

# Nuclear octupole shapes in Actinides with Fayans functionals

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UNIVERSITY OF JYVÄSKYLÄ



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# 1) At the heart of nuclei



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$$\begin{aligned}\epsilon_t^{even} &= (C_{t0}^\rho + \rho_0^\gamma C_{tD}^\rho) \rho_t^2 + C_t^\tau \rho_t \tau_t + C_t^{\Delta\rho} \rho_t \Delta\rho_t + C_t^{\nabla J} \rho_t \nabla J_t + C_t^J J_t^2 \\ \epsilon_t^{odd} &= (C_{t0}^s + \rho_0^\gamma C_{tD}^s) s_t^2 + \dots \quad t = 0,1\end{aligned}$$



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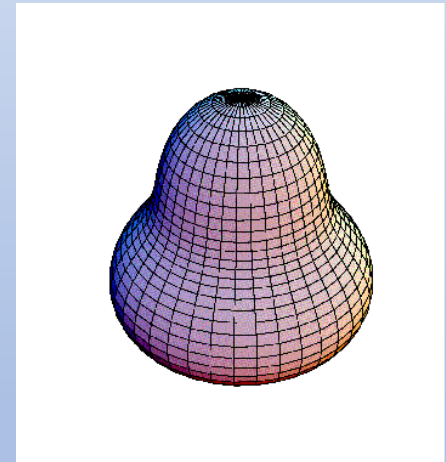


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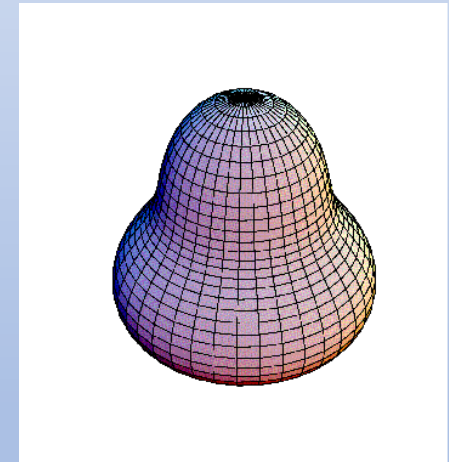


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- Fayans Pairing Term [3] -> adjusted Next-gen Fayans Functionals [4] [5] [6]







# 1) At the heart of nuclei

Skyrme

and

Fayans EDFs

$$\mathcal{E}_{\text{pair},q} = \frac{1}{4} \underline{V_{\text{pair},q}} \left( 1 - \frac{\rho_0}{\underline{\rho_{\text{pair}}}} \right) \underline{\rho_q^2} \quad (q = p, n)$$

$$\mathcal{E}_{\text{Sk},t} = C_t^{\rho\rho}(\rho_0)\rho_t^2 + C_t^{\rho\tau}\rho_t\tau_t + C_t^{\rho\Delta\rho}\rho_t\Delta\rho_t + C_t^{\rho\nabla J}\rho_t\nabla\cdot\mathbf{J}_t + C_t^{J^2}\mathbf{J}_t^2$$

$$\mathcal{E}_C = e^2 \int d^3r d^3r' \rho_p(\mathbf{r}) \frac{1}{|\mathbf{r} - \mathbf{r}'|} \rho_p(\mathbf{r}')$$

$$\mathcal{E}_{C,\text{ex}} = -\frac{3}{4}e^2 \left(\frac{3}{\pi}\right)^{1/3} \rho_p^{4/3}.$$

$$\mathcal{E}_{\text{Fy},q}^{\text{pair}} = \frac{2\varepsilon_F}{3\rho_{\text{sat}}}\rho_q^2 \left[ f_{\text{ex}}^\xi + h_+^\xi x_{\text{pair}}^\gamma + \underline{h_\nabla^\xi r_s^2 (\nabla x_{\text{pair}})^2} \right]$$

$$x_t = \frac{\rho_t}{\rho_{\text{sat}}}, \quad x_{\text{pair}} = \frac{\rho_0}{\rho_{\text{pair}}}$$

$$\mathcal{E}_{\text{Fy}}^{\text{v}} = \frac{1}{3}\varepsilon_F\rho_{\text{sat}} \left[ a_+^{\text{v}} \frac{1-h_{1+}^{\text{v}}x_0^\sigma}{1+h_{2+}^{\text{v}}x_0^\sigma} x_0^2 + a_-^{\text{v}} \frac{1-h_{1-}^{\text{v}}x_0}{1+h_{2-}^{\text{v}}x_0} x_1^2 \right]$$

$$\mathcal{E}_{\text{Fy}}^{\text{s}} = \frac{1}{3}\varepsilon_F\rho_{\text{sat}} \frac{a_+^{\text{s}} r_s^2 (\nabla x_0)^2}{1+h_+^{\text{s}}x_0^\sigma + h_\nabla^{\text{s}} r_s^2 (\nabla x_0)^2}$$

$$\mathcal{E}_{\text{Fy}}^{\text{ls}} = \frac{4\varepsilon_F r_s^2}{3\rho_{\text{sat}}} (\kappa\rho_0\nabla\cdot\mathbf{J}_0 + \kappa'\rho_1\nabla\cdot\mathbf{J}_1 + g\mathbf{J}_0^2 + g'\mathbf{J}_1^2)$$

$$\mathcal{E}_{C,\text{ex}} = -\frac{3}{4}e^2 \left(\frac{3}{\pi}\right)^{1/3} \rho_p^{4/3} (1 - h_C x_0^\sigma)$$

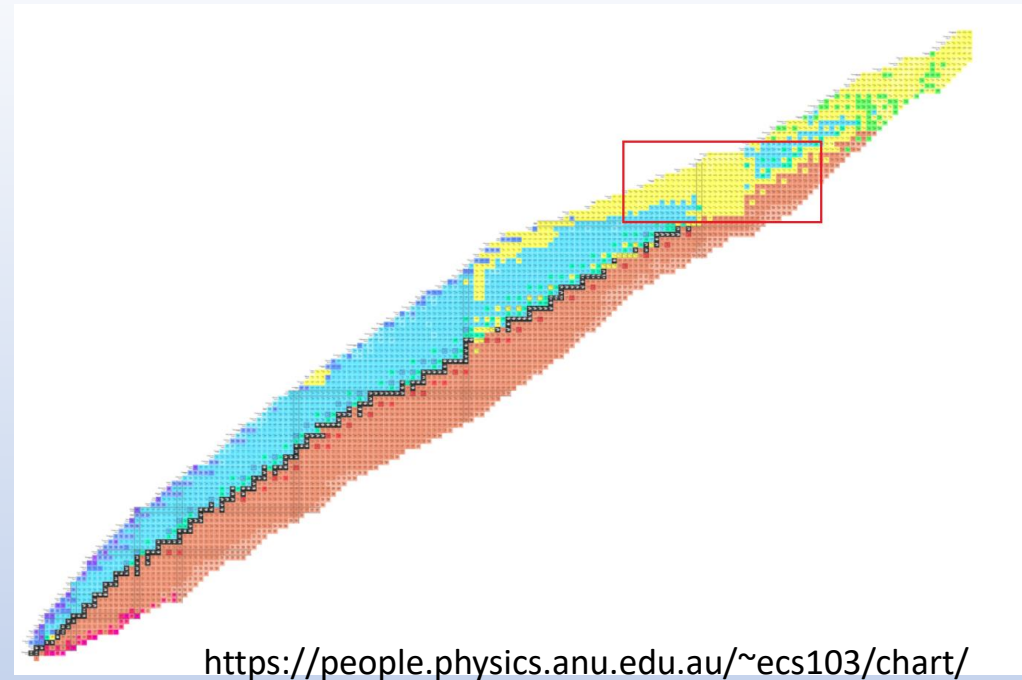


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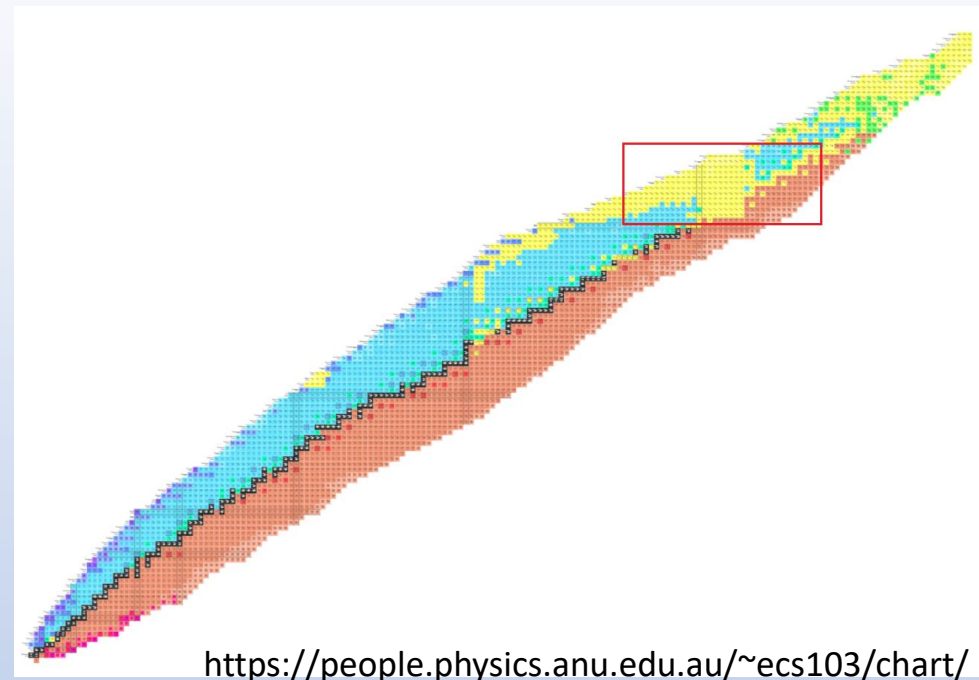
- Actinides and superheavy clusters expected to present  $\beta_3$  [7] [8]





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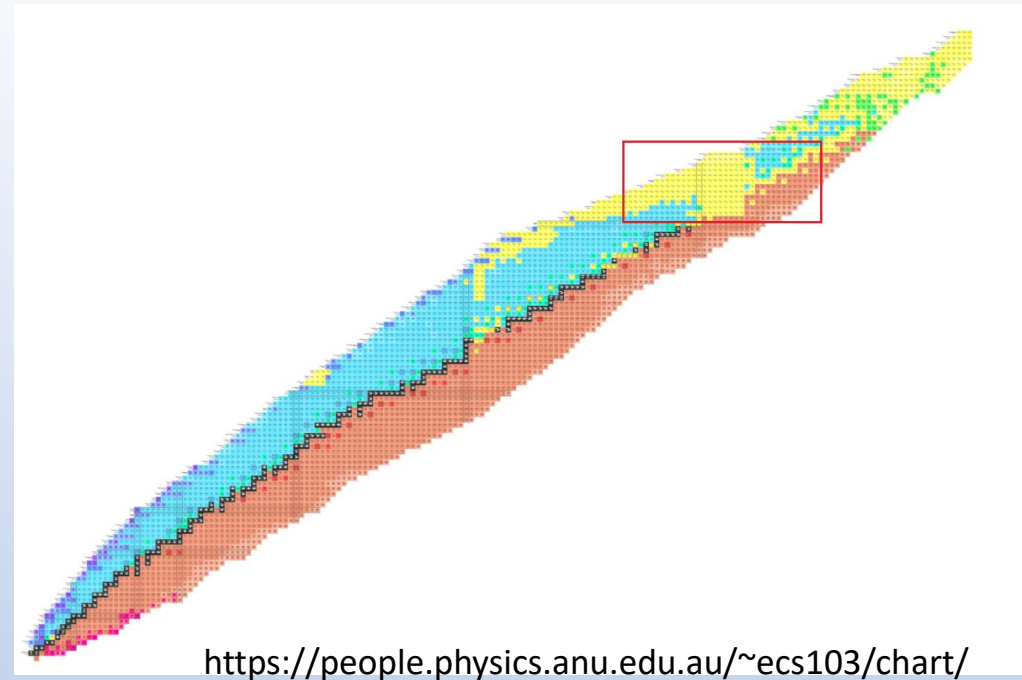
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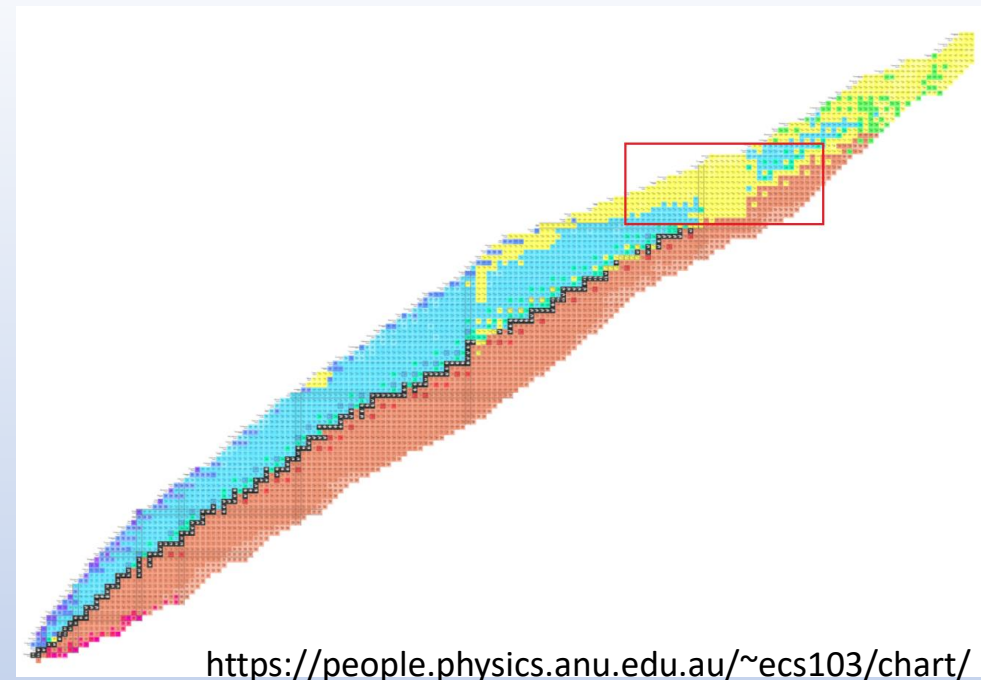
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- Ground state energy,  $\beta_2$ ,  $\beta_3$ ,  $\Delta_{1;2n}$ , rms radii, etc.

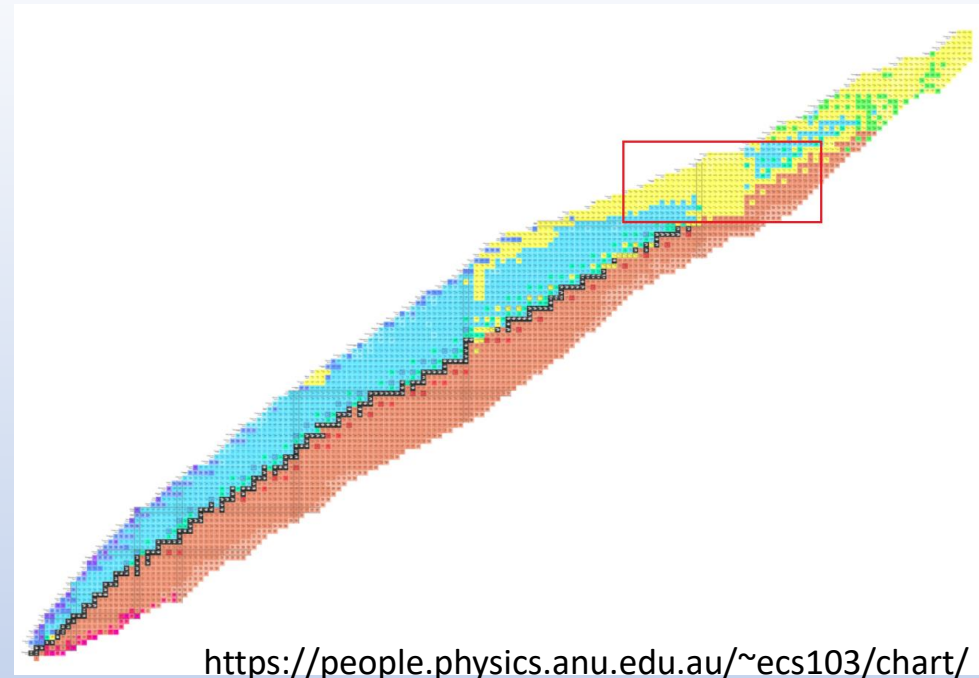




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- Comparison to current-gen EDFs and studies on pear-shaped nuclei [9]





