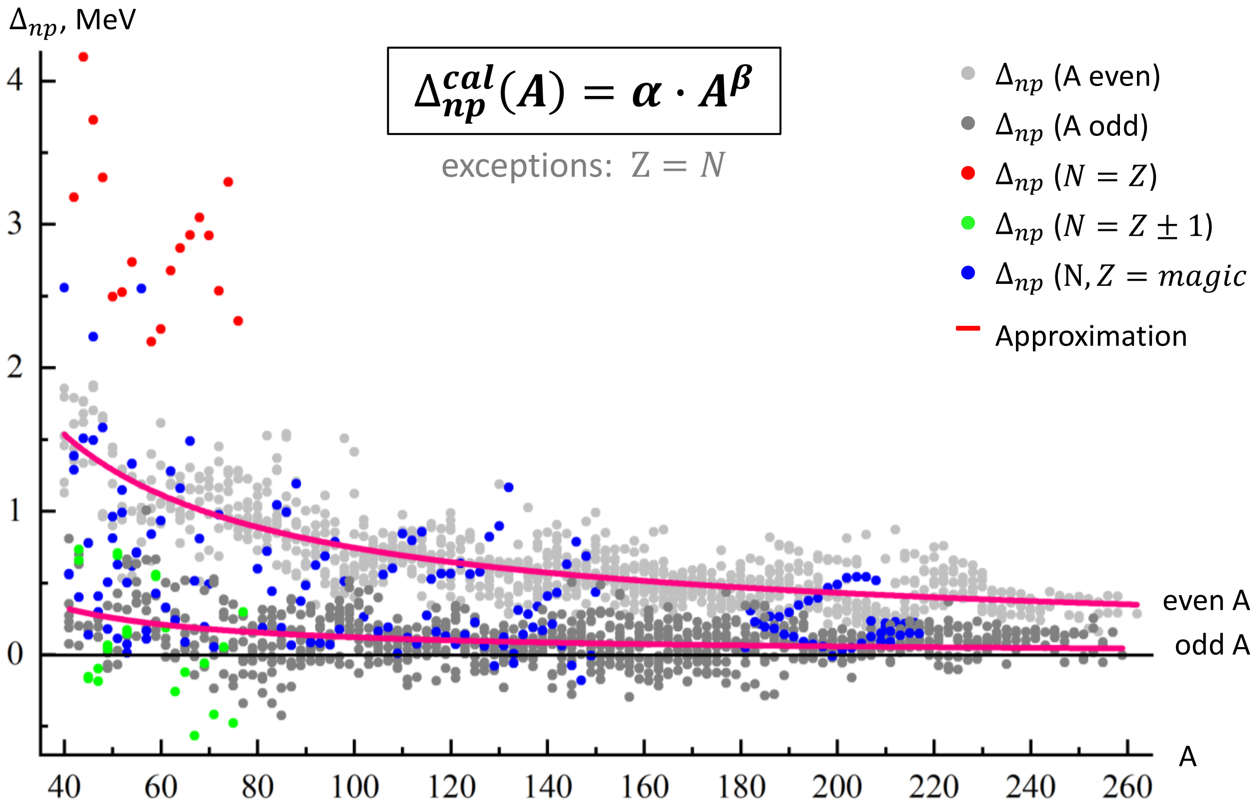


	RMSD, keV
Result by Δ_{np}	381
Result by Δ_{np} + ML	376
Weizsaecker-Skyrme WS+RBF (macro-microscopic) [Na-Na Ma et al., 2019. Chinese Phys. C. 2019. 43]	298
Hartree-Fock + Skyrme HFB-24 model (microscopic) [Goriely S. et al., Phys. Rev. Lett. 2017. 102. 152503]	715
Finite-Range Droplet Model FRDM (macro-microscopic) [Moller P. et al., ADNDT. 59. 185]	791

Binding energy predictions



New approximations – AME2020 data



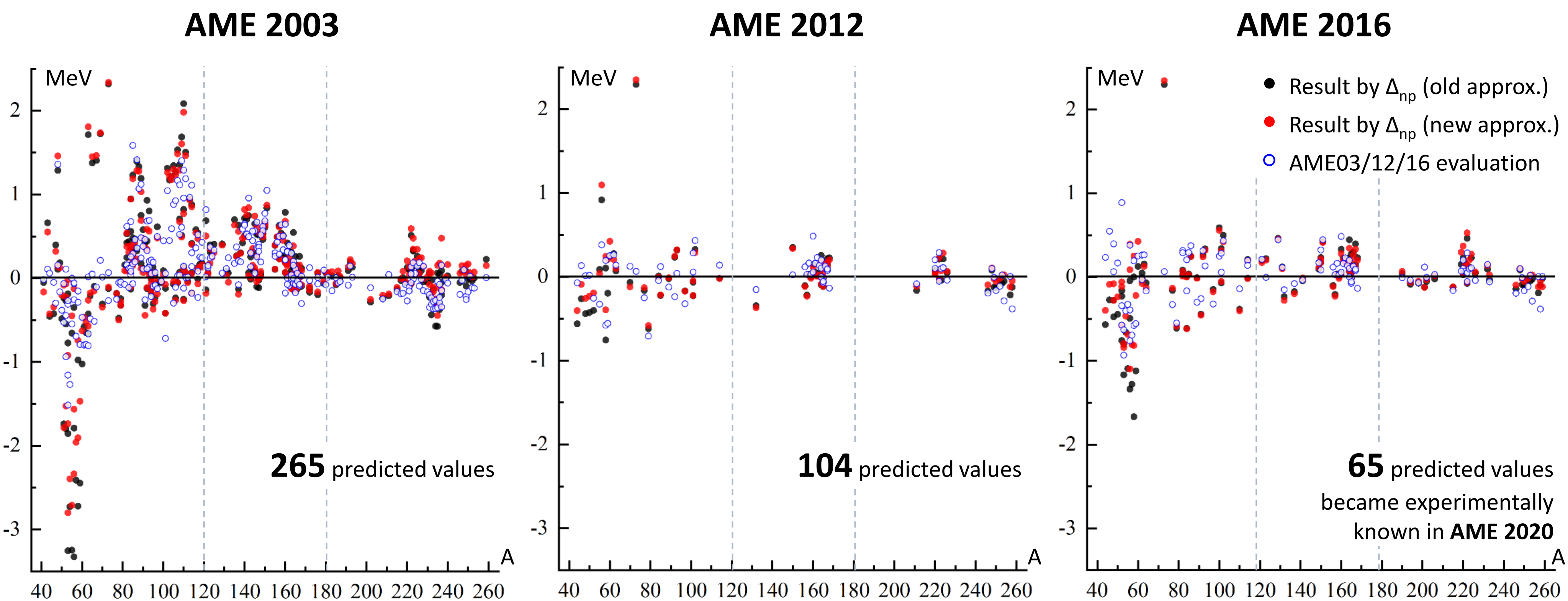
AME	A even 2003	A even 2012	A even 2016	A even 2020	A odd 2003	A odd 2012	A odd 2016	A odd 2020
α, MeV	29,751 ± 2,788	26,061 ± 2,077	25,186 ± 2,062	28,218 ± 2,169	44,251 ± 21,926	24,380 ± 10,548	25,158 ± 10,636	17,277 ± 6,628
β	-0,799 ± 0,021	-0,770 ± 0,018	-0,764 ± 0,018	-0,789 ± 0,017	-1,294 ± 0,116	-1,164 ± 0,099	-1,167 ± 0,097	-1,076 ± 0,088
RMSD, MeV	0,211	0,185	0,193	0,181	0,182	0,163	0,165	0,158

«A» dependence discussion in np pairwise correlations

- $\sim A^{-1/3}$
  [Wang, Liu J. Phys. Conf. Ser. 420 (2013) 012057]
  [Hilaire et al. Phys. Lett. B 531 (2002) 61-66]
- $\sim A^{-2/3}$
  [Madland, Nix Nucl. Phys. A 476 (1988) 1-38]
- $\sim A^{-1}$
  [Jensen at al. Nucl. Phys. A 431 (1984) 393-418]
- $\sim A^{-1}$ for even A, $const$ for odd A
  [Jiang et al. Phys. Rev. C 85 (2012) 054303]
- $\sim A^{-1}$ – nucleon interactions are of short duration and $|\Psi|^2$ is constant inside the nucleus; $\sim A^{-1/3(-2/3)}$ – wave function concentrates on the nuclear surface
  [Nemirovsky, Adamchuk Nucl. Phys. 39 (1962) 551-562]

