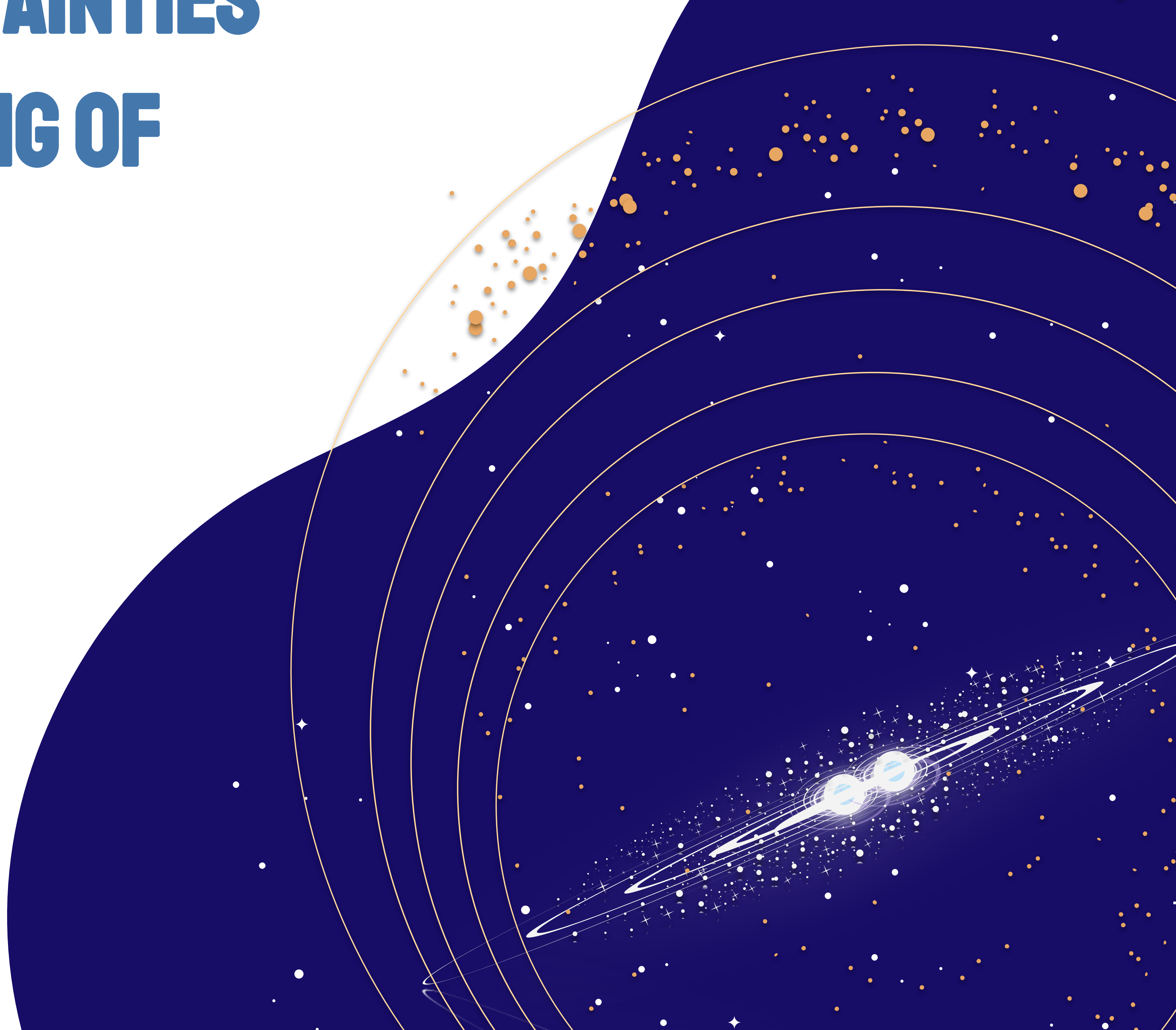
Statistical Framework for Nuclear Parameter Uncertainties in Nucleosynthesis Modeling of R-Process and I-Process