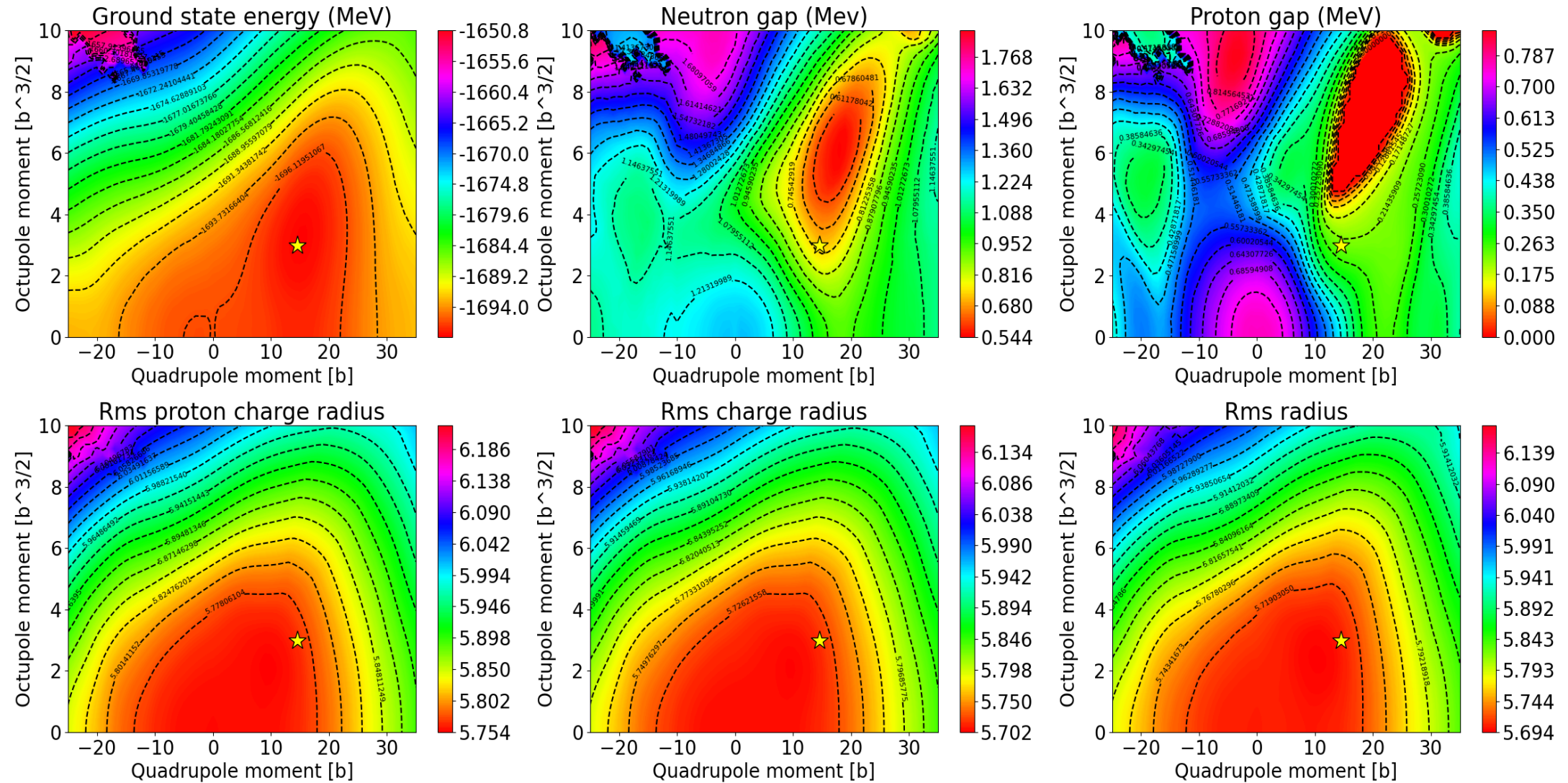
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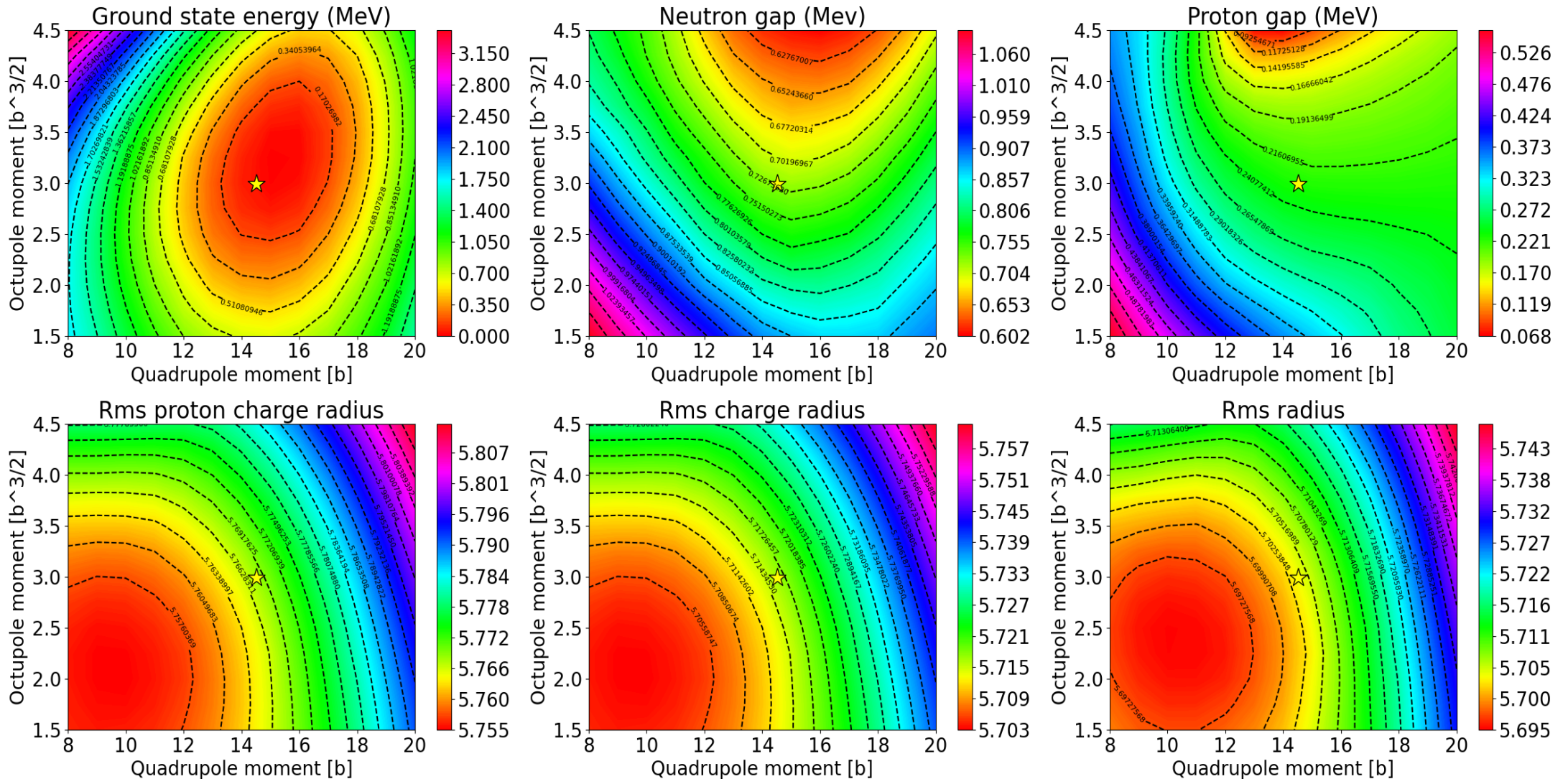
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224Th





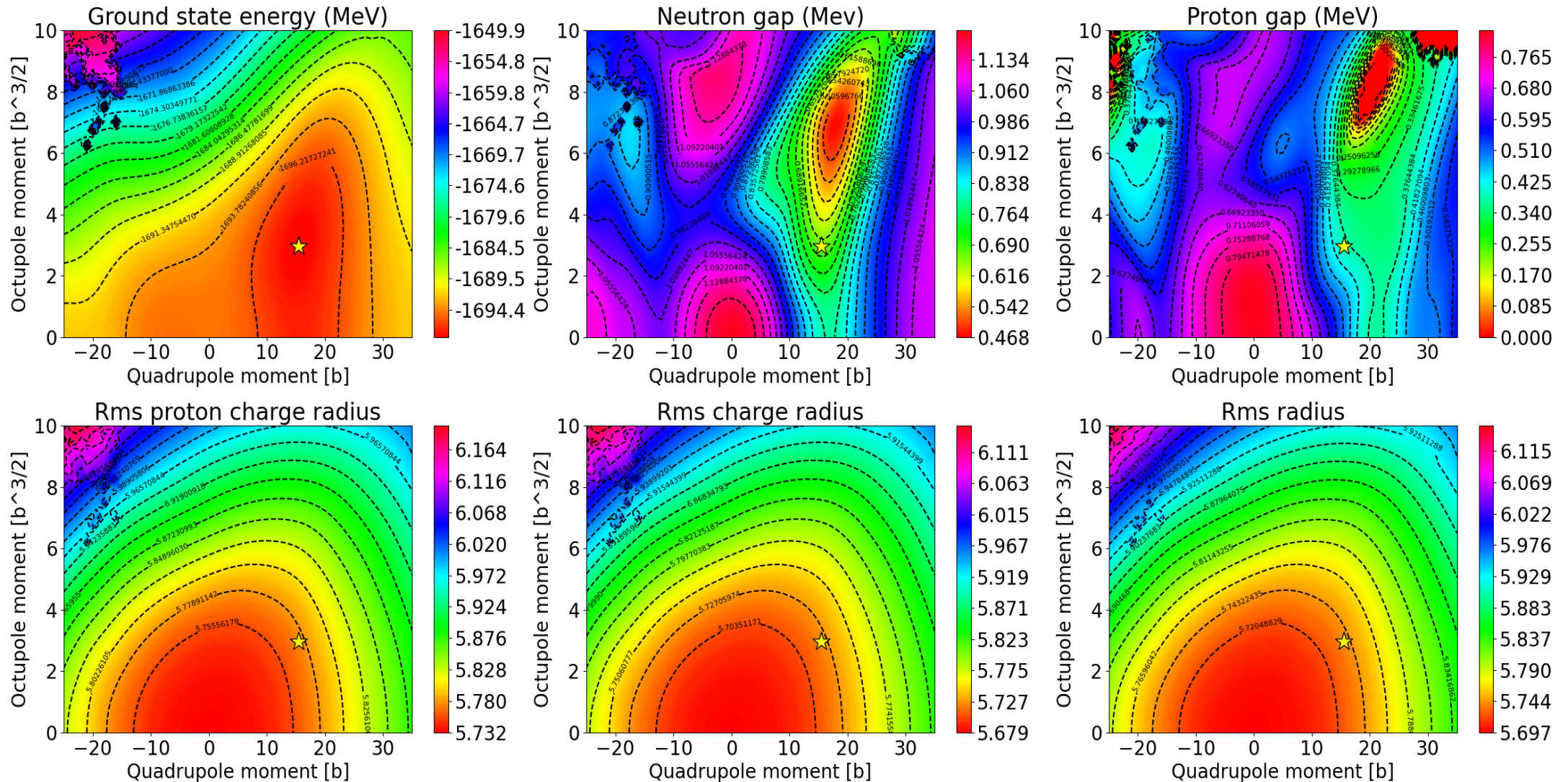
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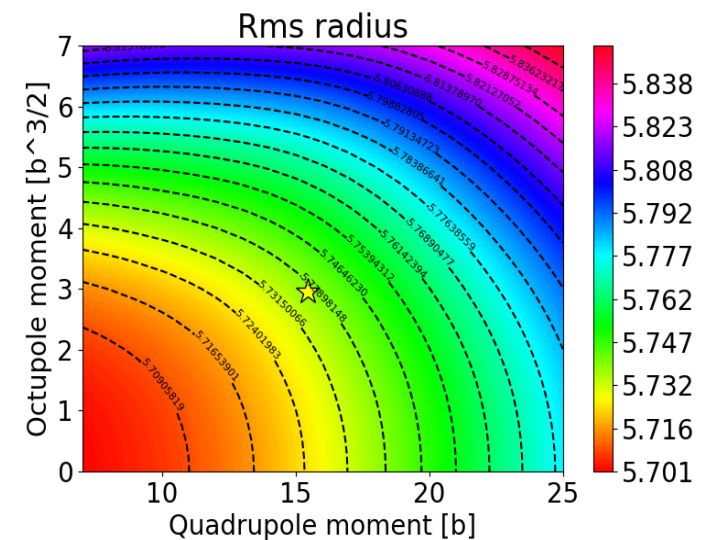
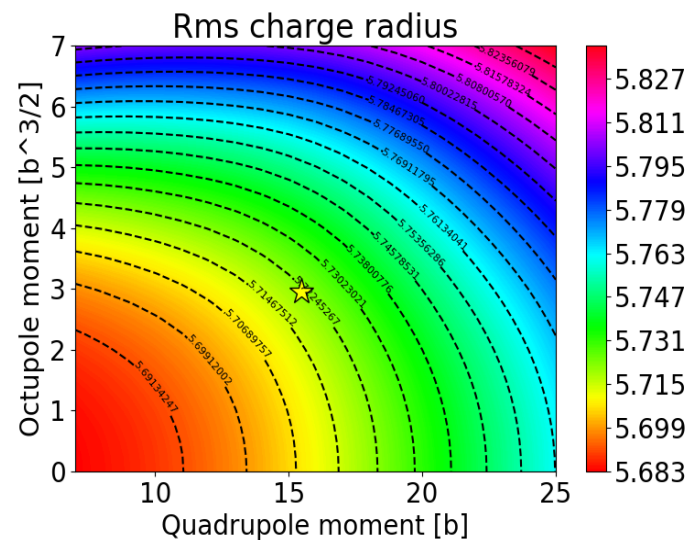
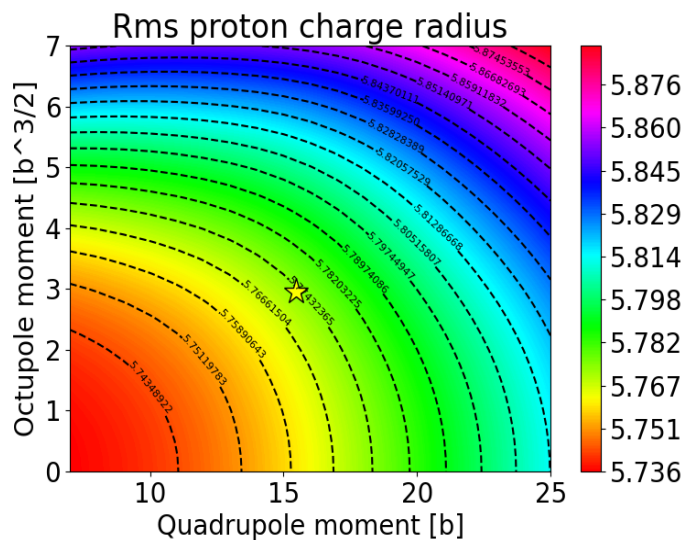
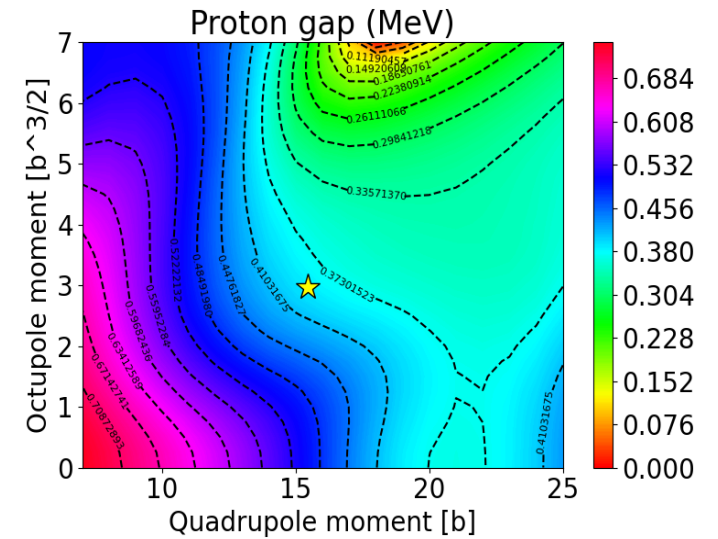
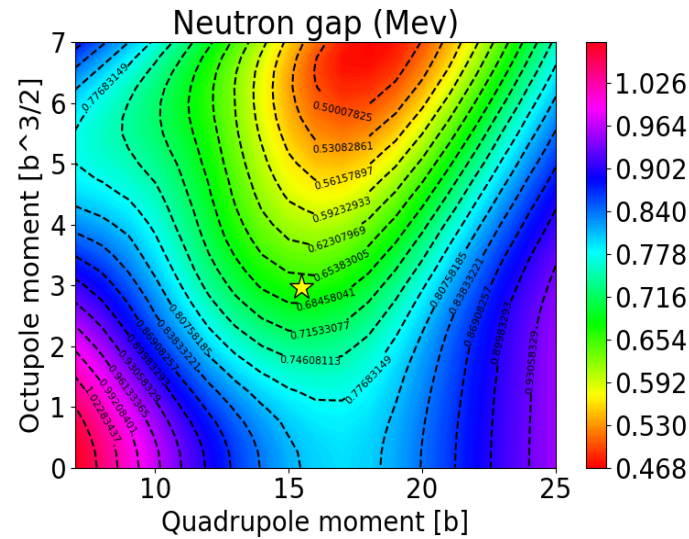
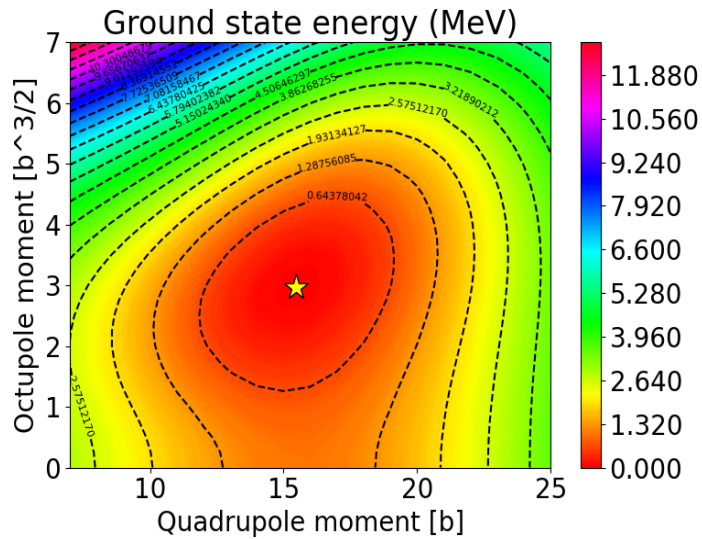
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- 1) Even-even computation around expected Q2-Q3 for min(E) of odd nucleus