Method reliability – results based on AME 2003, 2012, 2016

Deviations of estimates and experimental data AME 2020

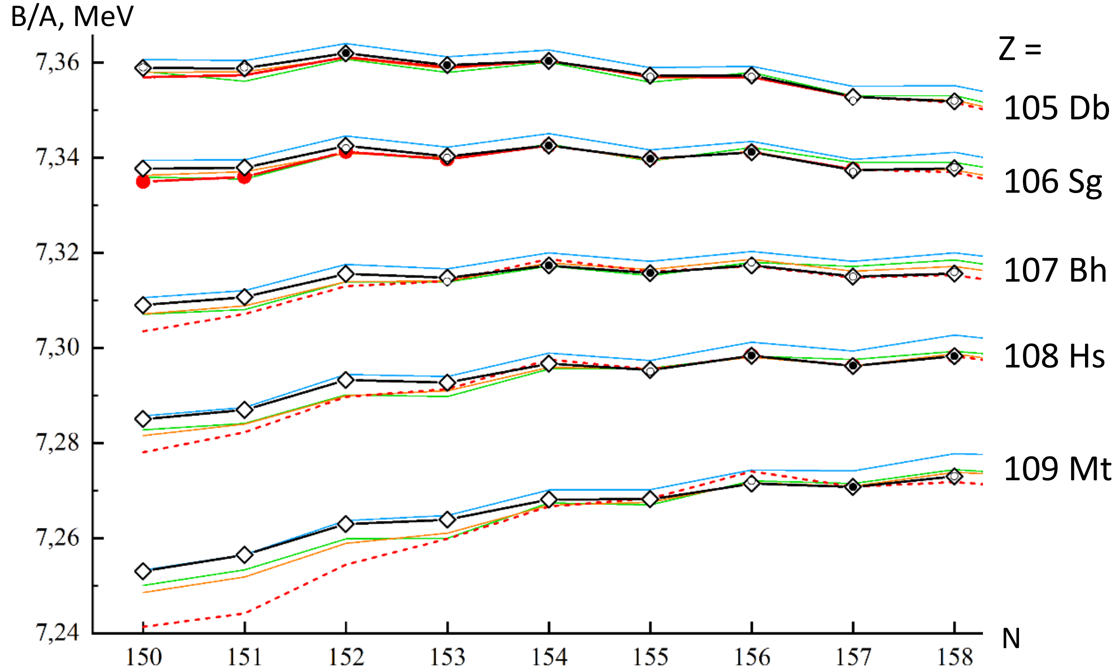


RMSD, keV [predictions – exp AME 2020]	**AME 2003** all	A ≥ 120	A ≥ 180	**AME 2012** all	A ≥ 120	A ≥ 180	**AME 2016** all	A ≥ 120	A ≥ 180
Result by Δ_{np} (old approx.)	747	308	201	466	192	139	381	149	127
Result by Δ_{np} (new approx.)	664	301	201	384	190	165	372	134	108
AME03/12/16 evaluation	455	315	178	293	169	139	223	162	169

2-15% improving predictions based on AME 2016 accuracy in different A-zones

Binding energy predictions for SHE (B/A)

1. Result by Δ_{np} approximation only



- ◇ - New result by Δ_{np} with AME 2020

● AME 2020 exp

○ AME 2020 theory

-●- Old result by Δ_{np} with AME 2016

- - - Old result by Δ_{np} with AME 2016 + ML

— Weizsaecker-Skyrme WS+RBF (macro-microscopic) [Na-Na Ma et al., 2019. Chinese Phys. C. 2019. 43]

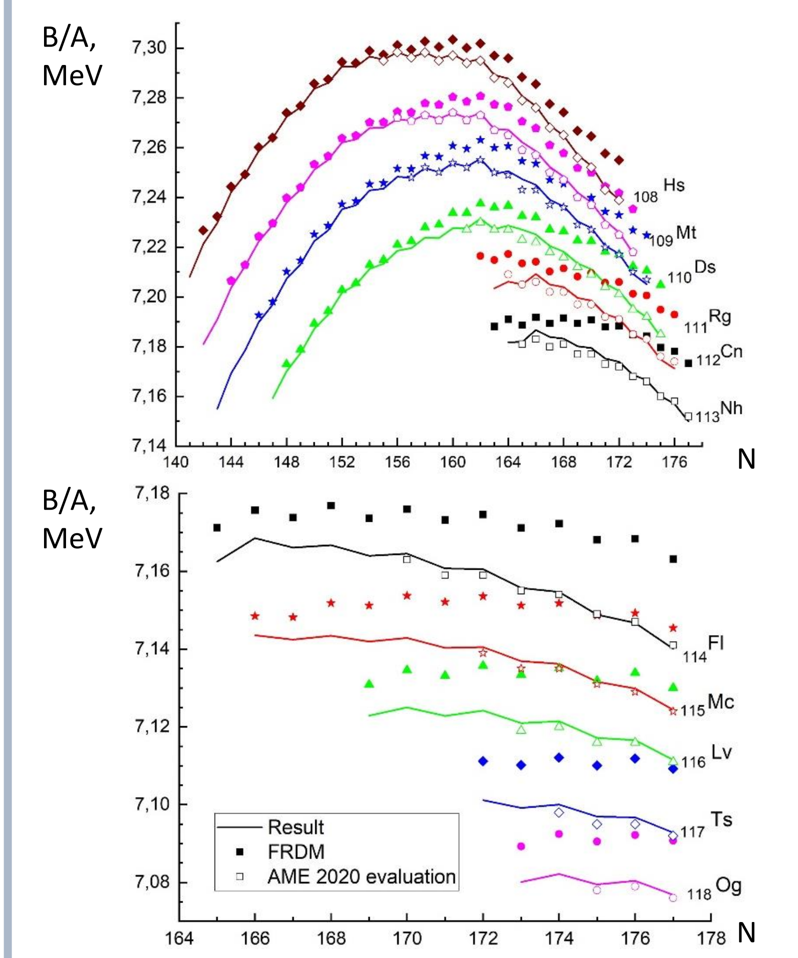
— Hartree-Fock + Skyrme HFB-24 model (microscopic) [Goriely S. et al., Phys. Rev. Lett. 2017. 102. 152503]

— Finite-Range Droplet Model FRDM (macro-microscopic) [Moller P. et al., ADNDT. 59. 185]

2. Result by Δ_{np} + Q_α

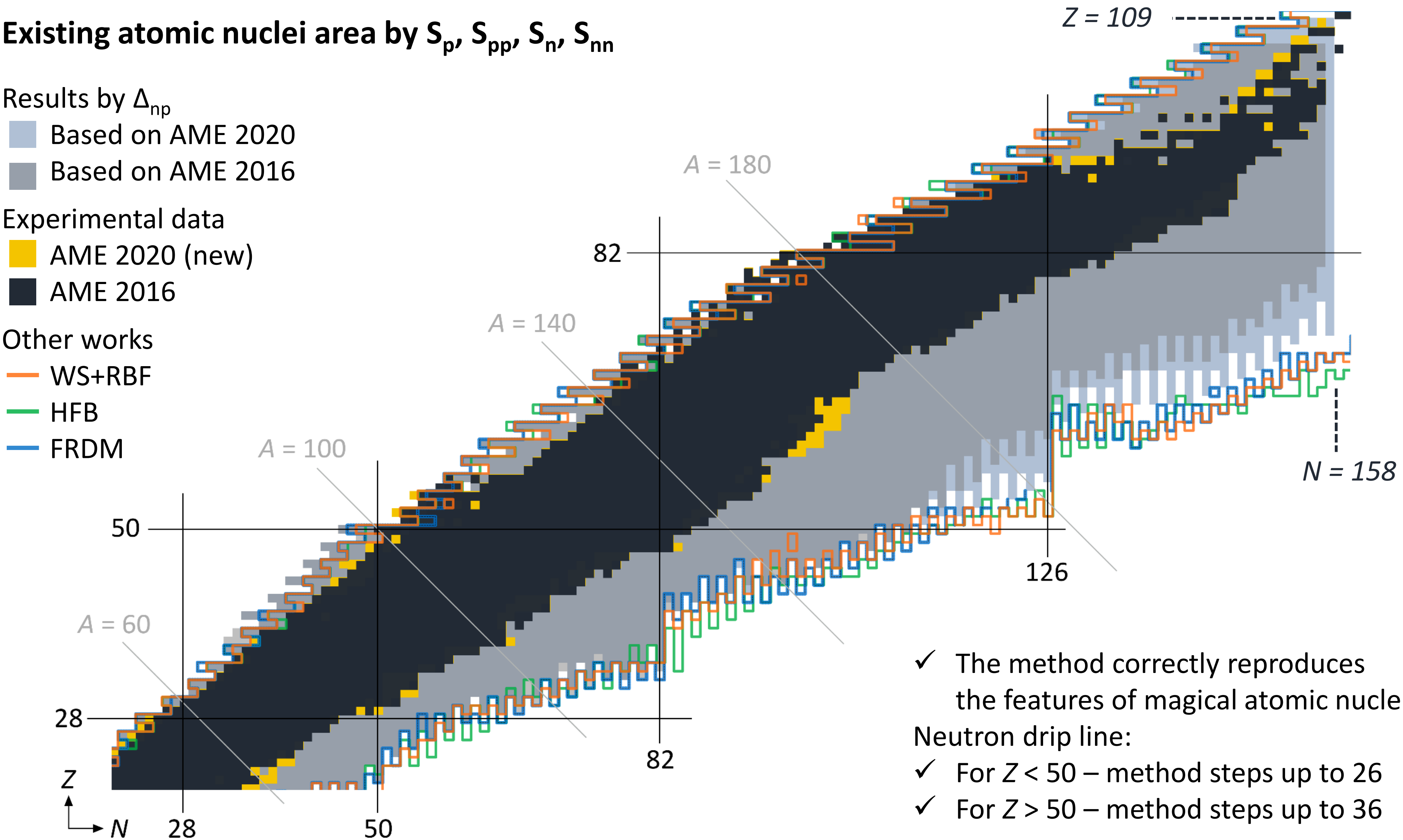
«Alpha decay characteristics of SHE»

Ivan Mostakov et al. (poster section)



Results for drip lines

Existing atomic nuclei area by S_p, S_{pp}, S_n, S_{nn}



- ✓ The method correctly reproduces the features of magical atomic nuclei

Neutron drip line:

- ✓ For $Z < 50$ – method steps up to 26
- ✓ For $Z > 50$ – method steps up to 36

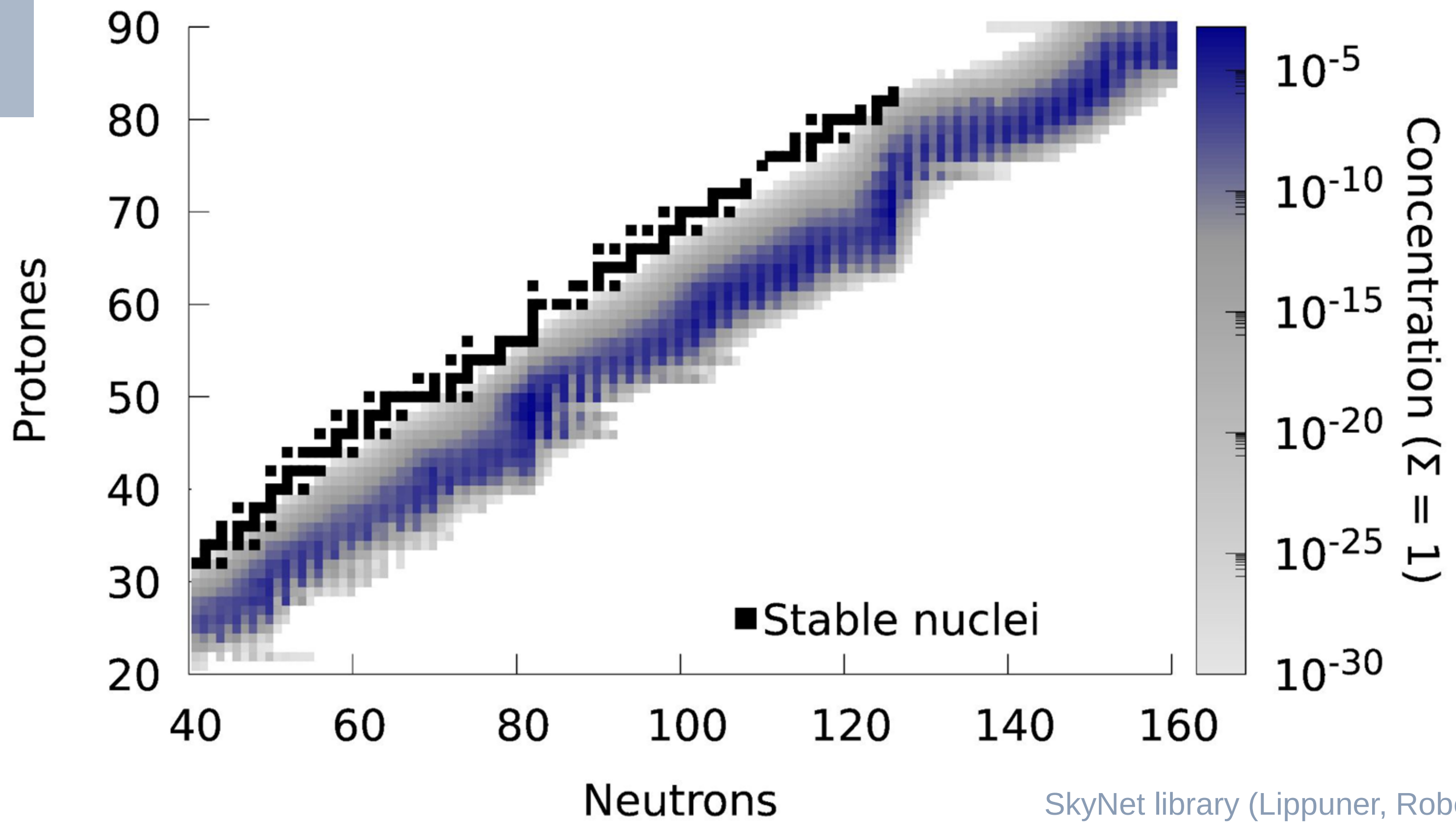
Method validation through r-process simulation

«Sensitivity of r-process simulation to choice of the mass model»
Negrebetskiy Vasily (poster section)

Nucleosynthesis simulations depend on theoretical values of **reaction rates**:

$$\frac{dy_i}{dt} = \sum_{k \in K_i} \lambda_k g_k \prod_{l \in L_k} y_l$$

Results of simplified r-process model with standard REACLIB rates

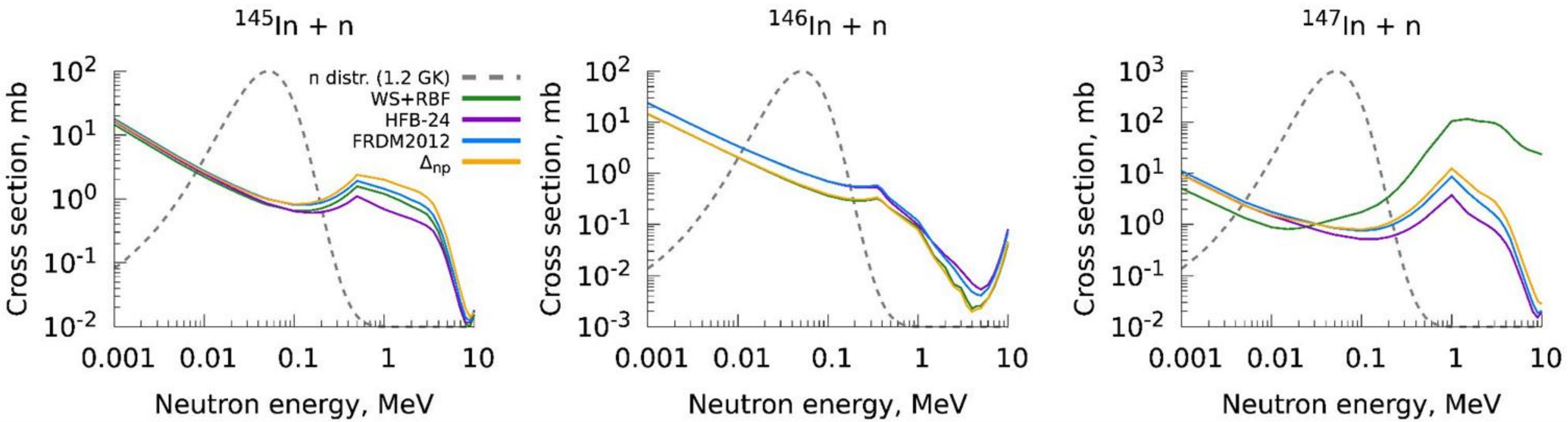


SkyNet library (Lippuner, Roberts, ApJS 2017)

Neutron capture cross sections calculation

Binding energies are essential values for statistical model of nuclear reaction.