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- 1) Even-even computation around expected Q2-Q3 for min(E) of odd nucleus
- 2) Select reasonable blocking orbitals candidates

90\_Th\_210\_FYdrHFB neutron blocking

num=	1	block=	1	state=	1	1	Eqp=	0.98849777	(1-2N)E=	-0.43803999	Ovlp=	0.48581159	1-[	5,	3,	0]
num=	2	block=	1	state=	2	2	Eqp=	1.03132448	(1-2N)E=	-0.79448565	Ovlp=	0.50056312	1+[	6,	2,	0]
num=	3	block=	2	state=	1	154	Eqp=	1.03849441	(1-2N)E=	0.59329136	Ovlp=	0.66069727	3-[	5,	4,	1]
num=	4	block=	1	state=	3	3	Eqp=	1.09072859	(1-2N)E=	0.31649926	Ovlp=	0.61462786	1-[	5,	4,	1]
num=	5	block=	2	state=	2	155	Eqp=	1.12867326	(1-2N)E=	-0.92131424	Ovlp=	0.53585210	3+[	6,	3,	1]
num=	6	block=	3	state=	1	290	Eqp=	1.33024372	(1-2N)E=	-1.16652448	Ovlp=	0.60205808	5+[	6,	2,	2]
num=	7	block=	2	state=	3	156	Eqp=	1.33143102	(1-2N)E=	-1.08108058	Ovlp=	0.51947902	3-[	5,	3,	2]
num=	8	block=	3	state=	2	291	Eqp=	1.36263221	(1-2N)E=	-1.21421565	Ovlp=	0.57512942	5-[	5,	3,	2]
num=	9	block=	4	state=	1	410	Eqp=	1.65087848	(1-2N)E=	-1.53015780	Ovlp=	0.58929986	7+[	6,	3,	3]
num=	10	block=	5	state=	1	515	Eqp=	2.11694535	(1-2N)E=	-2.00442036	Ovlp=	0.76908035	9+[	6,	2,	4]
num=	11	block=	5	state=	2	516	Eqp=	2.62695340	(1-2N)E=	2.52311239	Ovlp=	0.83796064	9+[	6,	0,	4]
num=	12	block=	1	state=	4	4	Eqp=	2.63183142	(1-2N)E=	1.52769455	Ovlp=	0.76577608	1-[	5,	5,	0]
num=	13	block=	1	state=	5	5	Eqp=	2.67050206	(1-2N)E=	-1.69863083	Ovlp=	0.62843667	1-[	5,	1,	0]
num=	14	block=	2	state=	4	157	Eqp=	2.74809493	(1-2N)E=	-2.68508005	Ovlp=	0.71099017	3-[	5,	1,	2]
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num=	16	block=	1	state=	6	6	Eqp=	2.78133078	(1-2N)E=	-2.70752540	Ovlp=	0.69568921	1-[	5,	0,	1]
num=	17	block=	6	state=	2	607	Eqp=	2.95067683	(1-2N)E=	2.77257885	Ovlp=	0.91231534	11+[	6,	0,	6]





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num=	8	block=	3	state=	2	291	Eqp=	1.36263221	(1-2N)E=	-1.21421565	Ovlp=	0.57512942	5-[	5,	3,	2]
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num=	11	block=	5	state=	2	516	Eqp=	2.62695340	(1-2N)E=	2.52311239	Ovlp=	0.83796064	9+[	6,	0,	4]
num=	12	block=	1	state=	4	4	Eqp=	2.63183142	(1-2N)E=	1.52769455	Ovlp=	0.76577608	1-[	5,	5,	0]
num=	13	block=	1	state=	5	5	Eqp=	2.67050206	(1-2N)E=	-1.69863083	Ovlp=	0.62843667	1-[	5,	1,	0]
num=	14	block=	2	state=	4	157	Eqp=	2.74809493	(1-2N)E=	-2.68508005	Ovlp=	0.71099017	3-[	5,	1,	2]
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- 3) Unconstrained calculation for each possible configuration



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- 3) Unconstrained calculation for each possible configuration
- 4) Lowest E -> Ground state



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num=	4	block=	1	state=	3	3	Eqp=	1.09072859	(1-2N)E=	0.31649926	Ovlp=	0.61462786	1-[	5,	4,	1]
num=	5	block=	2	state=	2	155	Eqp=	1.12867326	(1-2N)E=	-0.92131424	Ovlp=	0.53585210	3+[	6,	3,	1]
num=	6	block=	3	state=	1	290	Eqp=	1.33024372	(1-2N)E=	-1.16652448	Ovlp=	0.60205808	5+[	6,	2,	2]
num=	7	block=	2	state=	3	156	Eqp=	1.33143102	(1-2N)E=	-1.08108058	Ovlp=	0.51947902	3-[	5,	3,	2]
num=	8	block=	3	state=	2	291	Eqp=	1.36263221	(1-2N)E=	-1.21421565	Ovlp=	0.57512942	5-[	5,	3,	2]
num=	9	block=	4	state=	1	410	Eqp=	1.65087848	(1-2N)E=	-1.53015780	Ovlp=	0.58929986	7+[	6,	3,	3]
num=	10	block=	5	state=	1	515	Eqp=	2.11694535	(1-2N)E=	-2.00442036	Ovlp=	0.76908035	9+[	6,	2,	4]
num=	11	block=	5	state=	2	516	Eqp=	2.62695340	(1-2N)E=	2.52311239	Ovlp=	0.83796064	9+[	6,	0,	4]
num=	12	block=	1	state=	4	4	Eqp=	2.63183142	(1-2N)E=	1.52769455	Ovlp=	0.76577608	1-[	5,	5,	0]
num=	13	block=	1	state=	5	5	Eqp=	2.67050206	(1-2N)E=	-1.69863083	Ovlp=	0.62843667	1-[	5,	1,	0]
num=	14	block=	2	state=	4	157	Eqp=	2.74809493	(1-2N)E=	-2.68508005	Ovlp=	0.71099017	3-[	5,	1,	2]
num=	15	block=	6	state=	1	606	Eqp=	2.76648130	(1-2N)E=	-2.57569794	Ovlp=	0.90042656	11+[	6,	1,	5]
num=	16	block=	1	state=	6	6	Eqp=	2.78133078	(1-2N)E=	-2.70752540	Ovlp=	0.69568921	1-[	5,	0,	1]
num=	17	block=	6	state=	2	607	Eqp=	2.95067683	(1-2N)E=	2.77257885	Ovlp=	0.91231534	11+[	6,	0,	6]

- 3) Unconstrained calculation for each possible configuration
- 4) Lowest E -> Ground state

Whole Q2-Q3 landscape unreasonable for non-ee nuclei; but isotopic chains can be built

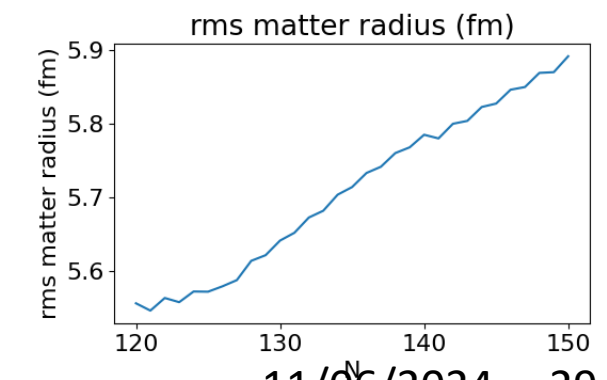
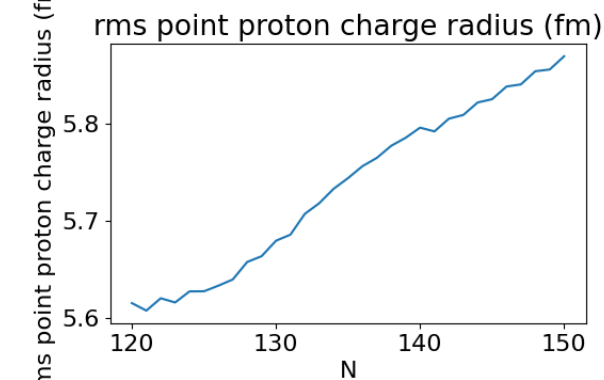
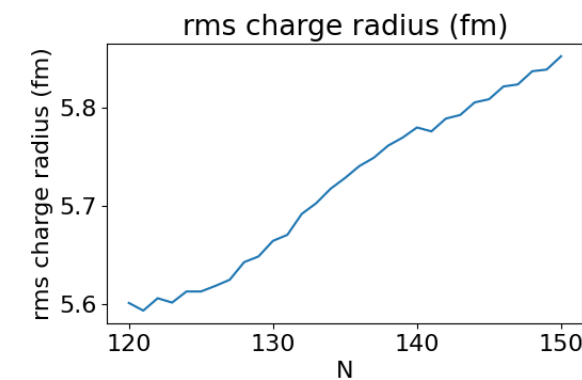
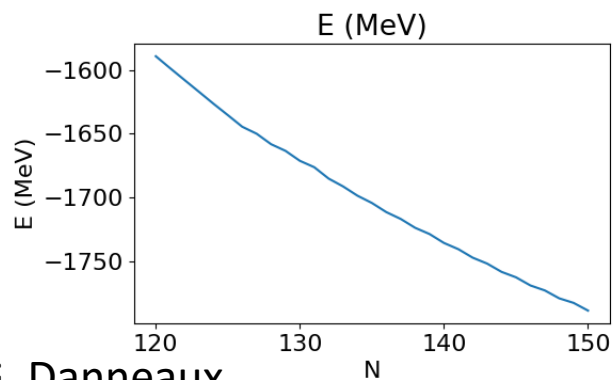
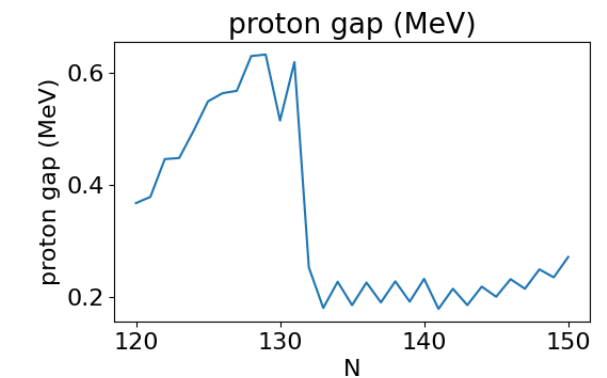
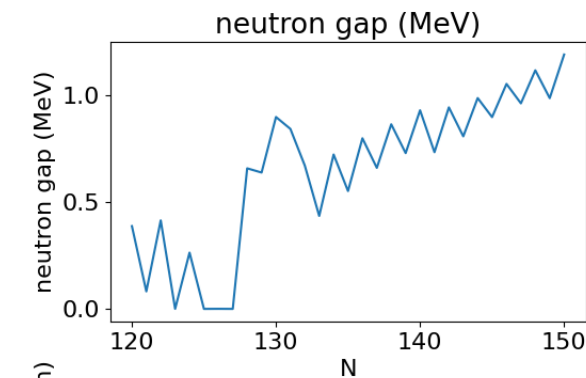
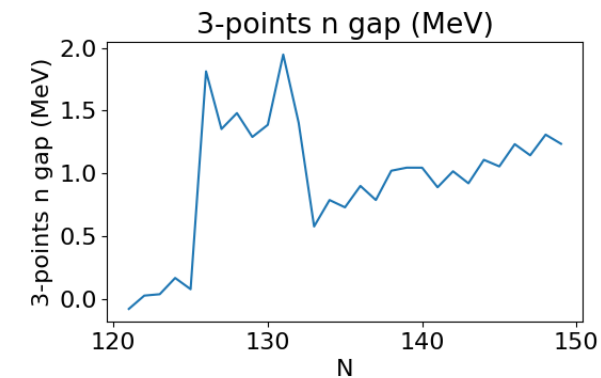
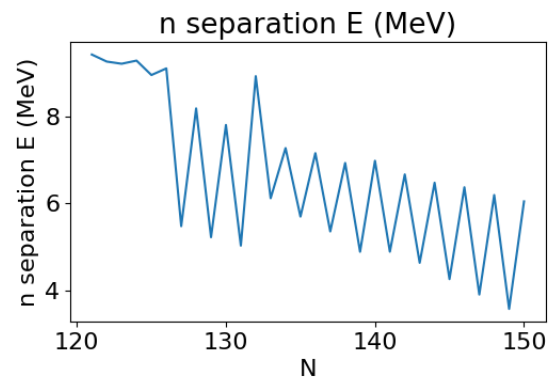
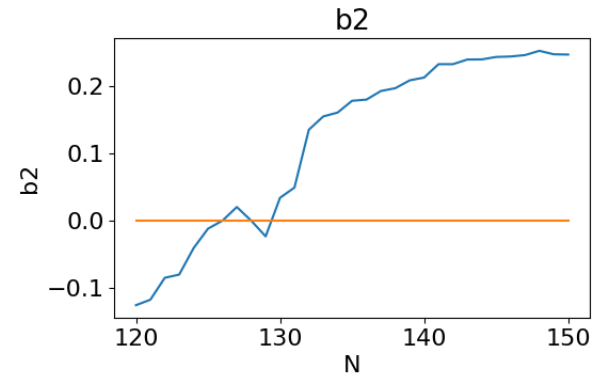
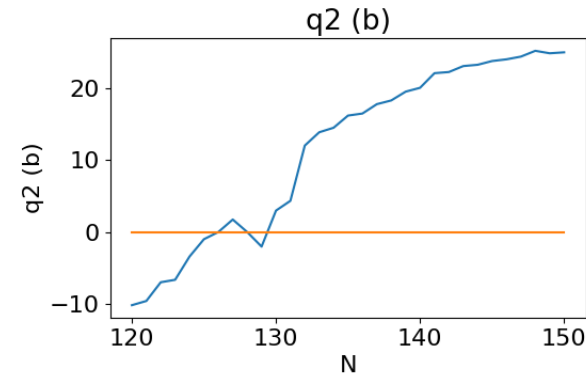
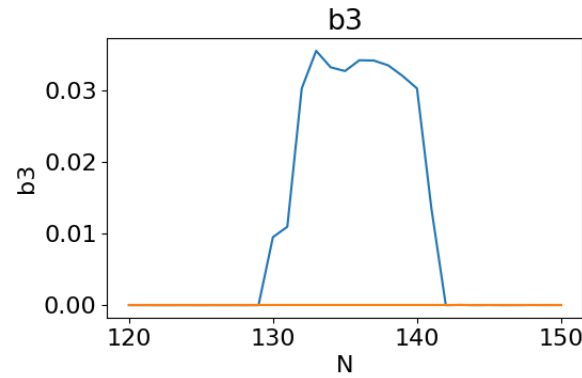
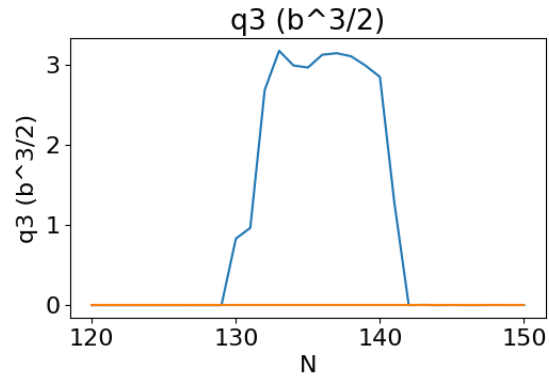