Neutron-rich Indium isotopes *(n,γ)* cross sections with different mass models



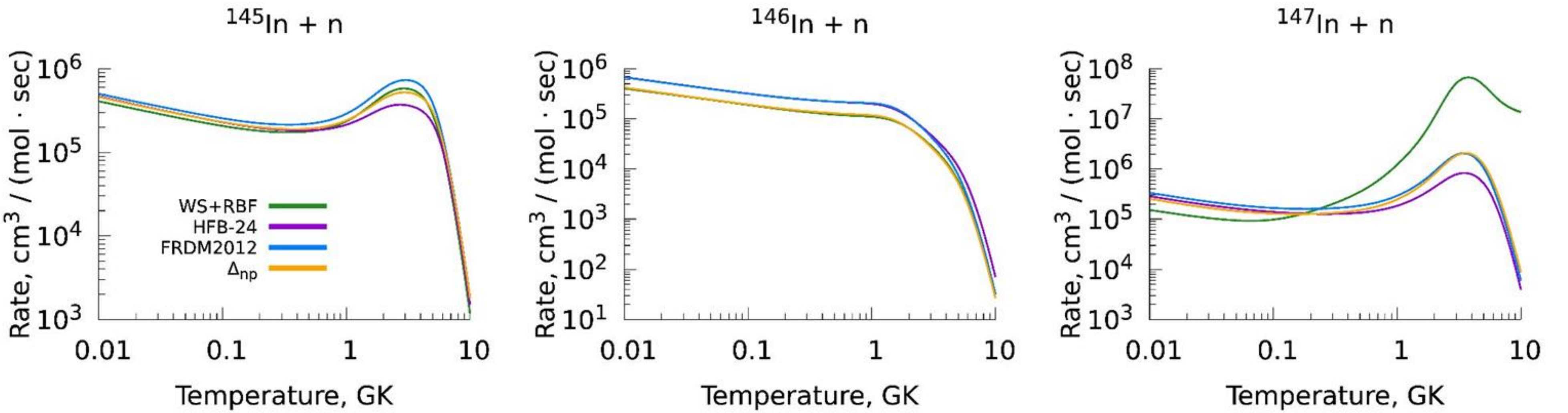
TALYS package (Koning et al., Nucl. D. Sheets. 2019)

Neutron capture rates calculation

Reaction rate calculation through cross sections:

$$\lambda(T) = \sqrt{\frac{8}{\pi m}} \frac{N_A}{(kT)^{3/2} G(T)} \int_0^\infty \sum_\mu \frac{(2I^\mu + 1)}{(2I^0 + 1)} \sigma^\mu(E) E \exp\left(-\frac{E + E_x^\mu}{kT}\right) dE$$

Neutron-rich Indium isotopes *(n,γ)* rates with different mass models

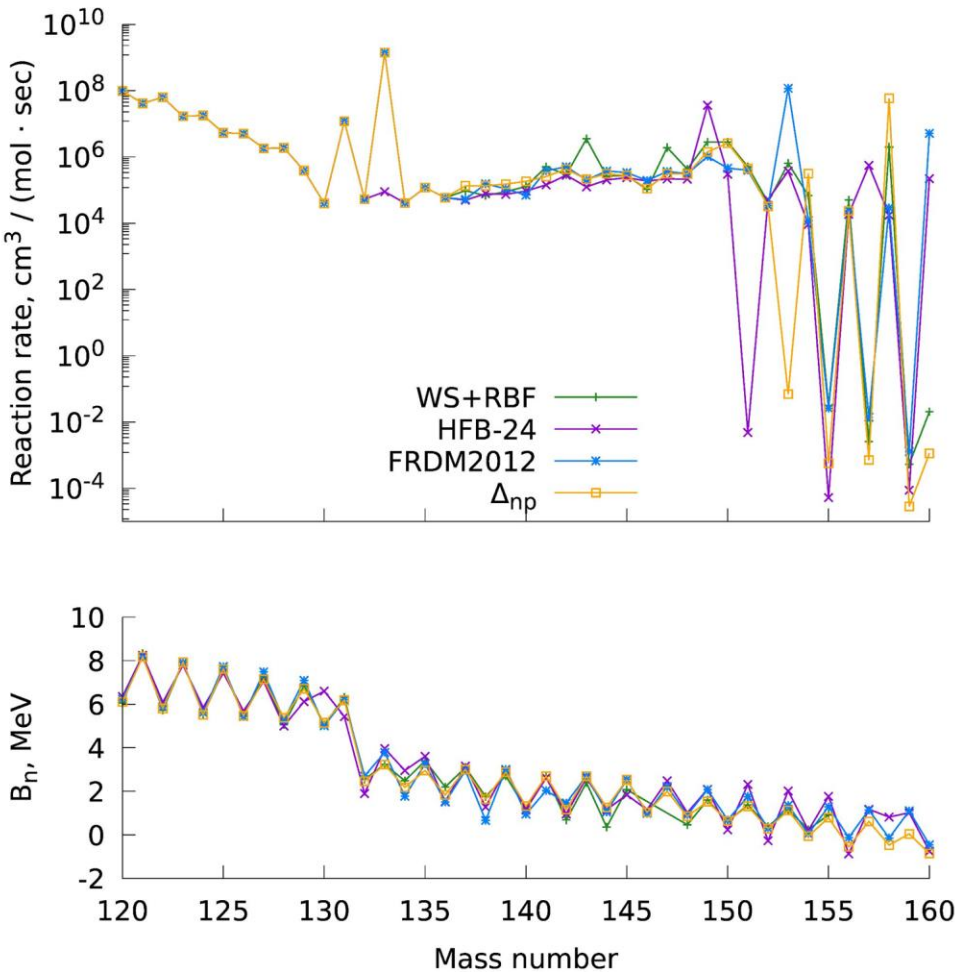


TALYS package (Koning et al., Nucl. D. Sheets. 2019)

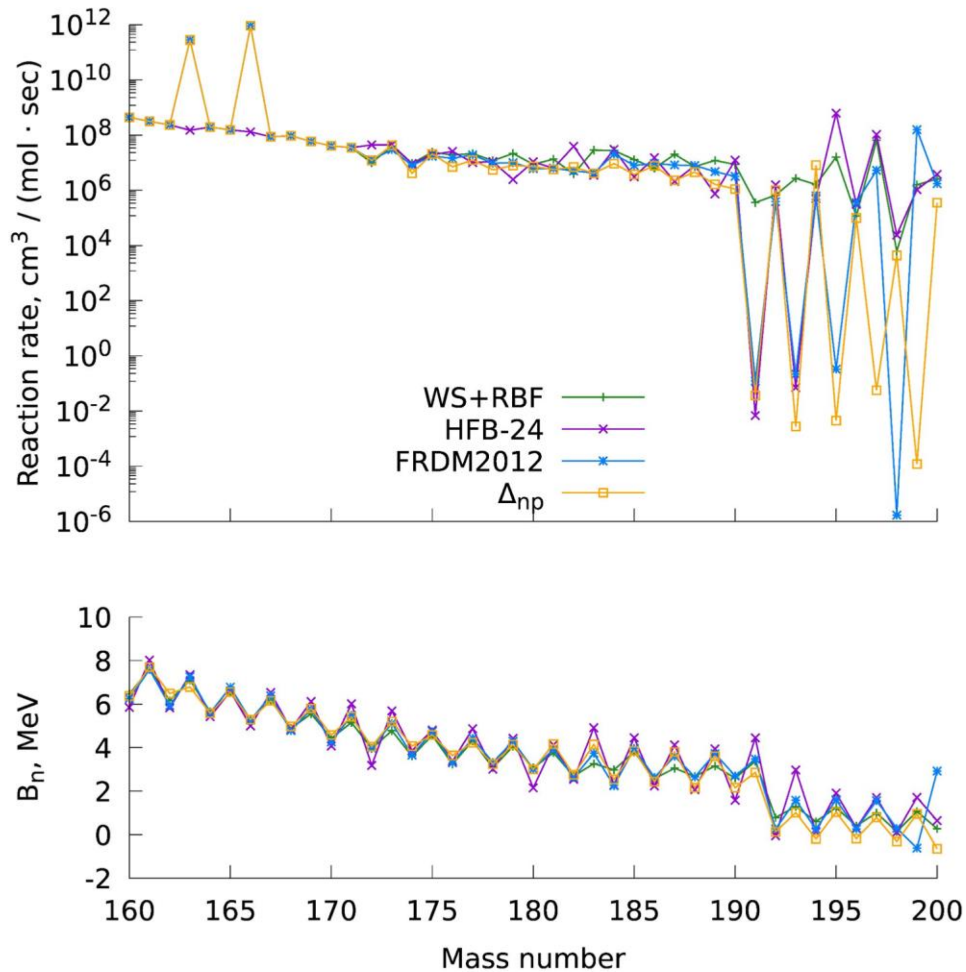
Sensitivity of (n,γ) rates to nuclear mass model