### 3) Fayans results in Actinides



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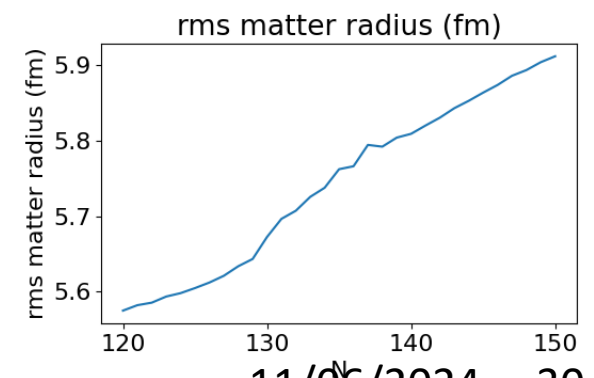
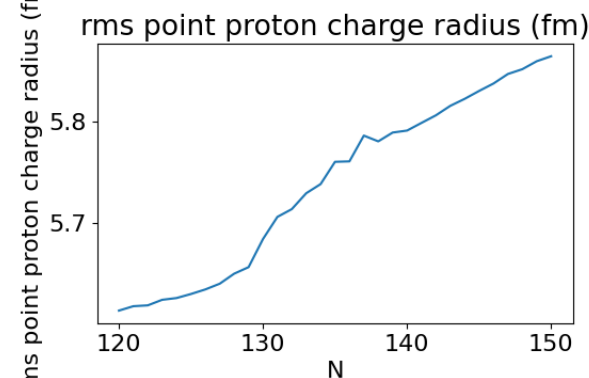
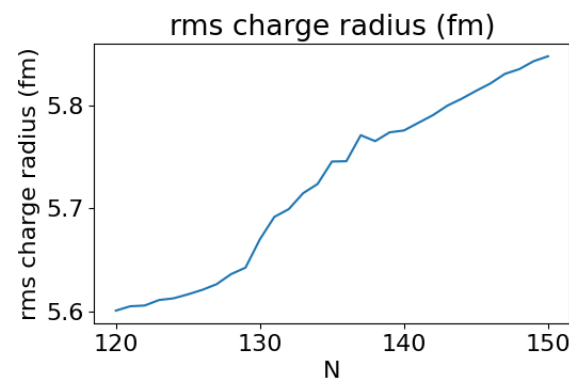
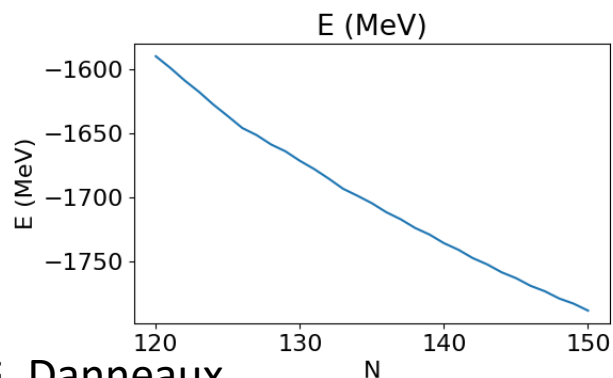
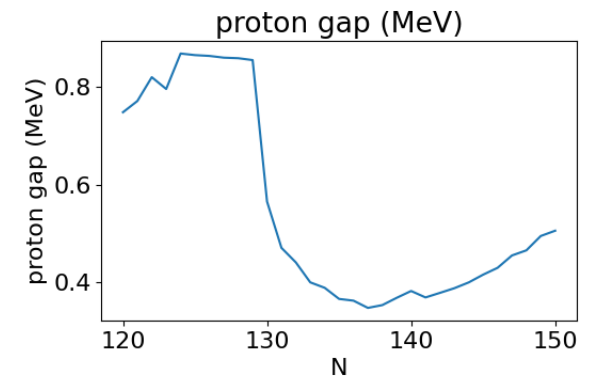
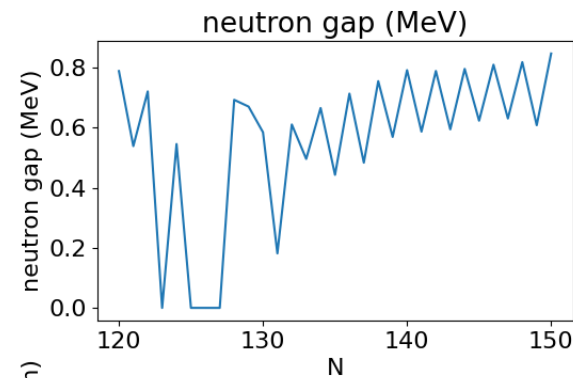
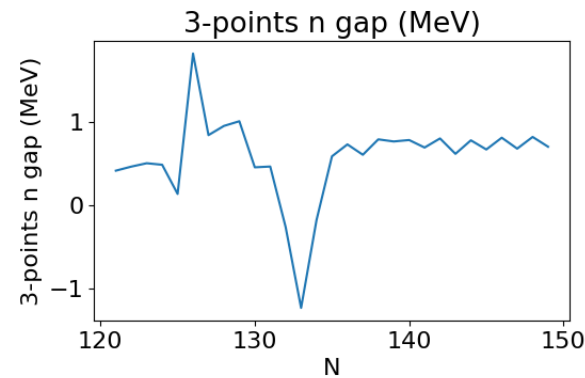
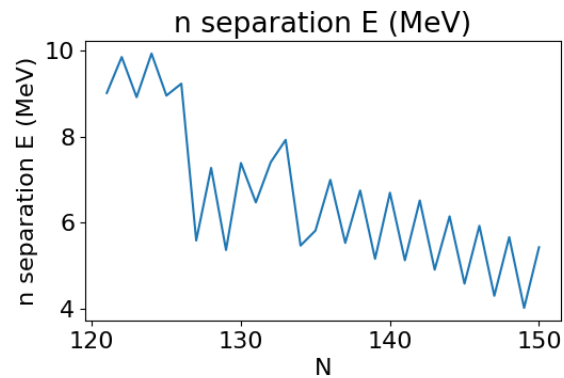
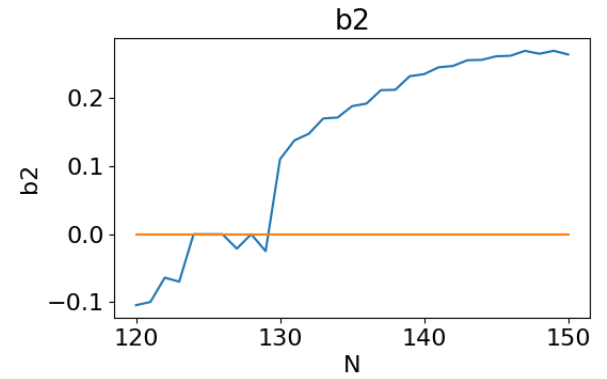
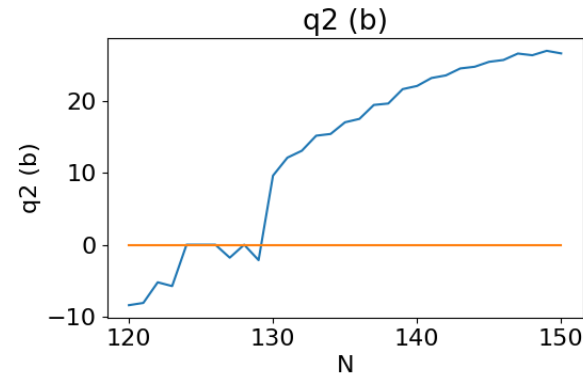
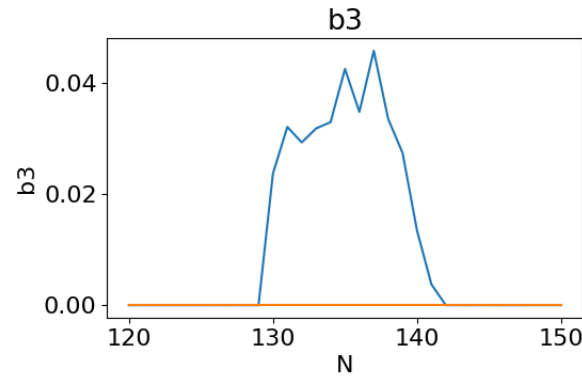
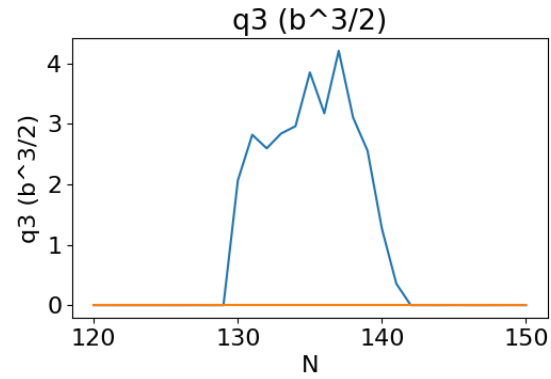
90\_Th\_120-150\_FYdrHFB





# 3) Fayans results in Actinides

90\_Th\_120-150\_FYstd





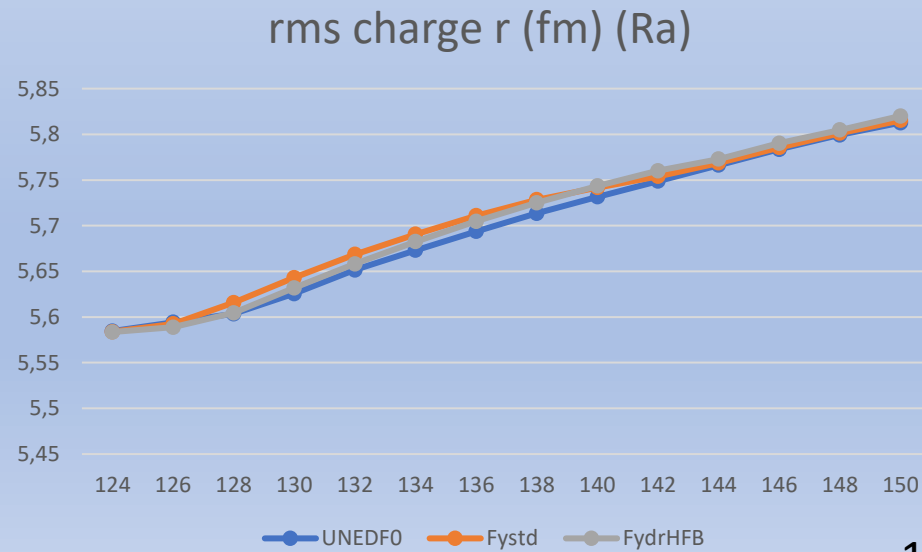
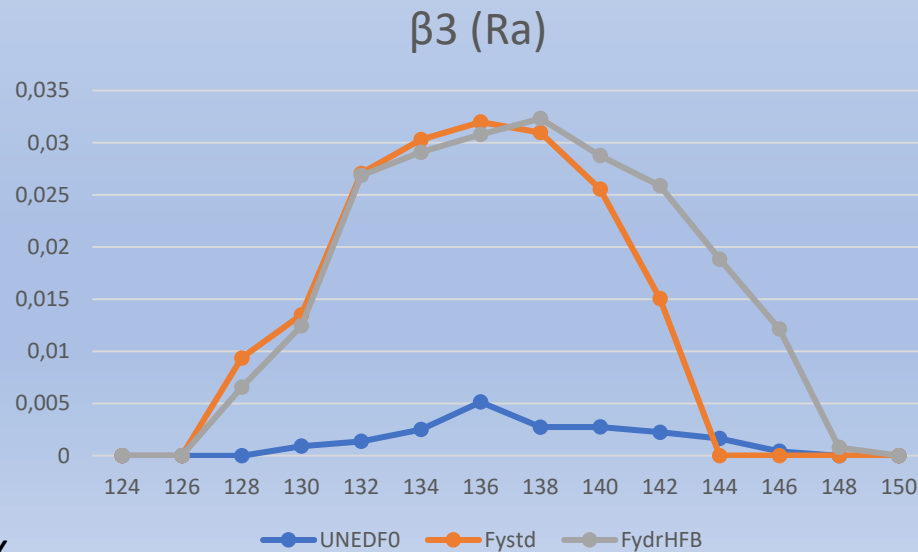
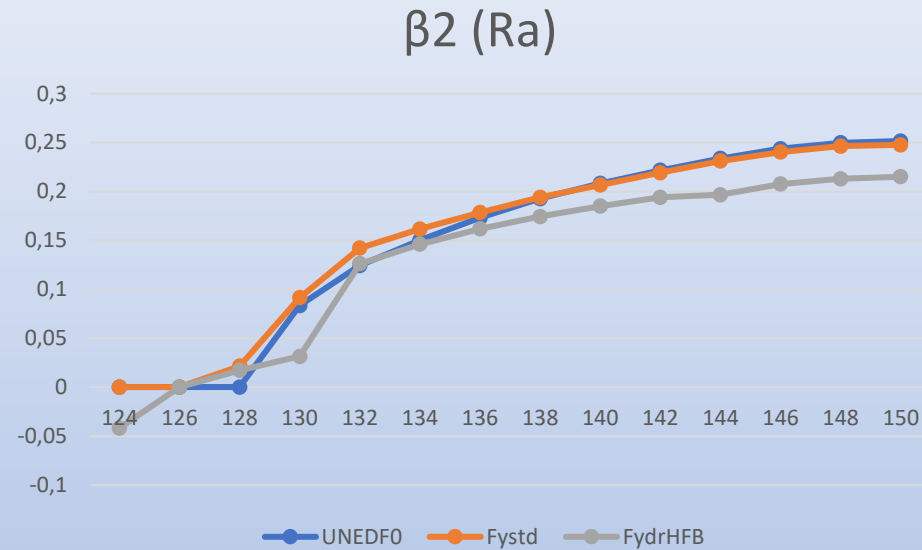
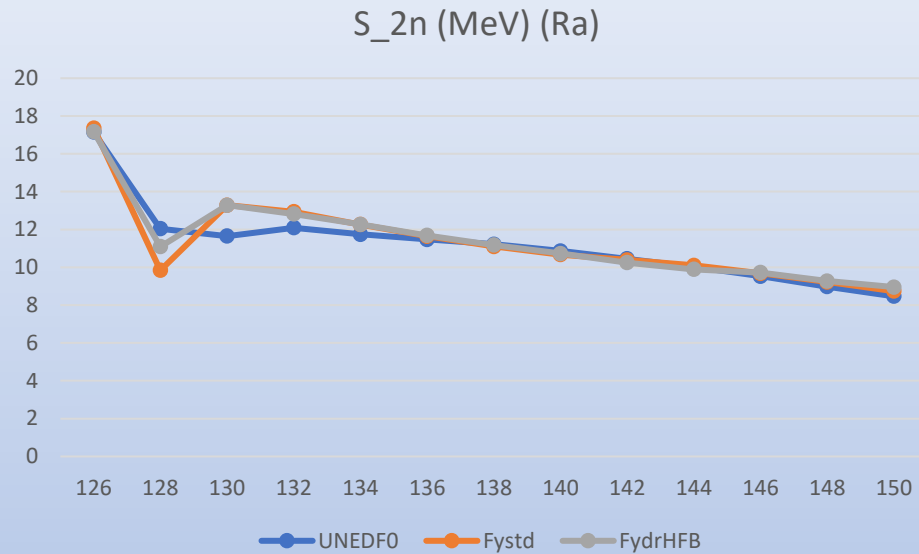
## 4) Comparisons

- Current-gen widely used EDFs: UNEDF(0;1;2), SLY4, etc



# 4) Comparisons

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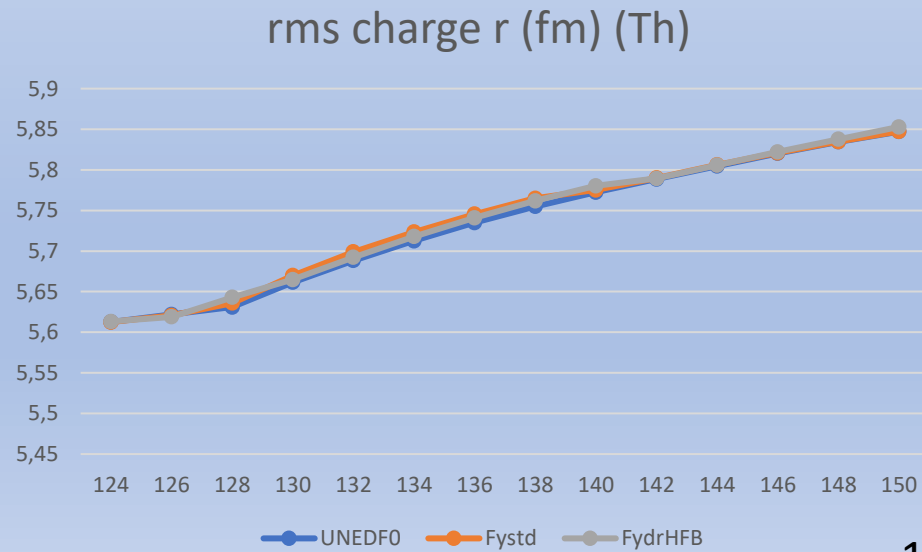
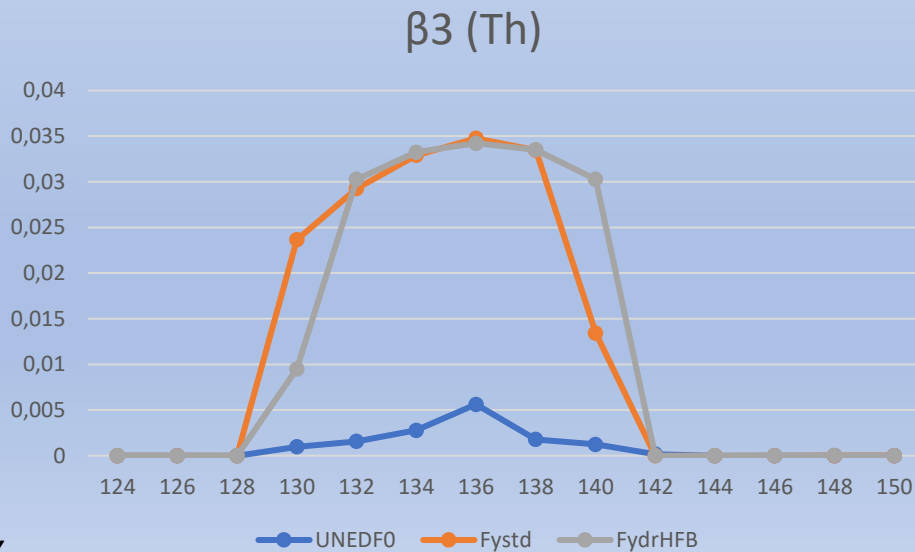
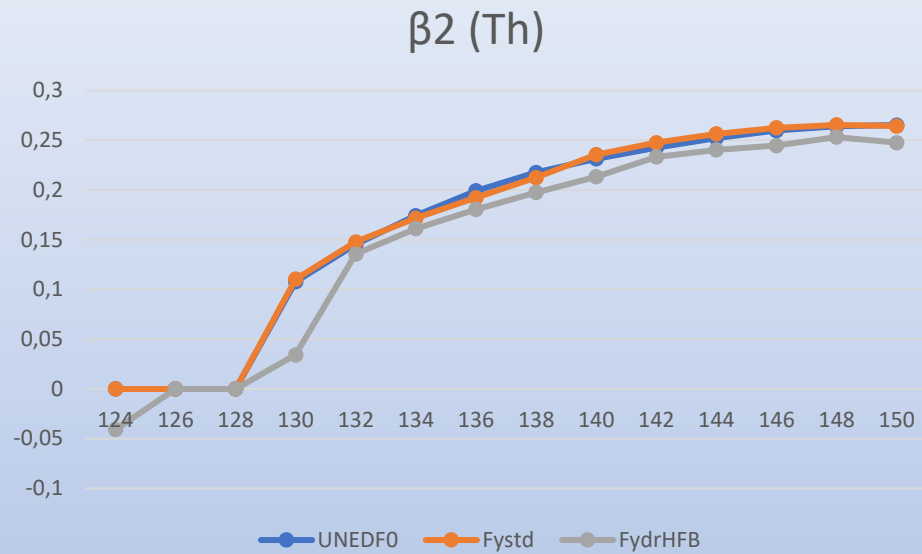
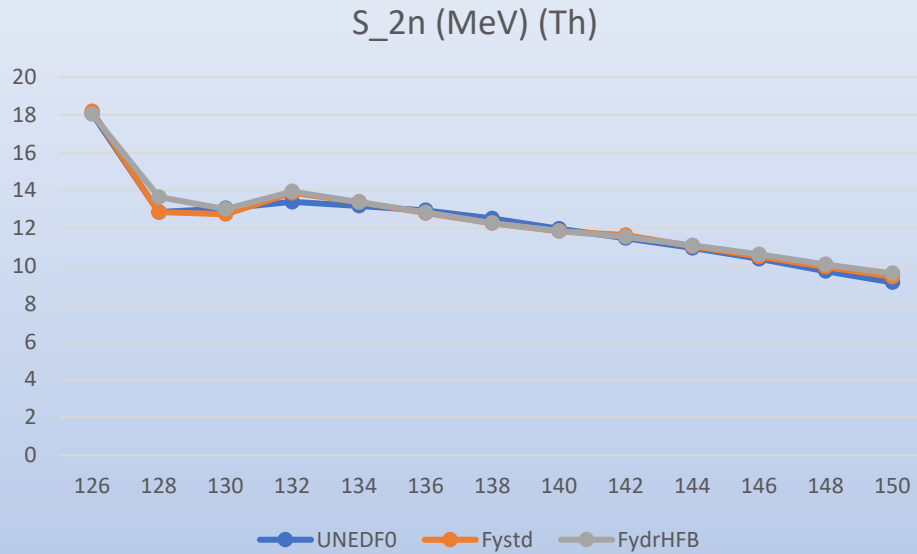