Theoretical rates of *(n,γ)* on neutron-rich isotopes

Indium



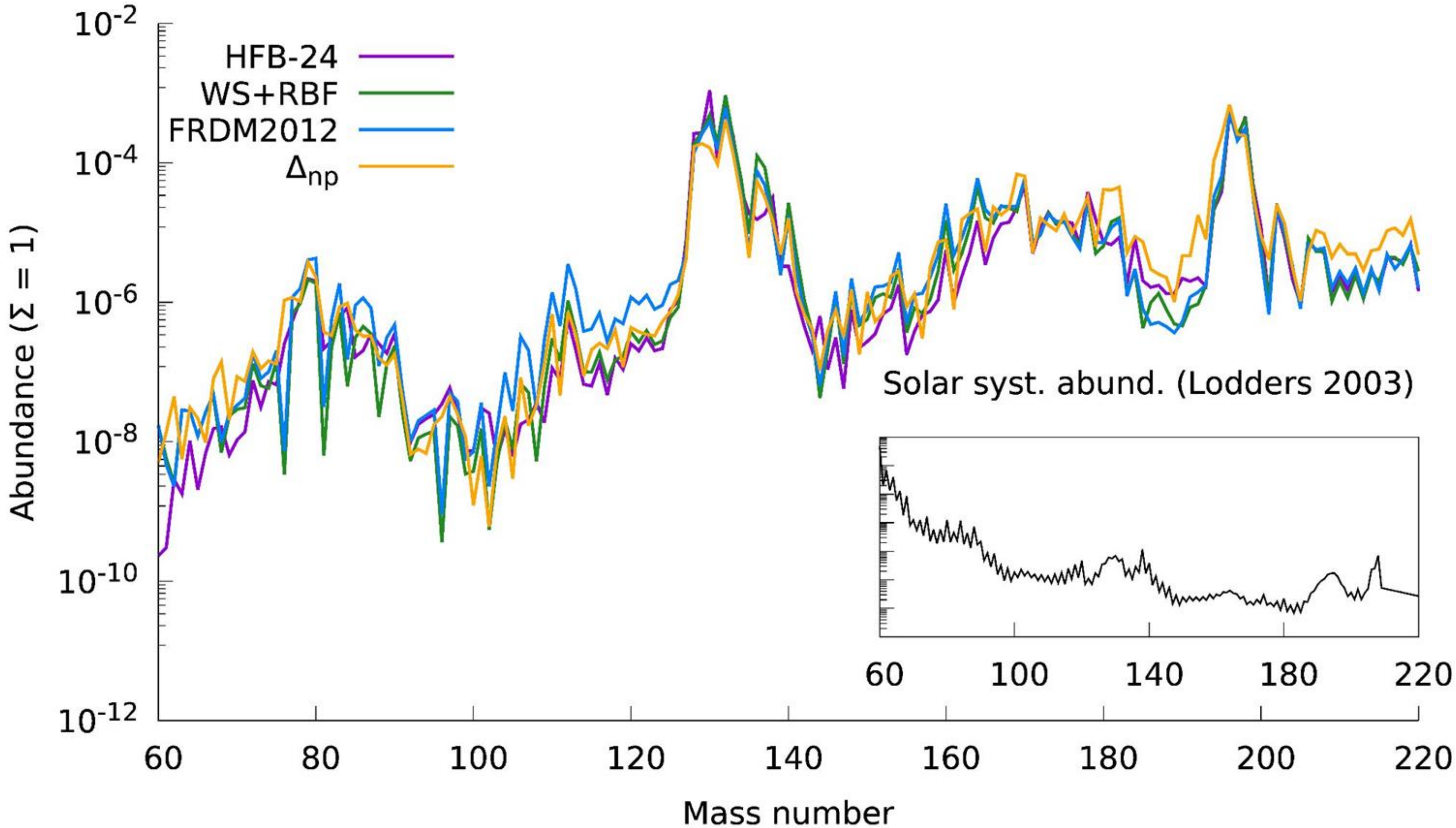
Terbium



r-process yields with different mass models

Preparation of nuclear mass table → Calculation of cross sections and rates (TALYS) → Replacement of REACLIB rates → Calculation of r-process yields (Skynet)

Results of r-process simulation with four mass models

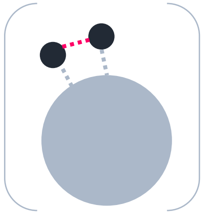


Conclusions

- ✓ Previous binding energies predictions based on Δ_{np} are verified with new experimental data from AME 2020. It is shown that the results accuracy is comparable to the other recent models
- ✓ A new approach to approximation is proposed. Based on several previous AME databases (2003, 2012 and 2016), it is shown that the new approximation improves result by 2-15%
- ✓ New predictions of binding energies based on AME 2020
- ✓ The calculation of the nucleosynthesis r-process product yield is shown. New predictions of binding energies are used to calculate the cross sections for the (*n*, *γ*) reaction

Thank you for your attention!

We would appreciate a detailed discussion about our work
Please feel free to contact!
vladimirova.elena@physics.msu.ru



Machine learning (ML) predictions

Preliminary results

<u>**Objective:** test the applicability of machine learning methods for estimating binding energies</u>

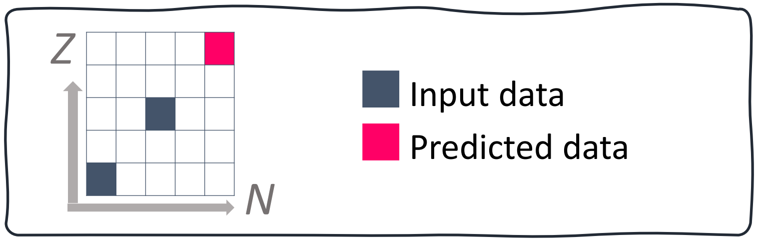
Results:

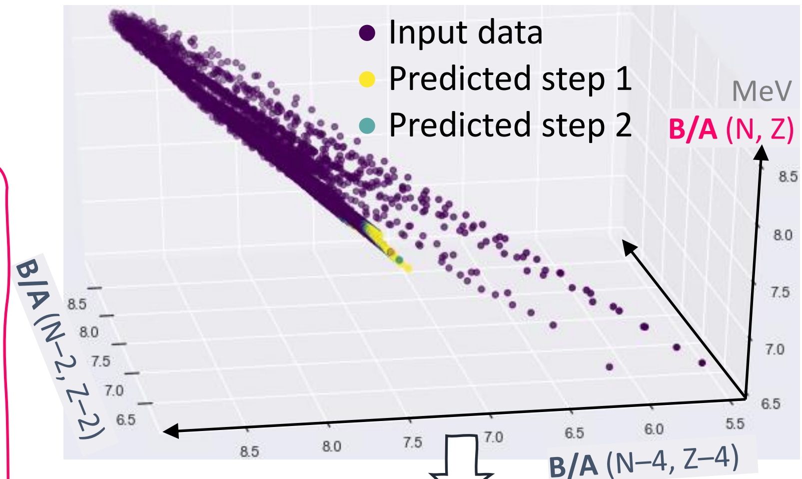
✓ The **best results are obtained with the SVR** algorithm (support vector regression)
As a first step, algorithms from the Scikit-learn (Python) library are used