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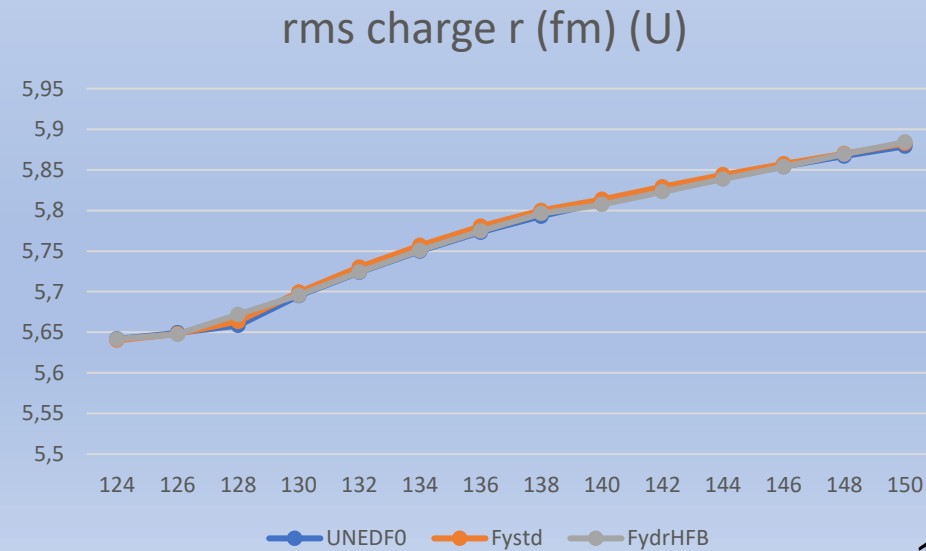
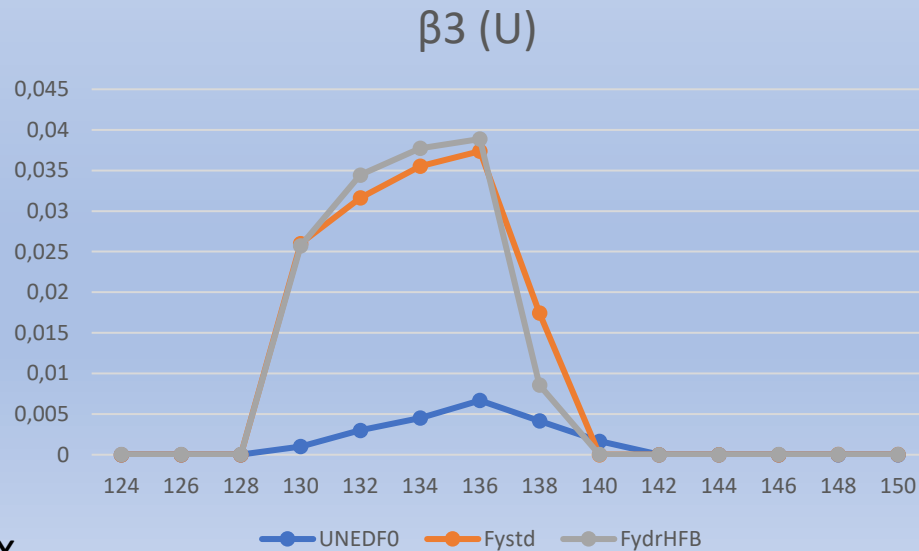
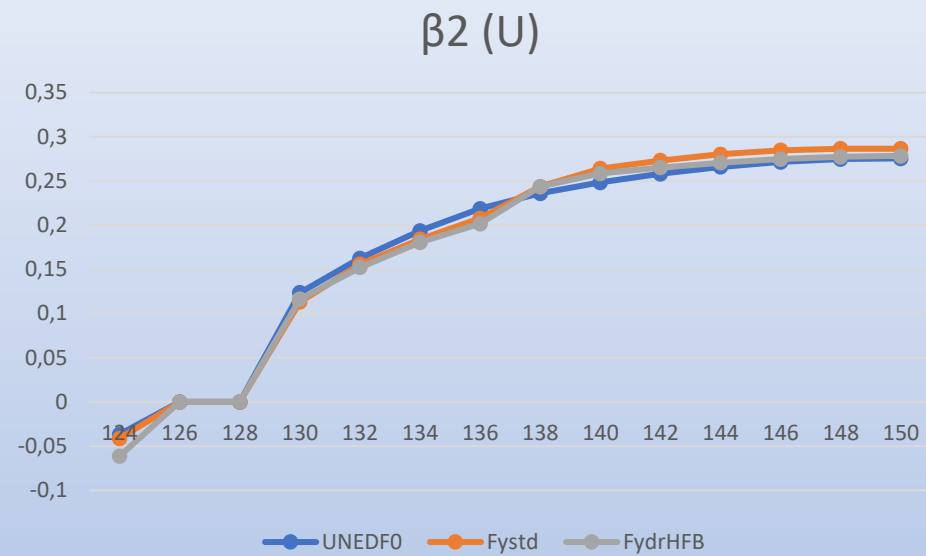
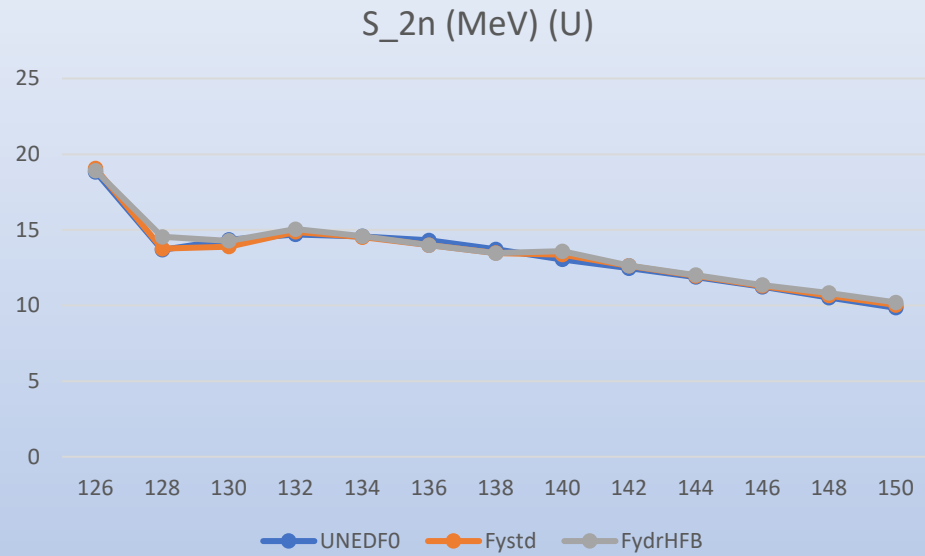
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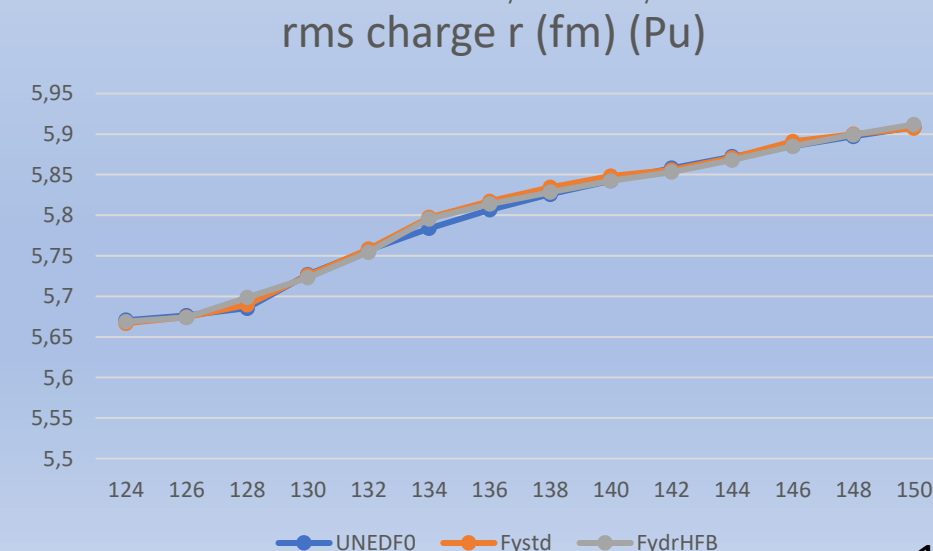
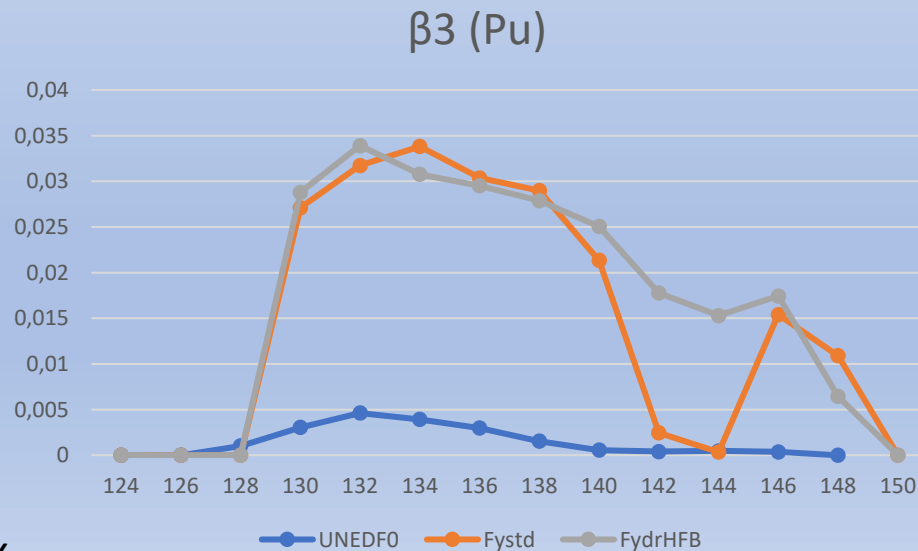
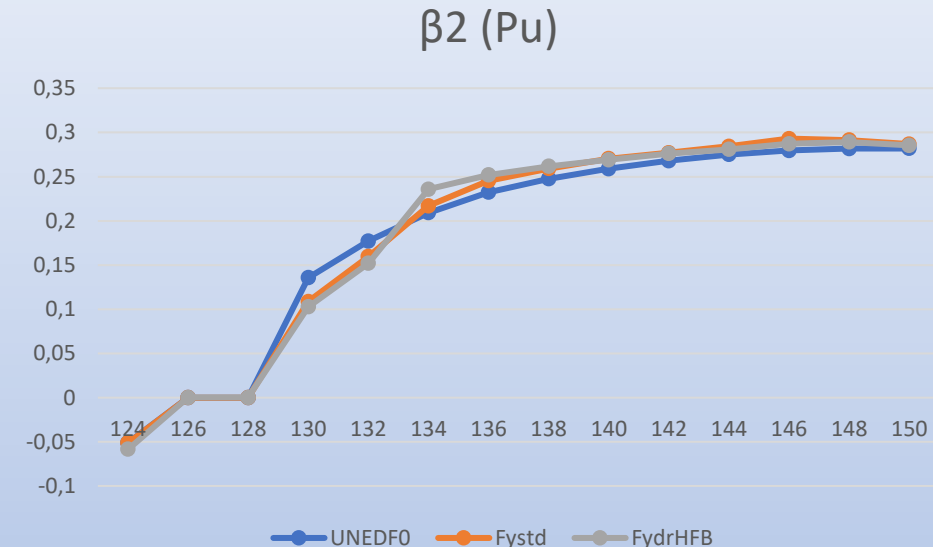
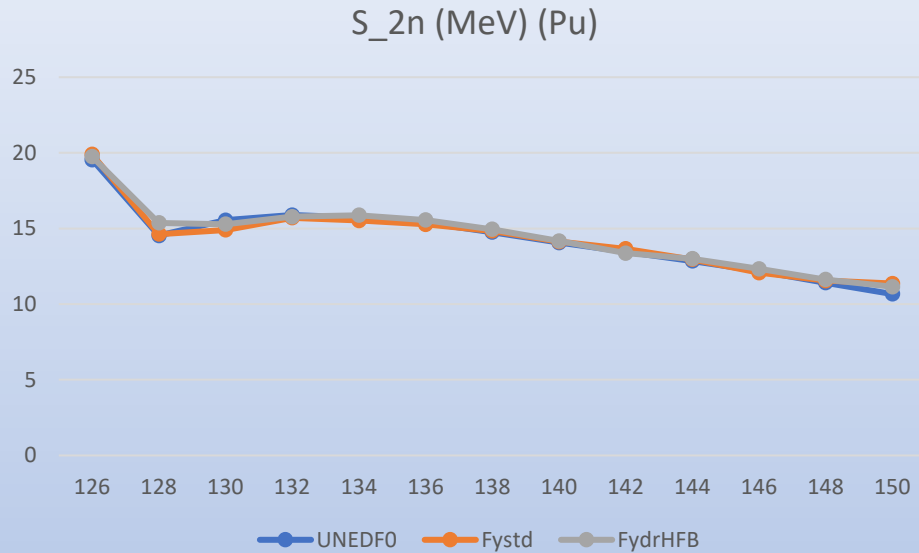
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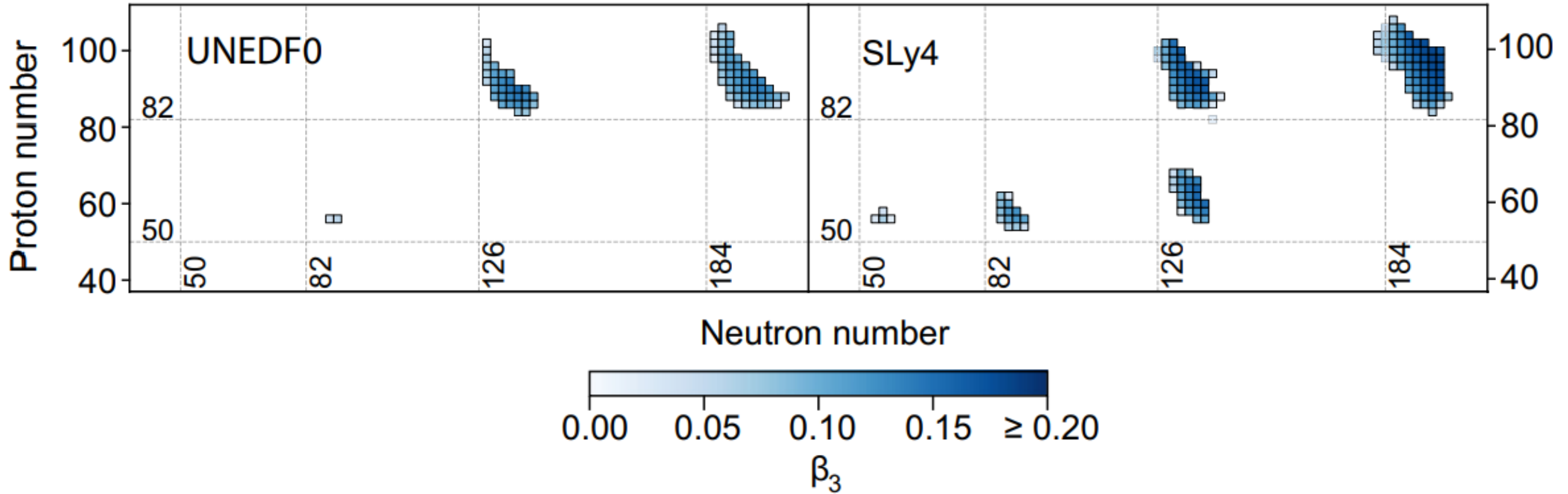