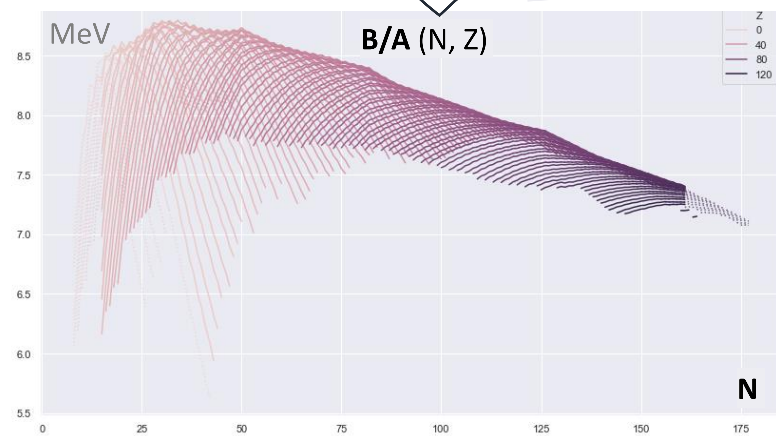
✓ The best results are obtained by using the energies of neighboring nuclei as input parameters to predict the energy of this nucleus: **B/A(N, Z) prediction based on the B/A of nuclei (N–2, Z–2) and (N–4, Z–4)**
Using as input parameters N, Z and their combinations to predict B, B/A, Δ_{np}, Q_{α} showed unstable results

✓ A significantly better result was obtained when **expanding the input array of experimental data AME 2016 by our estimates from local mass relations method** (steps $\leqslant$ 15)

✓ The result is stable for at least 2 iterations of the ML algorithm
1) 3911 training array rows → 97 predicted
2) 4008 training array rows → 90 predicted



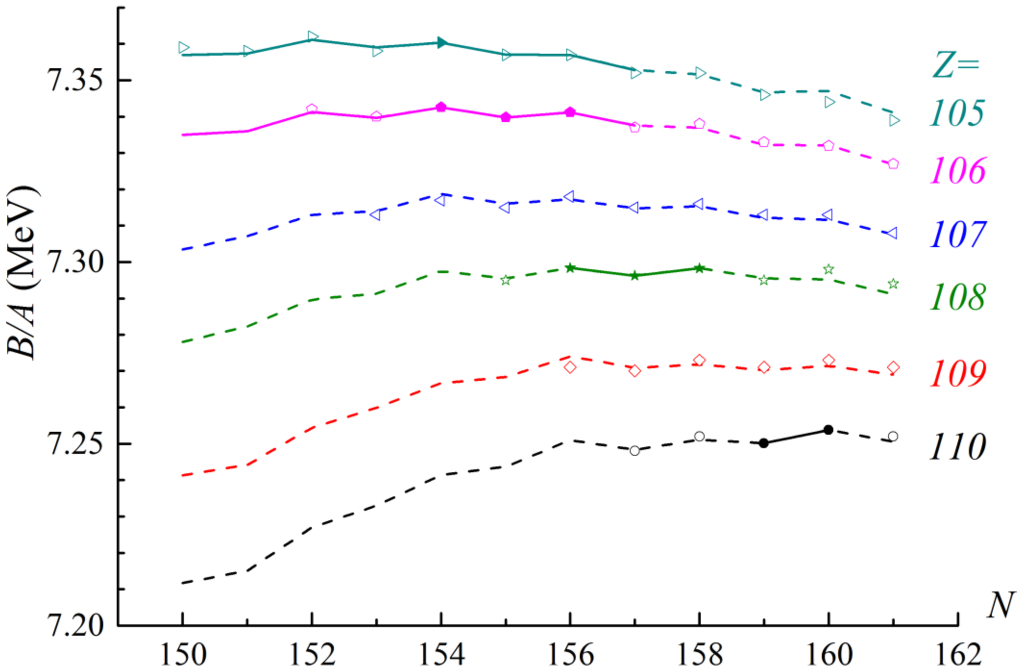




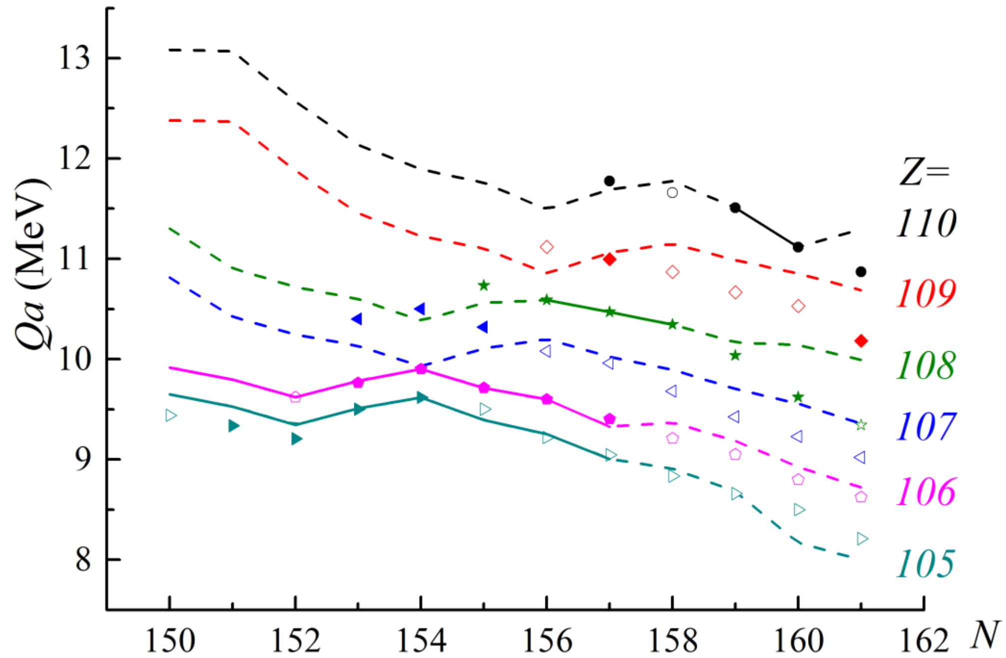
Predictions for SHE. Machine learning (ML)

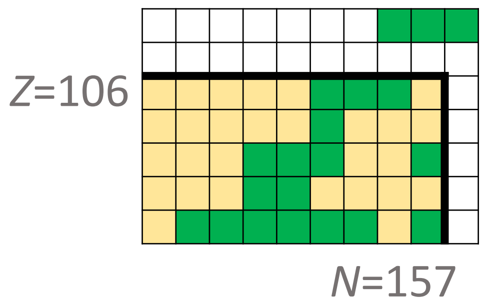
Preliminary results

Specific binding energies



Alpha decay energies





ML methods allowed to go beyond the boundaries of Z = 106, N = 157 (unattainable area for Δ_{np} estimates)

— Result by Δ_{np}

- - Experiment + Result by ML

● Experiment (AME16)

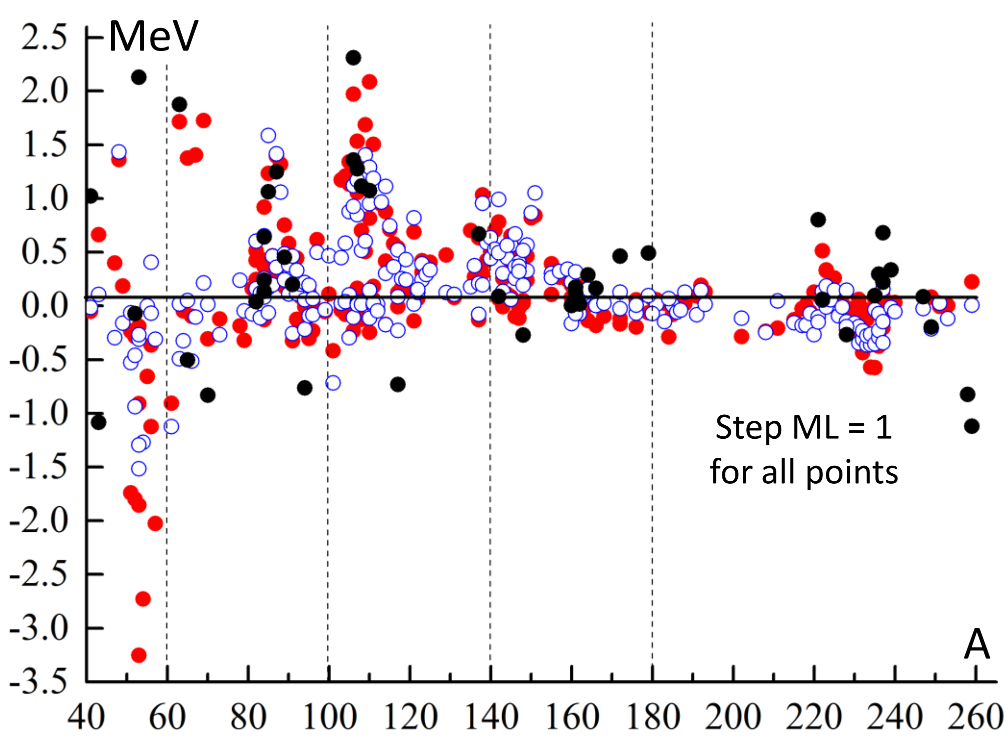
○ AME16 evaluation

Estimates based on AME (without expanding input array with Δ_{np})