## 4) Comparisons



# 4) Comparisons

- Survey of pear-shaped landscapes with Skyrme-based EDFs [9]

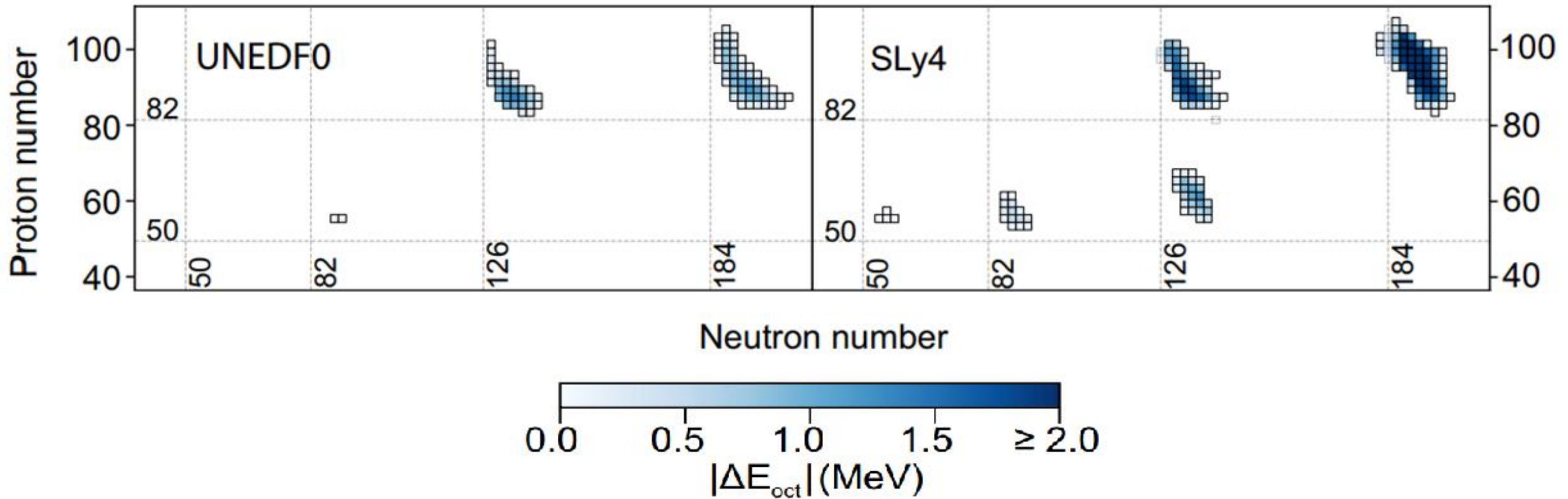


[9] Y. Cao, S.E. Agbemava, A.V. Afanasjev et al., Phys. Rev. C, 102, 12 (2020)



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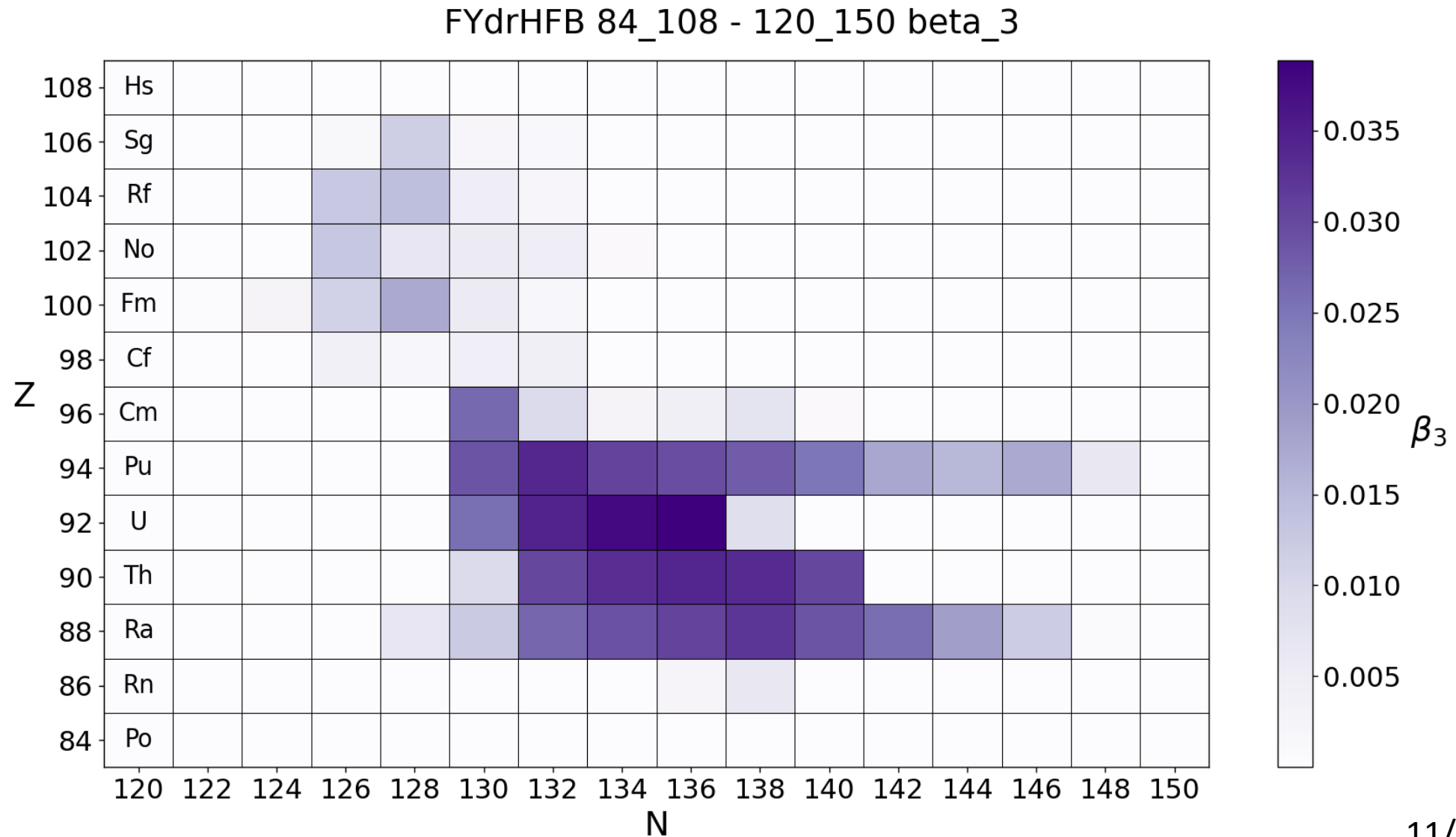
[9] Y. Cao, S.E. Agbemava, A.V. Afanasjev et al., Phys. Rev. C, 102, 12 (2020)



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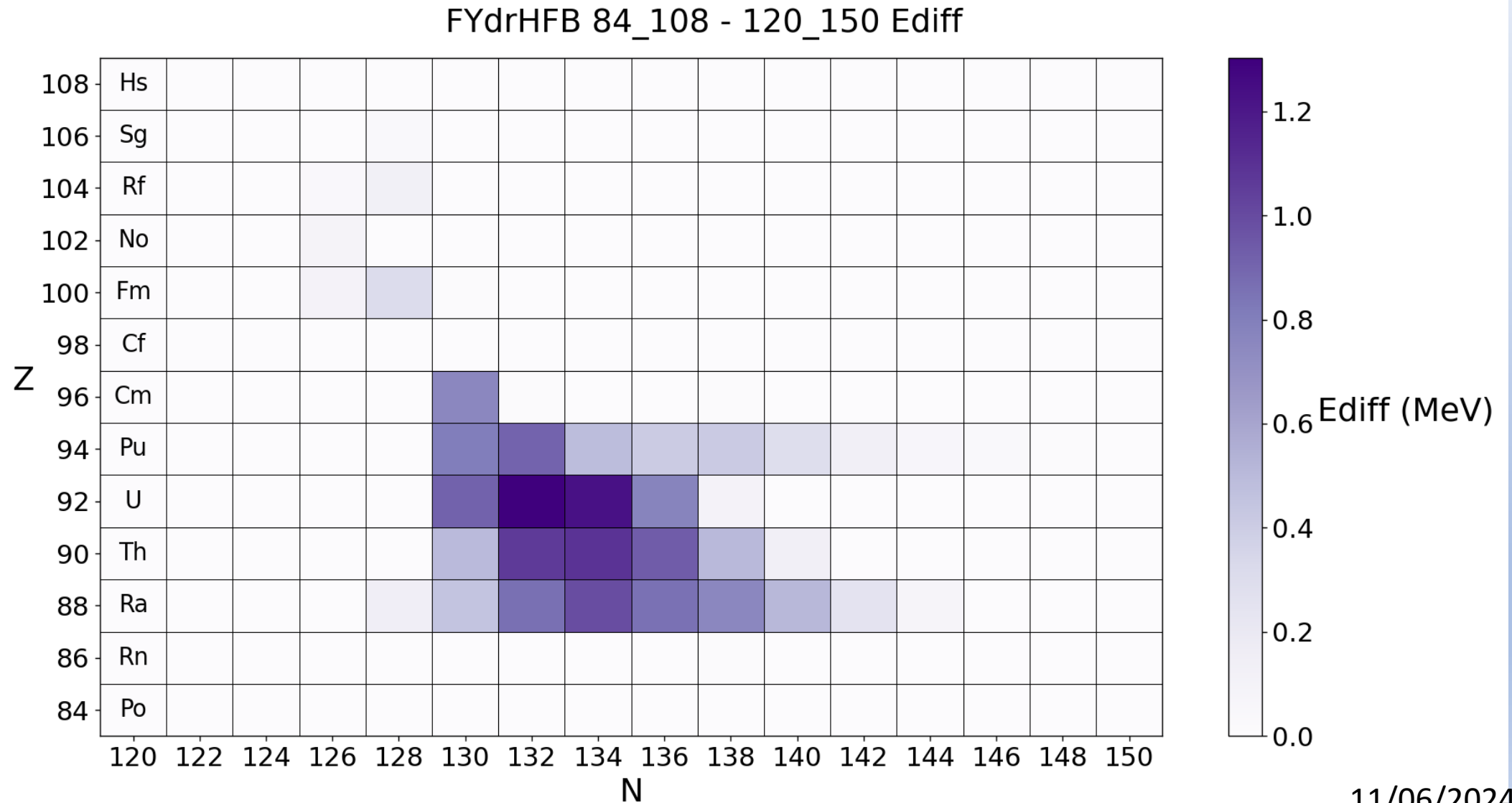






# 4) Comparisons

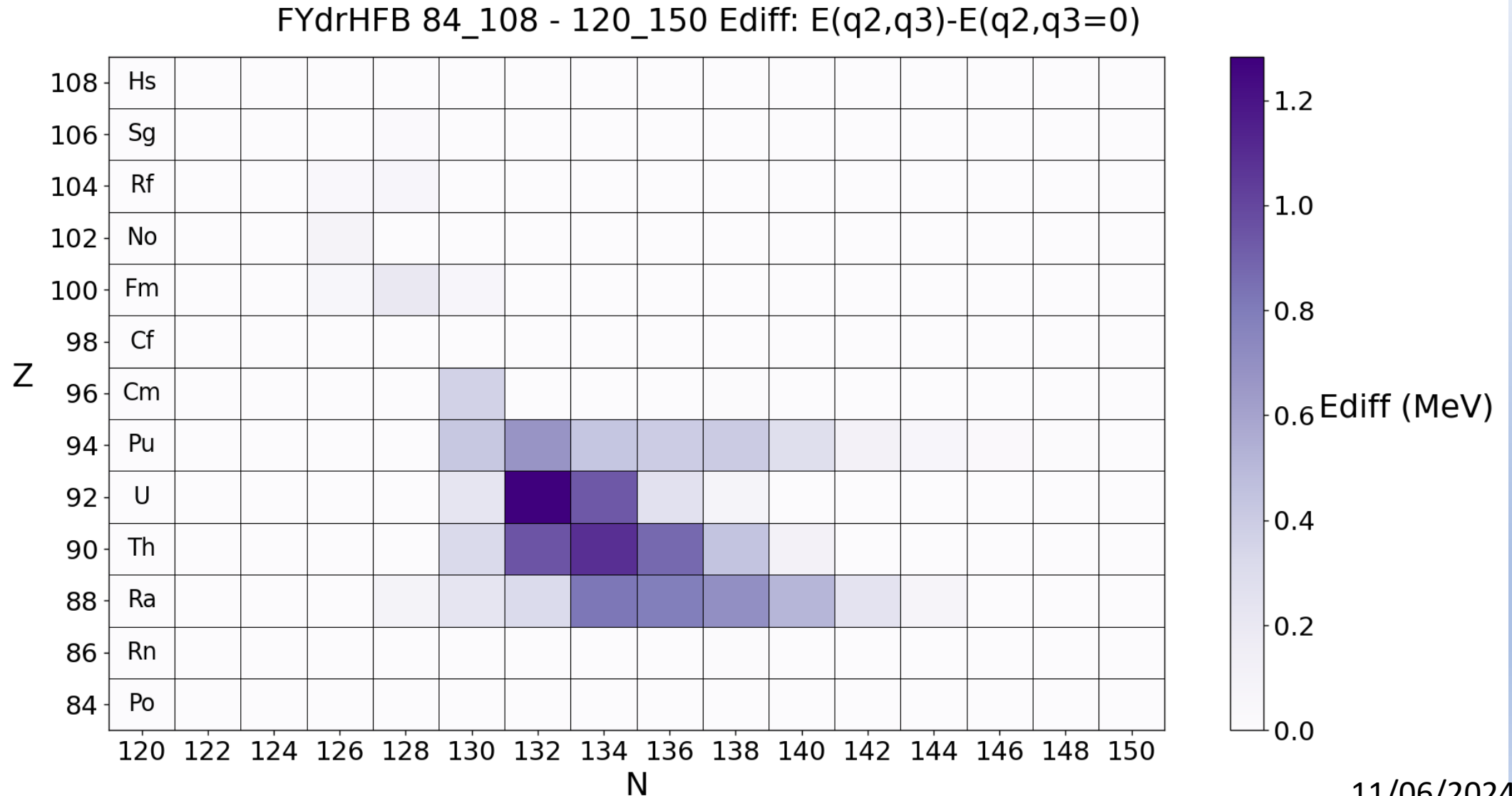
Difference in ground state energy gained from the inclusion of octupole deformation





# 4) Comparisons

Difference in ground state energy gained from the inclusion of octupole deformation

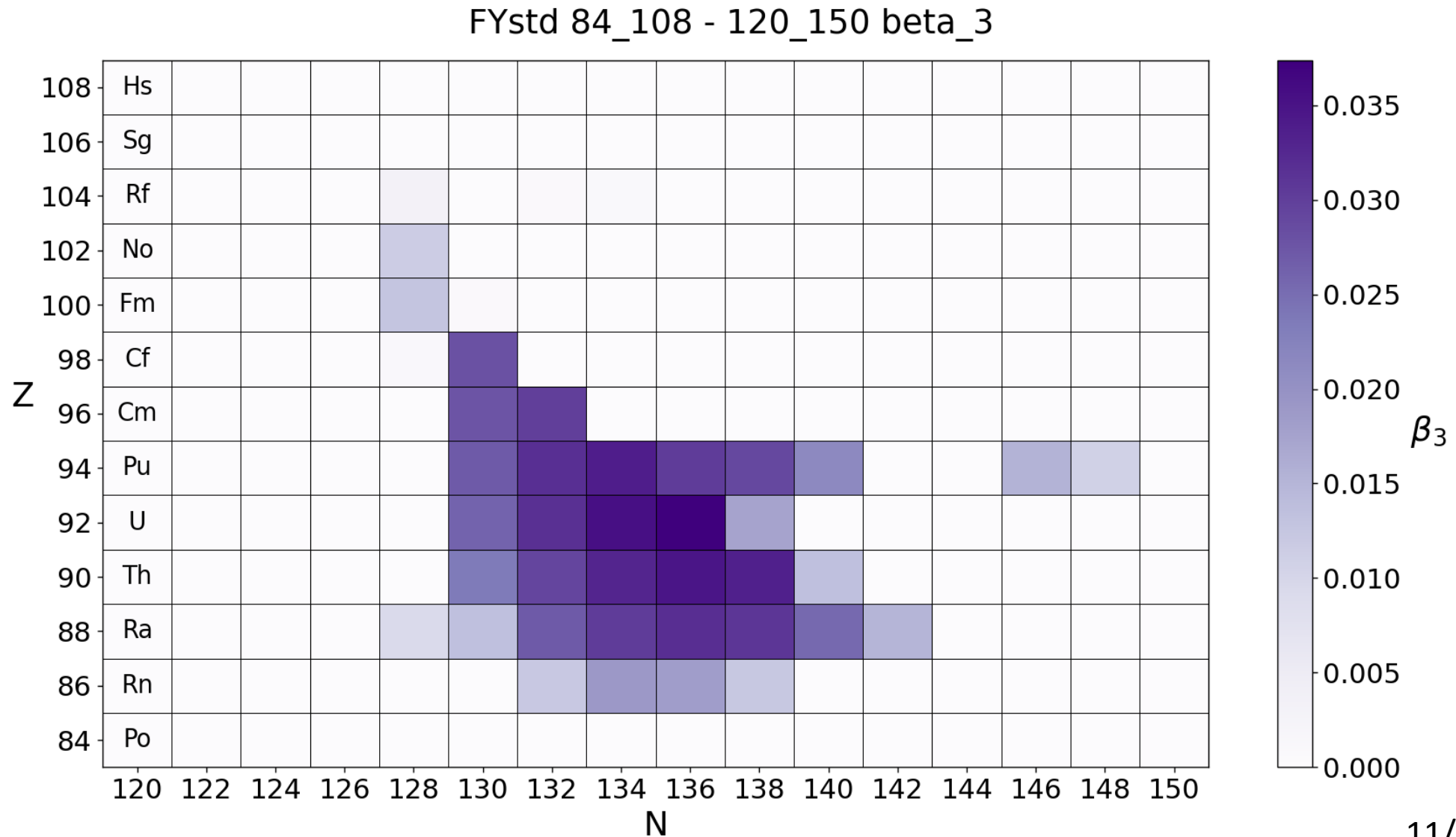




## 4) Comparisons



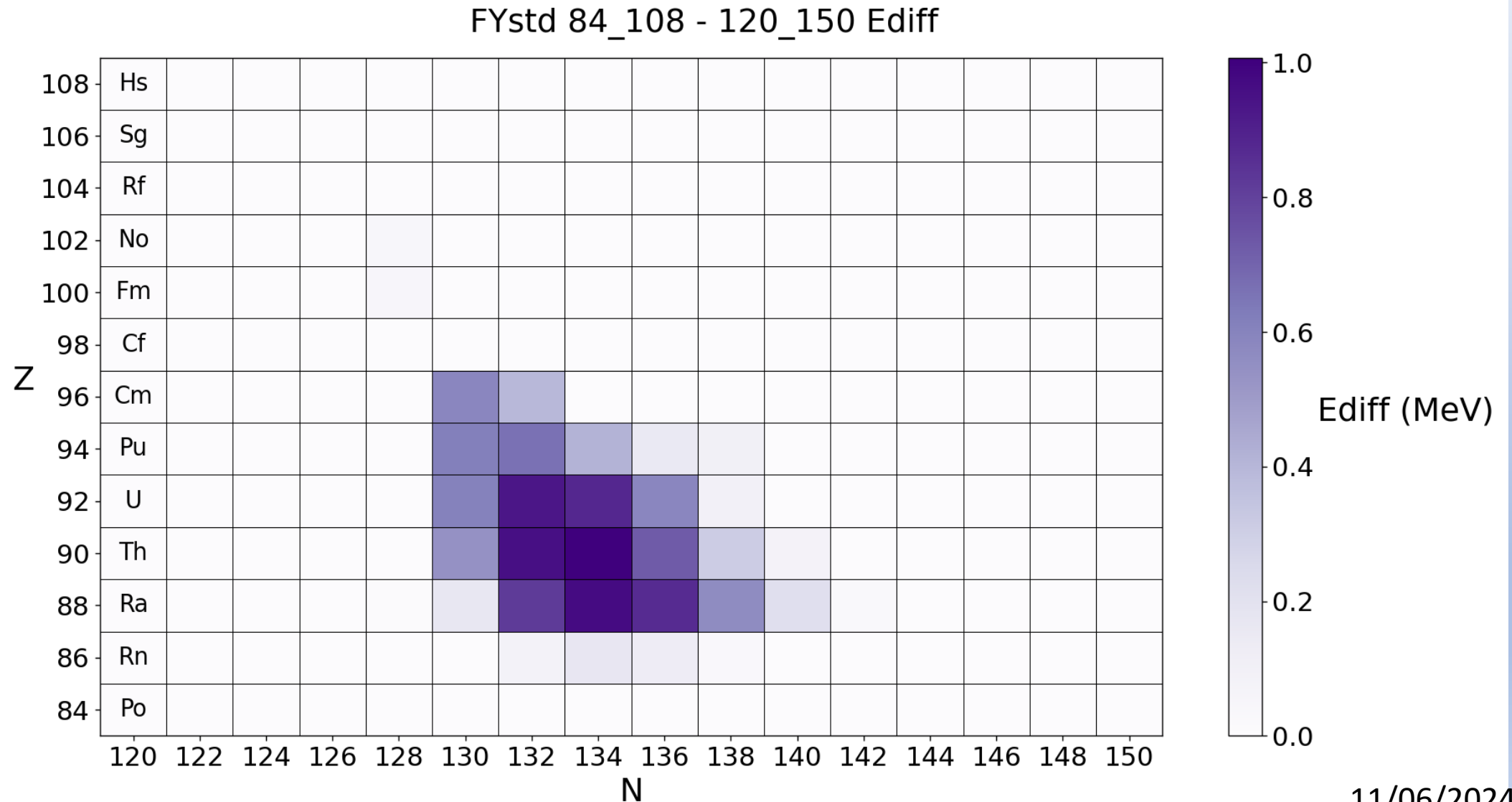
# 4) Comparisons





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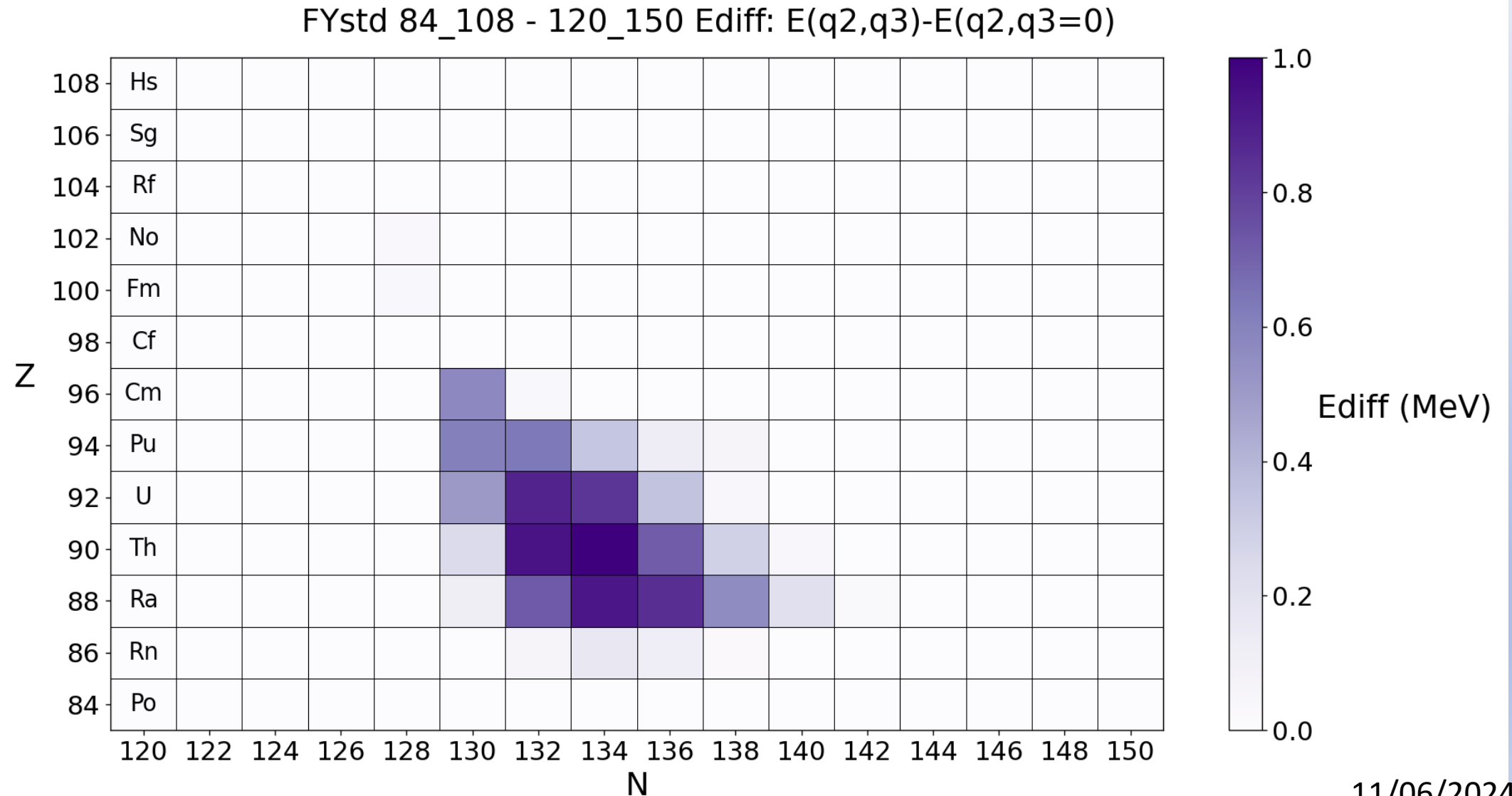
Difference in ground state energy gained from the inclusion of octupole deformation





# 4) Comparisons

Difference in ground state energy gained from the inclusion of octupole deformation





## 5) Conclusions



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- Returned predicted octupole clusters in Actinides with stronger  $\beta_3$
- Strong step towards better understanding of heavily-deformed nuclei complex processes s.a. systematics, spectra, nuclear Schiff moment, fission, etc.



Thank you for  
your attention

Thanks to my colleagues:

M. Kortelainen, R. Han; University of Jyväskylä. J. Dobaczewski; University of York. K. Bennaceur; IPNL



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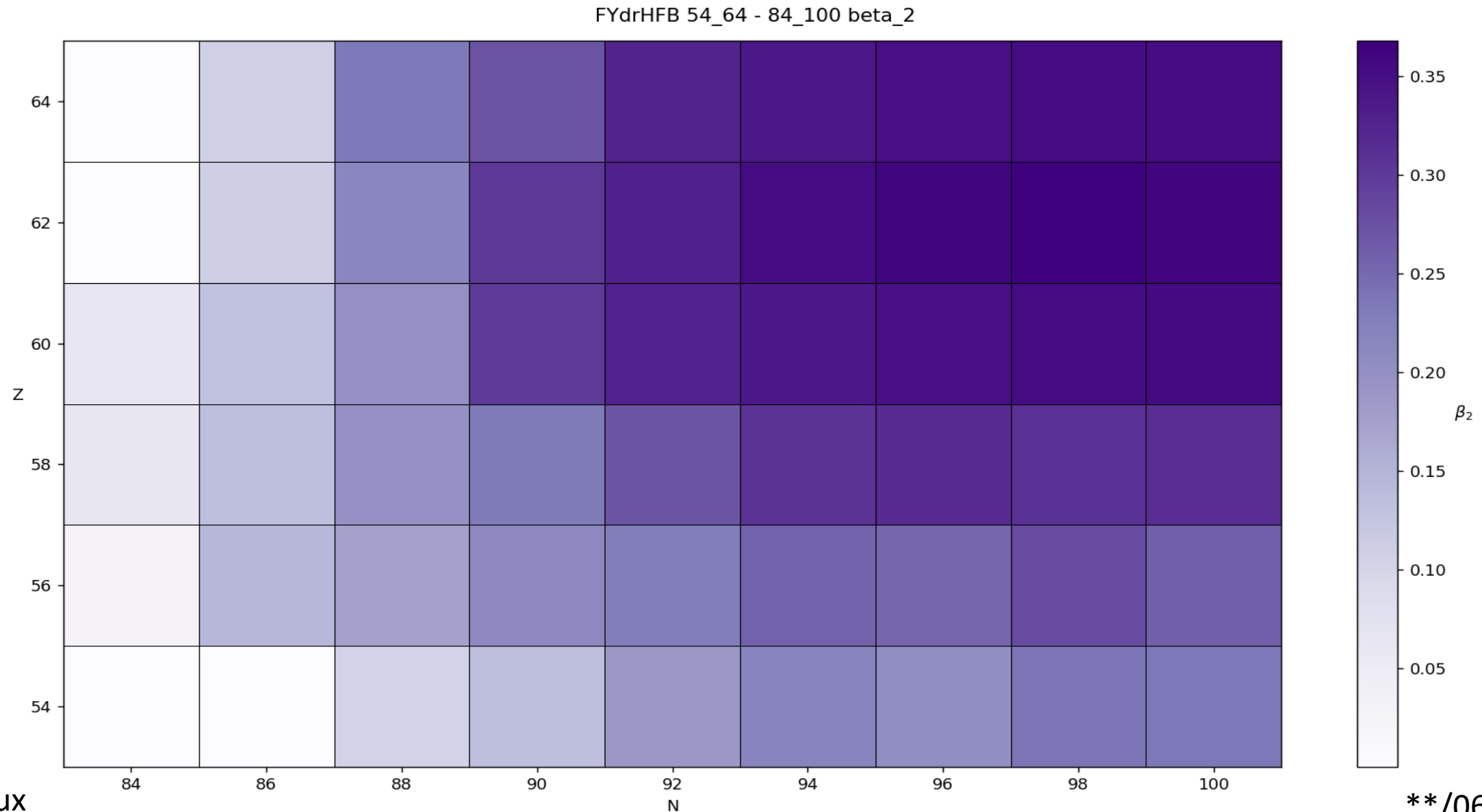