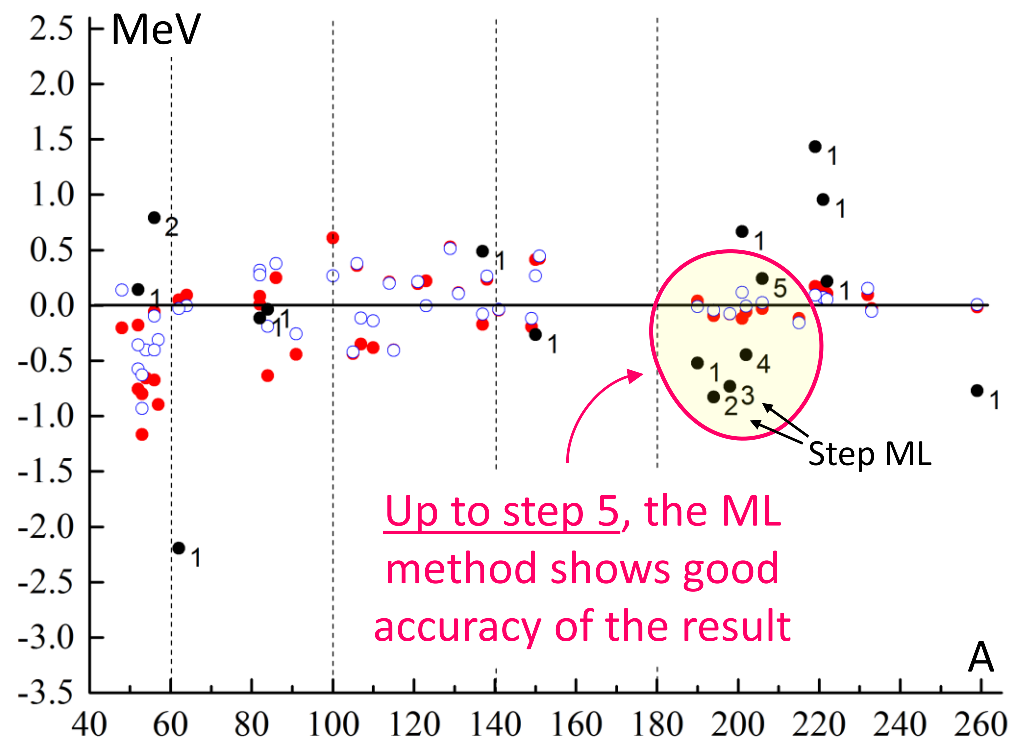
Preliminary results

Deviations of estimates and experimental data AME 2016

AME 2003



AME 2012



- ● Result by ML
- ● Result by Δ_{np}
- ○ AME03/12 evaluation

Результаты: полученные оценки энергий связи (NZ-диаграмма) – AME 2016

Оценки

Оценки

	128	129	130	131	132	133	134	135	136	137	138	139	140	141	142	143	144	145	146	147	148	149	150	151	152	153	154	155	156	157	158	159	160	
110																																		110
109																																		109
108																																		108
107																																		107
106	27	26	25	24	23	22	21	20	19	18	17	16	15	14	13	12	11	10	9	8	7	6	5	4	3	2				5				106
105	26	25	24	23	22	21	20	19	18	17	16	15	14	13	12	11	10	9	8	7	6	5	4	3	2	1		1	2	4				105
104	25	24	23	22	21	20	19	18	17	16	15	14	13	12	11	10	9	8	7	6	5	4	3	2				2	3					104
103	24	23	22	21	20	19	18	17	16	15	14	13	12	11	10	9	8	7	6	5	4	3	2	1			1	2	3	4				103
102	23	22	21	20	19	18	17	16	15	14	13	12	11	10	9	8	7	6	5	4	3	2							1					102
101	22	21	20	19	18	17	16	15	14	13	12	11	10	9	8	7	6	5	4	3	2	1		1	2	1		1						101
100	21	20	19	18	17	16	15	14	13	12	11	10	9	8	7	6	5	4		2														100
99	20	19	18	17	16	15	14	13	12	11	10	9	8	7	6	5	4	3	2	1		1	2	1						1				99
98	19	18	17	16	15	14	13	12	11	10	9		7	6		4		2												2				98
97	18	17	16	15	14	13	12	11	10	9	8	7	6	5	4	3	2	1						1				1	2	3				97
96	12	11	10	9	8	7	6	5	4			2																	3	4				96
95	8	7	6	5	4	3		1	2	3	2	1		1	1									1	2	3	4	5	6	7				95
94	7	6	5	4	3	2																				4	5	6	7	8				94
93	4	3	2	1		1						1											1	2	3	5	6	7	8	9				93
92	2																					1	2	3	4	6	7	8	9	10				92
91		1		1																	1	2	3	4	5	7	8	9	10	11				91
90																					2	3	4	5	6	8	9	10	11	12				90
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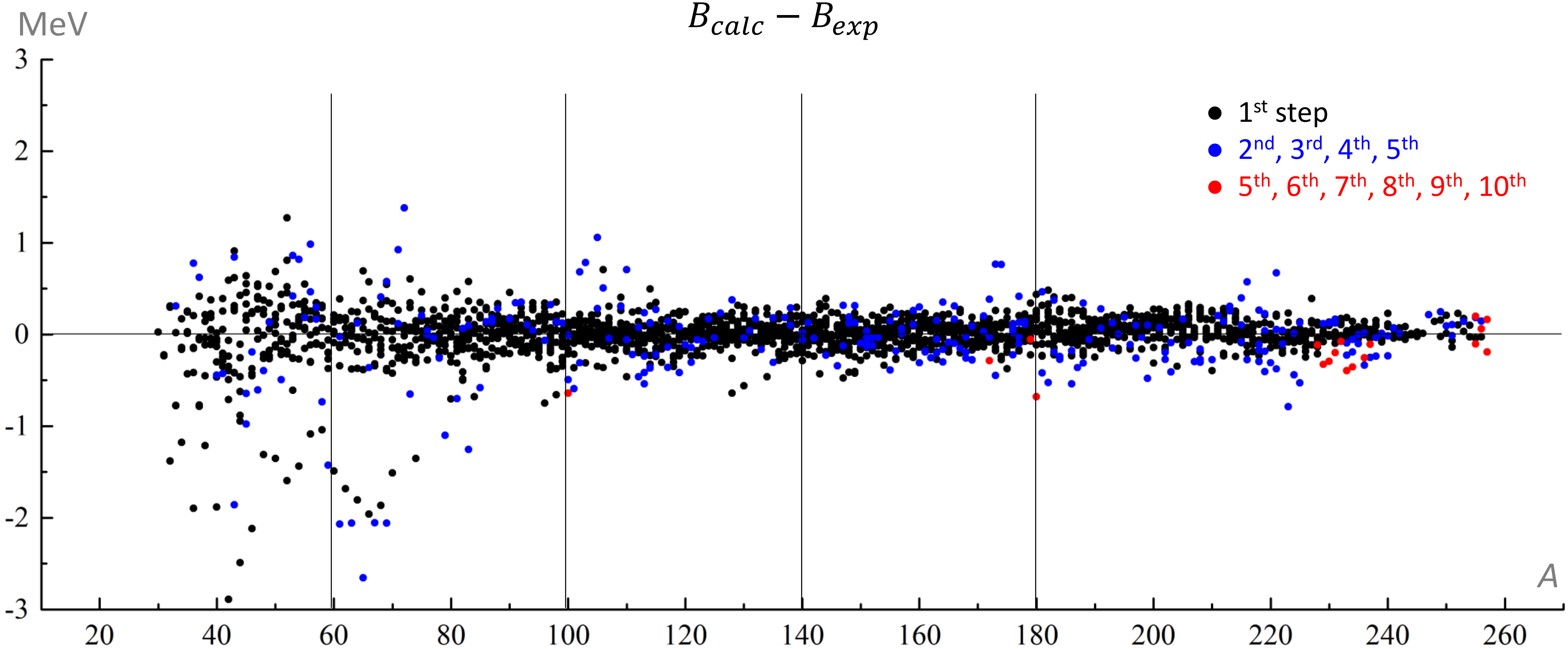
88																				1	4	5	6	7	8	10	11	12	13	14				88
87																				2	5	6	7	8	9	11	12	13	14	15				87
86																	1	2	3	4	6	7	8	9	10	12	13	14	15	16				86
85													1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18				85
84												1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19				84
	128	129	130	131	132	133	134	135	136	137	138	139	140	141	142	143	144	145	146	147	148	149	150	151	152	153	154	155	156	157	158	159	160	