# Cesium-centered cluster



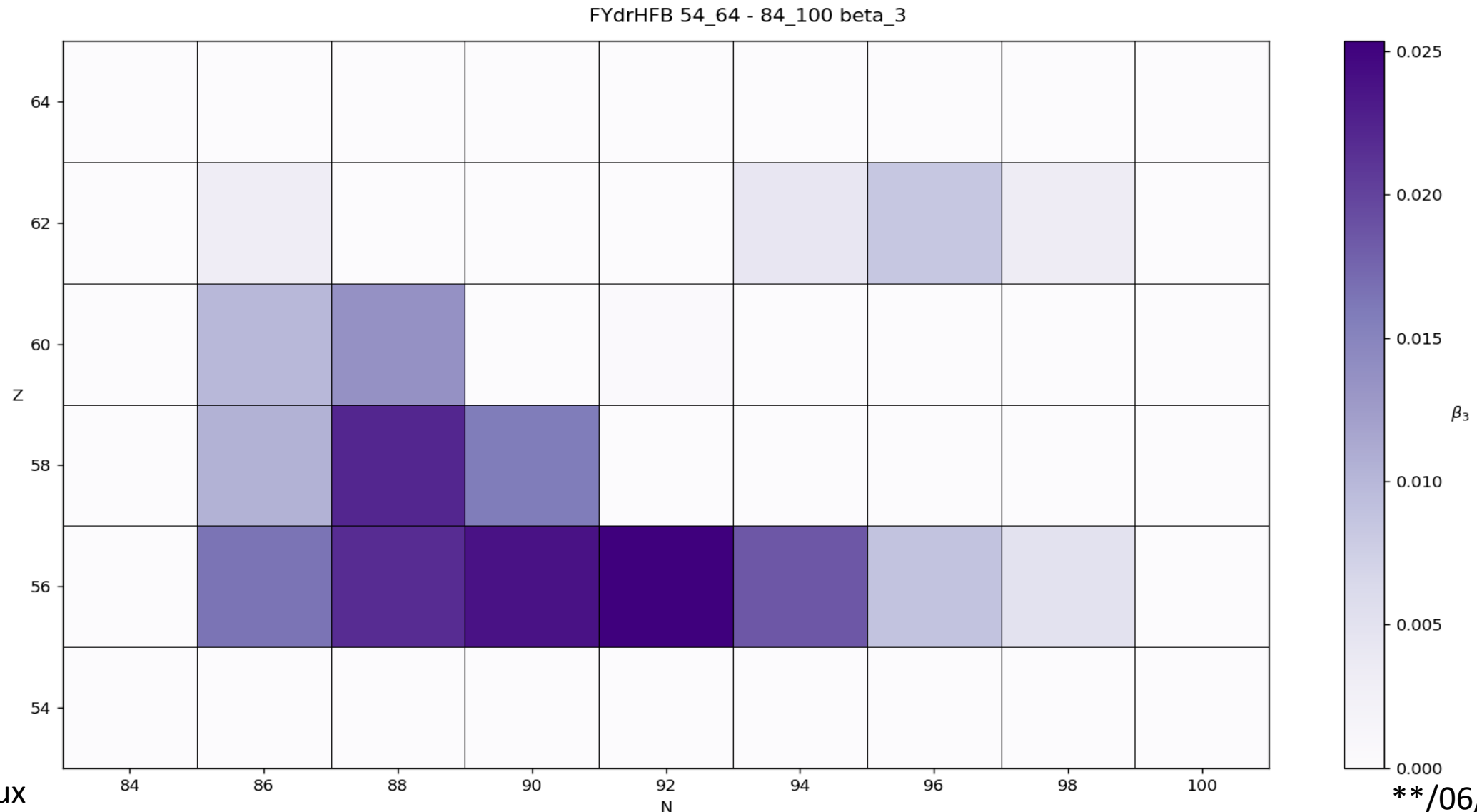


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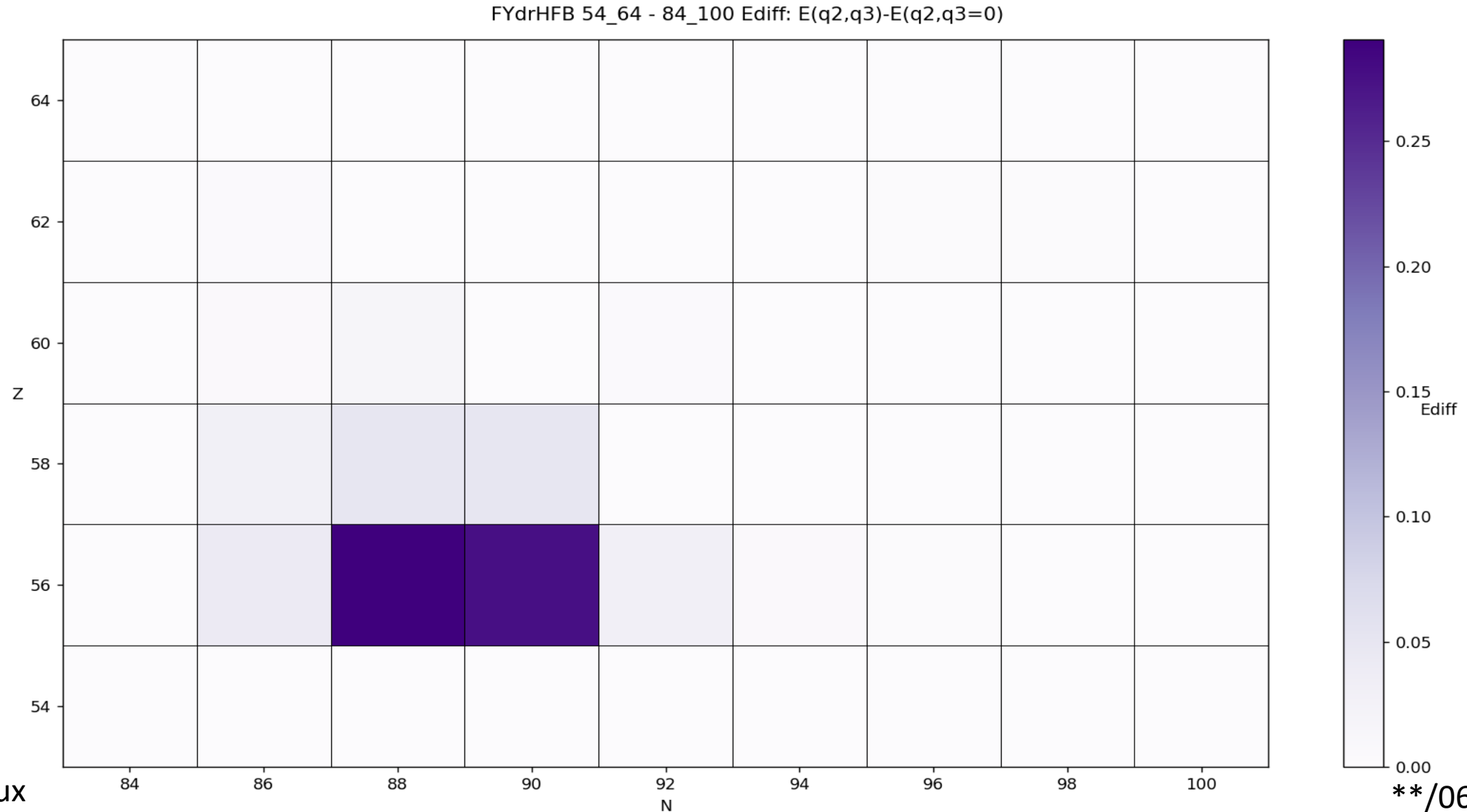
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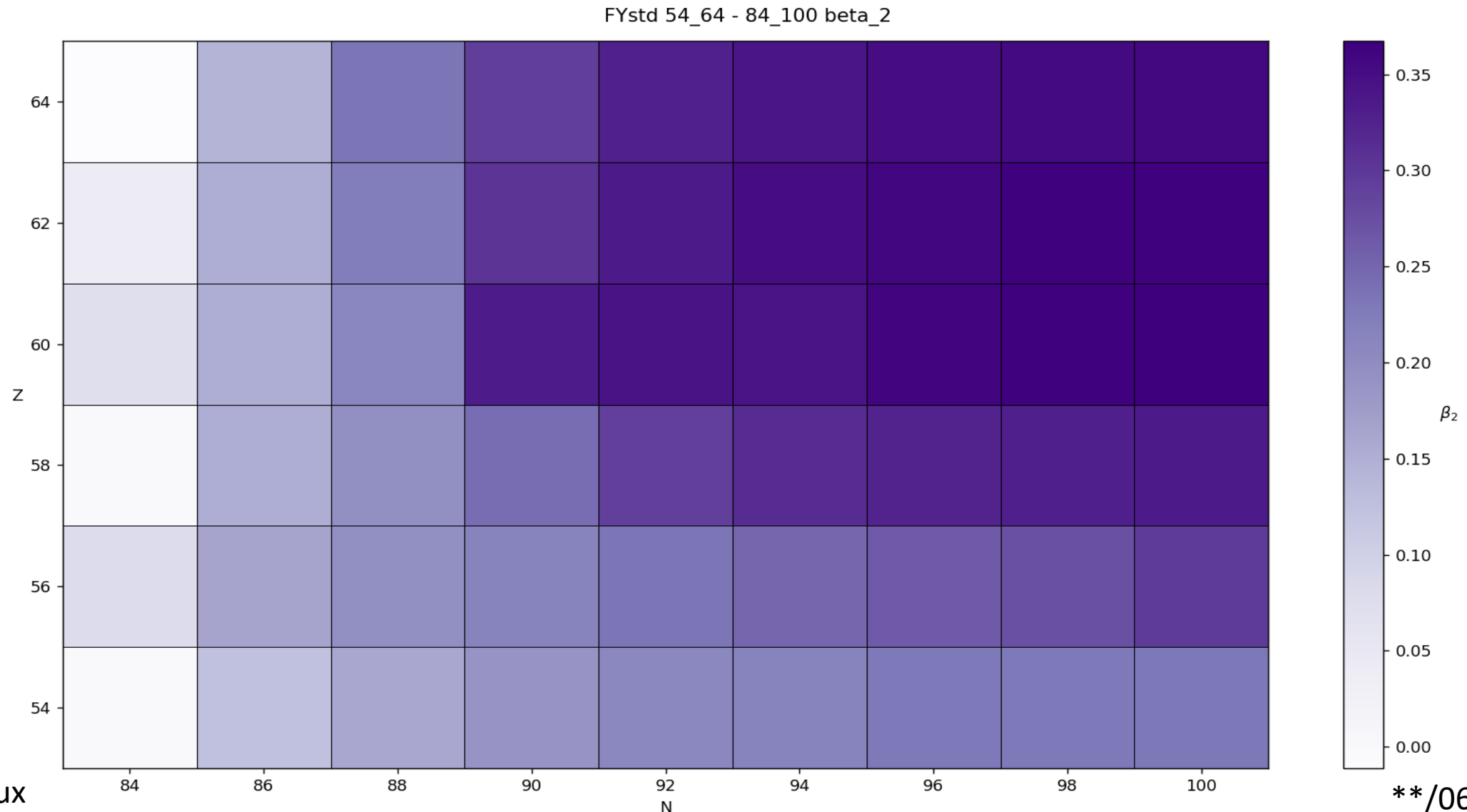




# Cesium-centered cluster

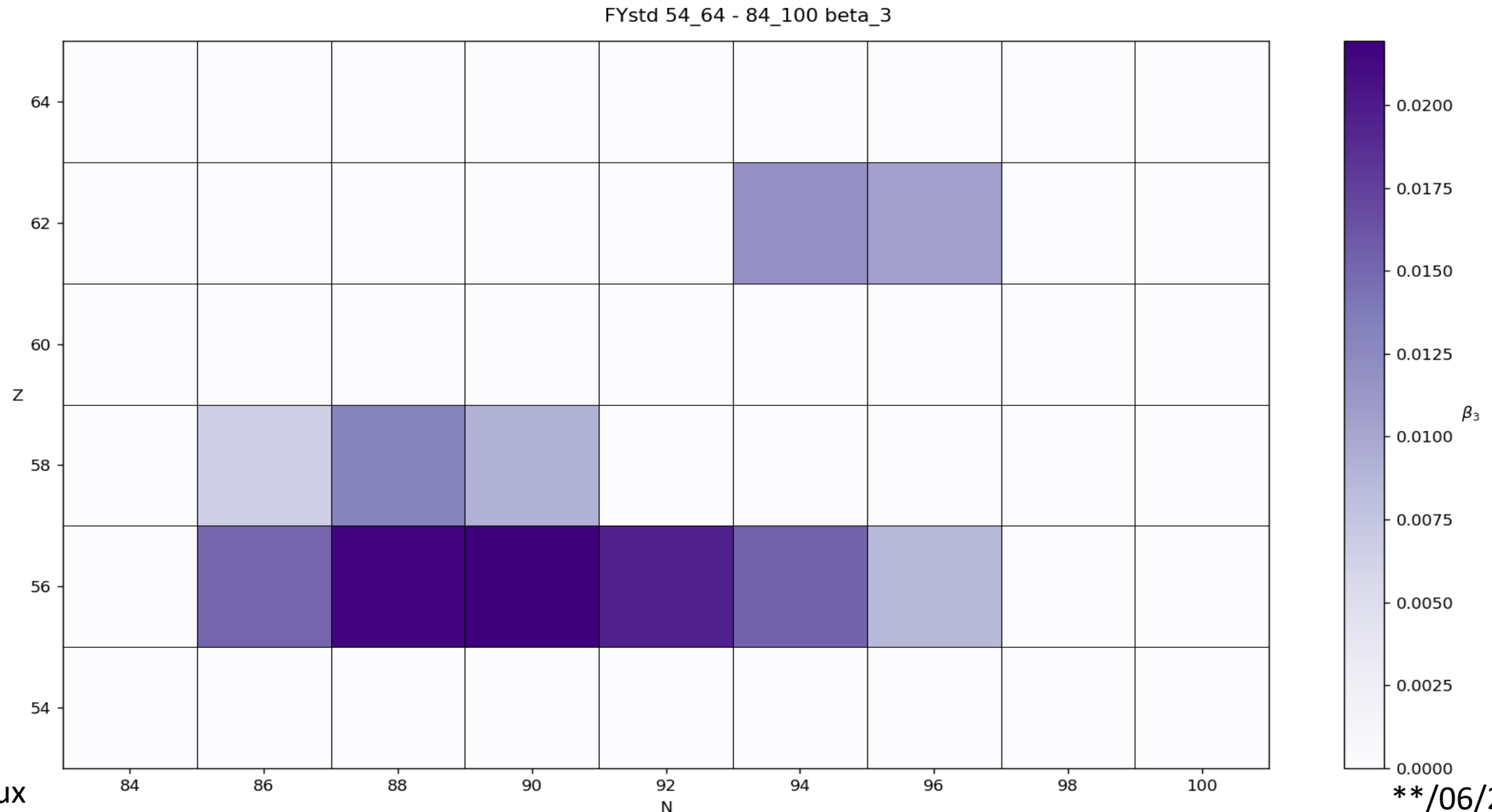


# Cesium-centered cluster



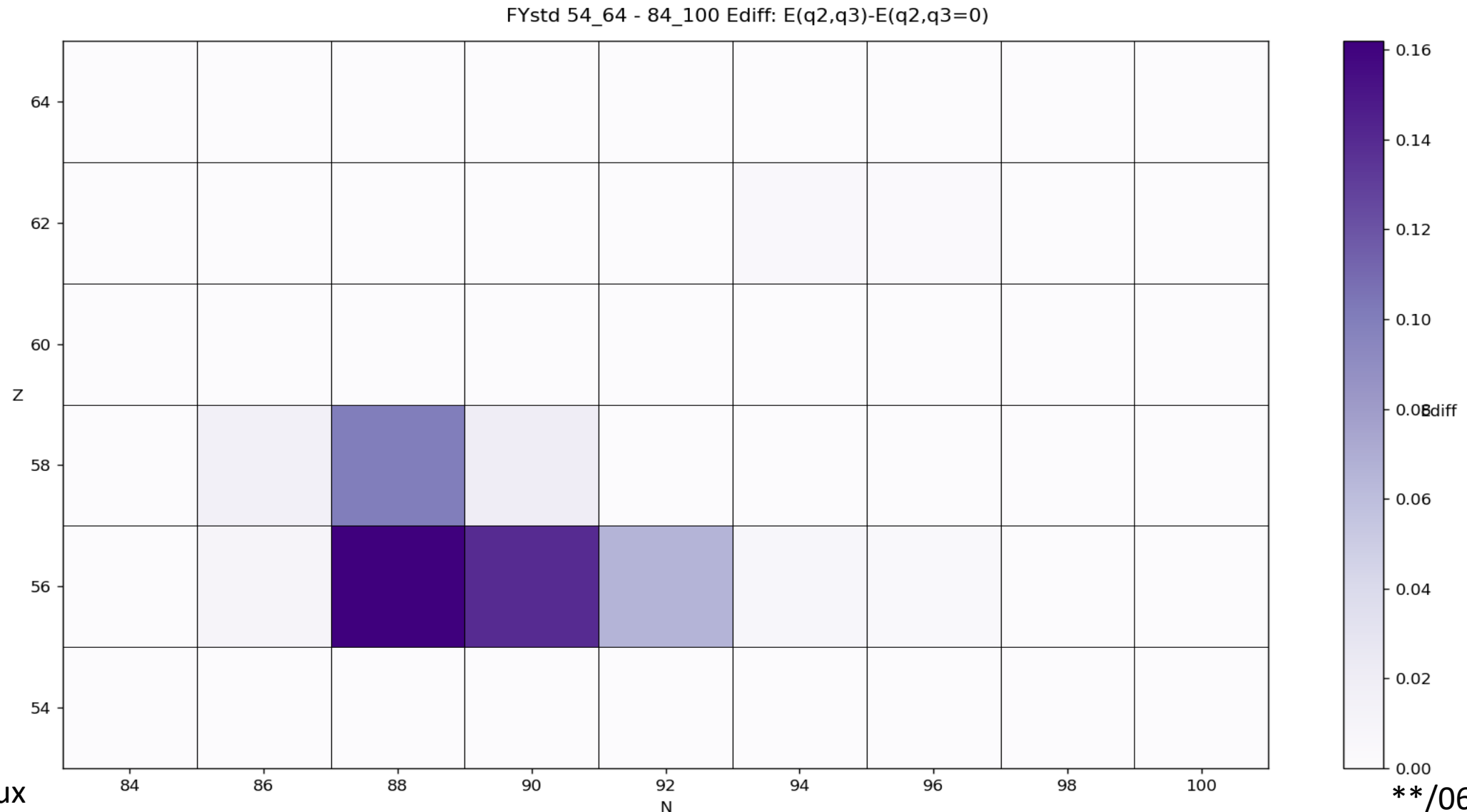


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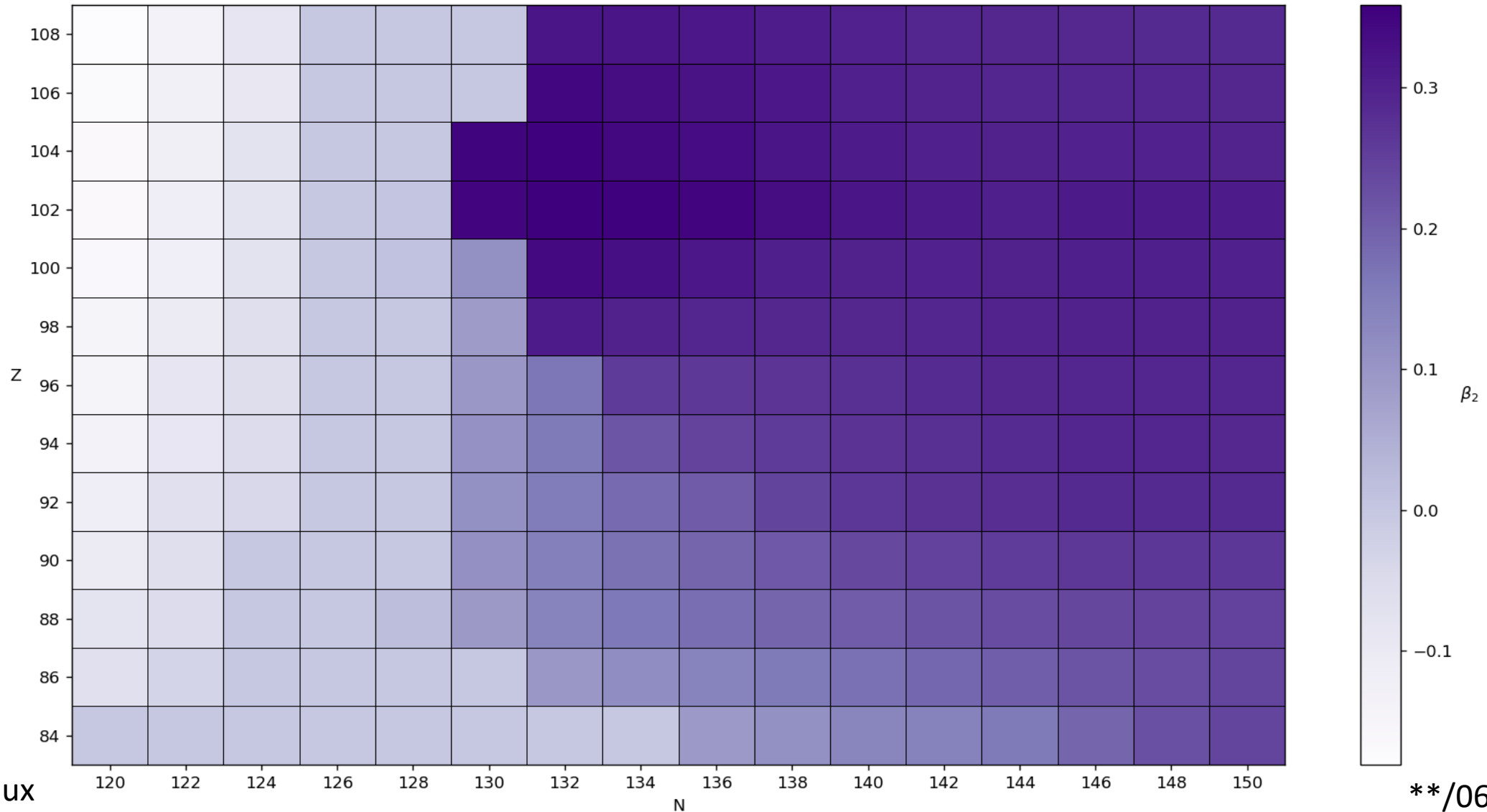


# Quadrupole



# Quadrupole

FYstd 84\_108 - 120\_150 beta\_2





# Quadrupole