Экспериментальные данные AME2016

Method reliability (AME 2016)

Deviations of binding energy

$B_{calc} - B_{exp}$



$\sigma = 594\ keV$ $\sigma_{\%} \approx 0{,}15\%$	$\sigma = 408\ keV$ $\sigma_{\%} \approx 0{,}06\%$	$\sigma = 179\ keV$ $\sigma_{\%} \approx 0{,}02\%$	$\sigma = 159\ keV$ $\sigma_{\%} \approx 0{,}01\%$	$\sigma = 167\ keV$ $\sigma_{\%} \approx 0{,}01\%$

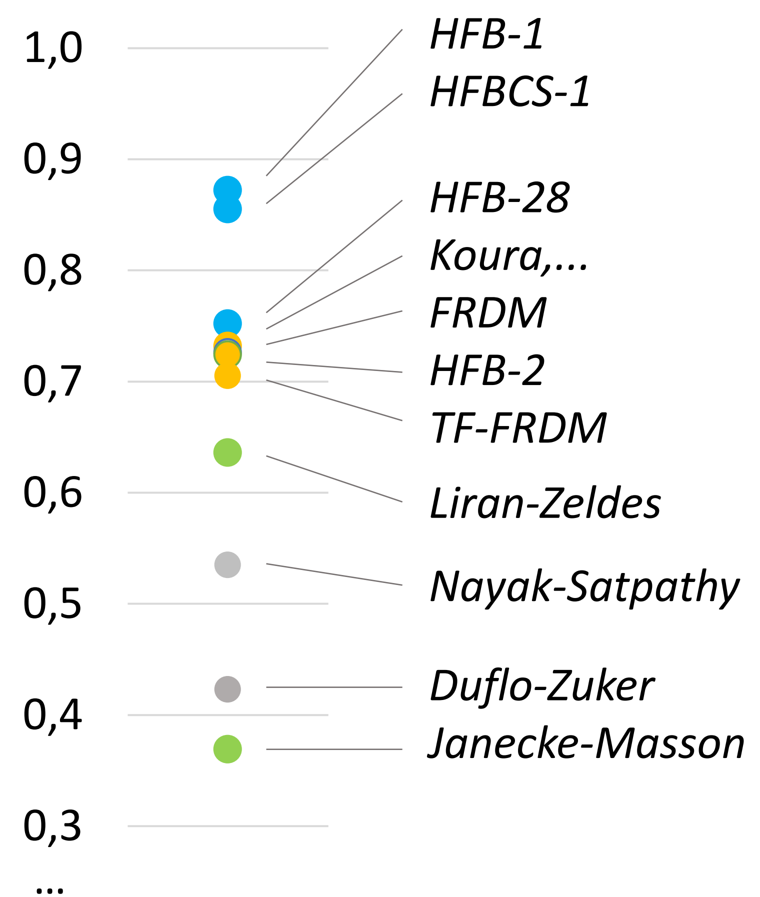
Подходы к предсказанию энергии связи

Определение энергии связи ядра

- **Микроскопические** — *~ эффективные потенциалы двухчастичного взаимодействия*
- **Макро-микроскопические** — *~ модель жидкой капли + уточняющие поправки*
- **Локальные массовые соотношения** — *~ использование известных энергий связи соседних ядер*

[**D. Lunney, J. M. Pearson, C. Thibault.** *Recent trends in the determination of nuclear masses* // Reviews Of Modern Physics 2003. Vol.75, N 3, p. 1021-1082]

Среднеквадратичное отклонение теоретической оценки от экспериментальных данных (2 135 точек), **МэВ**



Detailed illustration of the accuracy of currently used nuclear-mass models

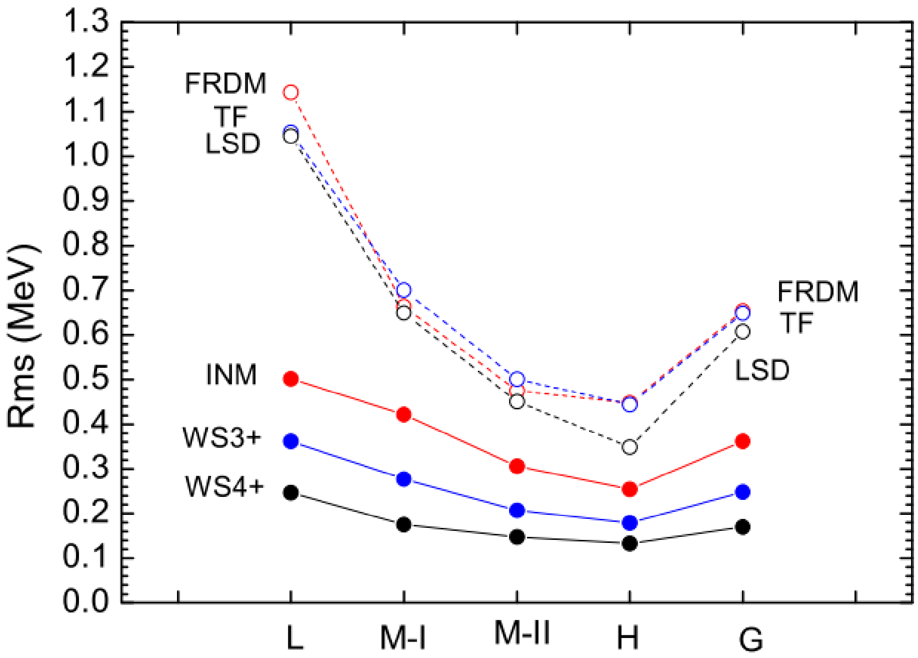


Fig. 1. (Color online) Dependence of the rms discrepancy on the region of nuclei for the FRDM, TF, LSD, INM, WS3+, and WS4+ models. The symbols: L, M-I, M-II, H and G denote the regions of light, medium-I, medium-II, heavy and global nuclei, respectively.

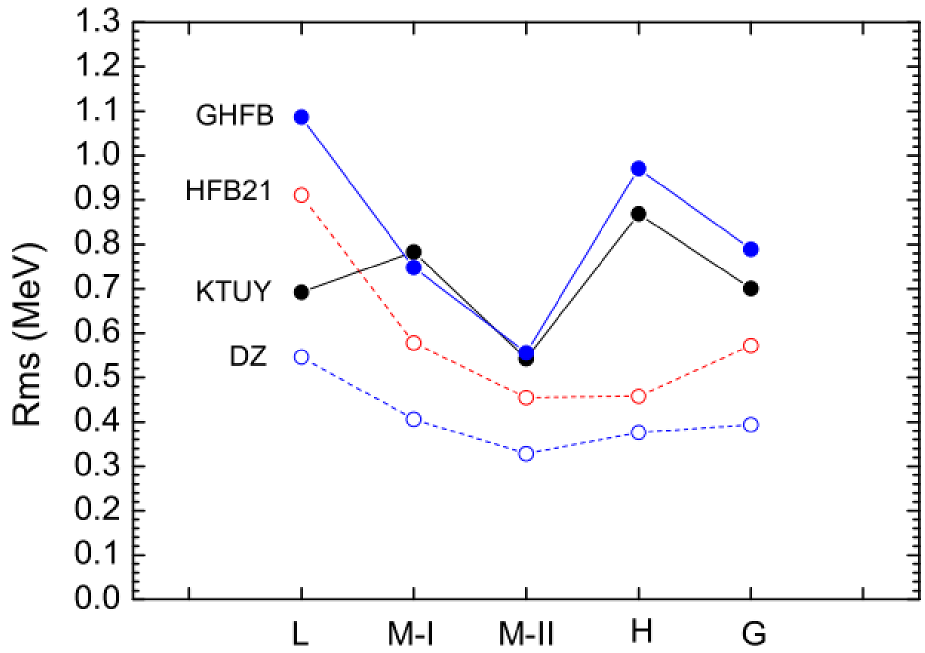


Fig. 2. (Color online) Same as in Fig. 1, but for the GHFB, HFB21, KTUY, and DZ models.

[Sobiczewski et al. Atomic Data and Nuclear Data Tables Vol. 119, 2018, pp. 1-32]