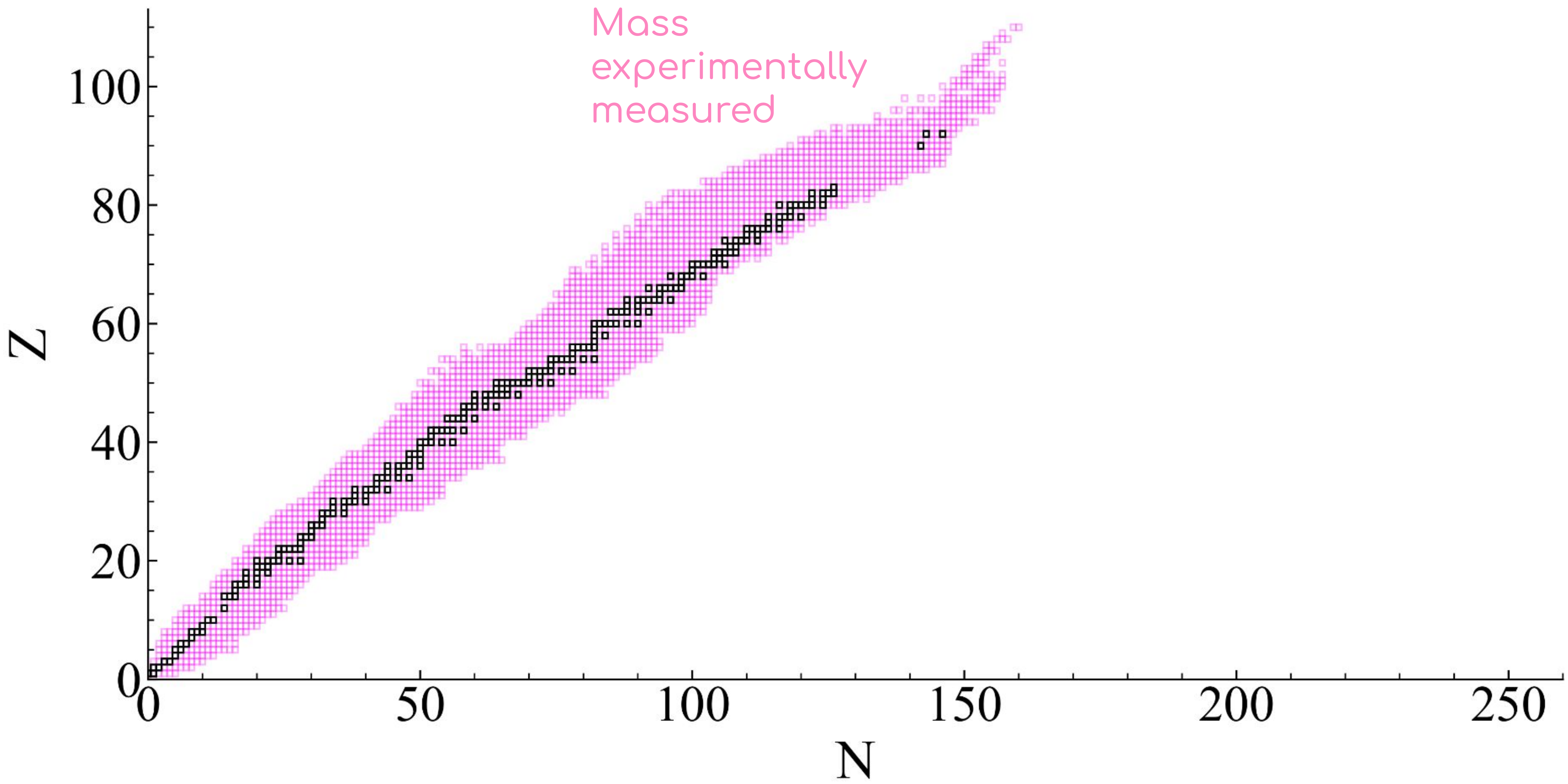
Sébastien Martinet

Co-authors: Arthur Choplin, Stéphane Goriely, Lionel Siess



Estimating Nuclear Uncertainties

Experimentally known masses vs r-process network needed



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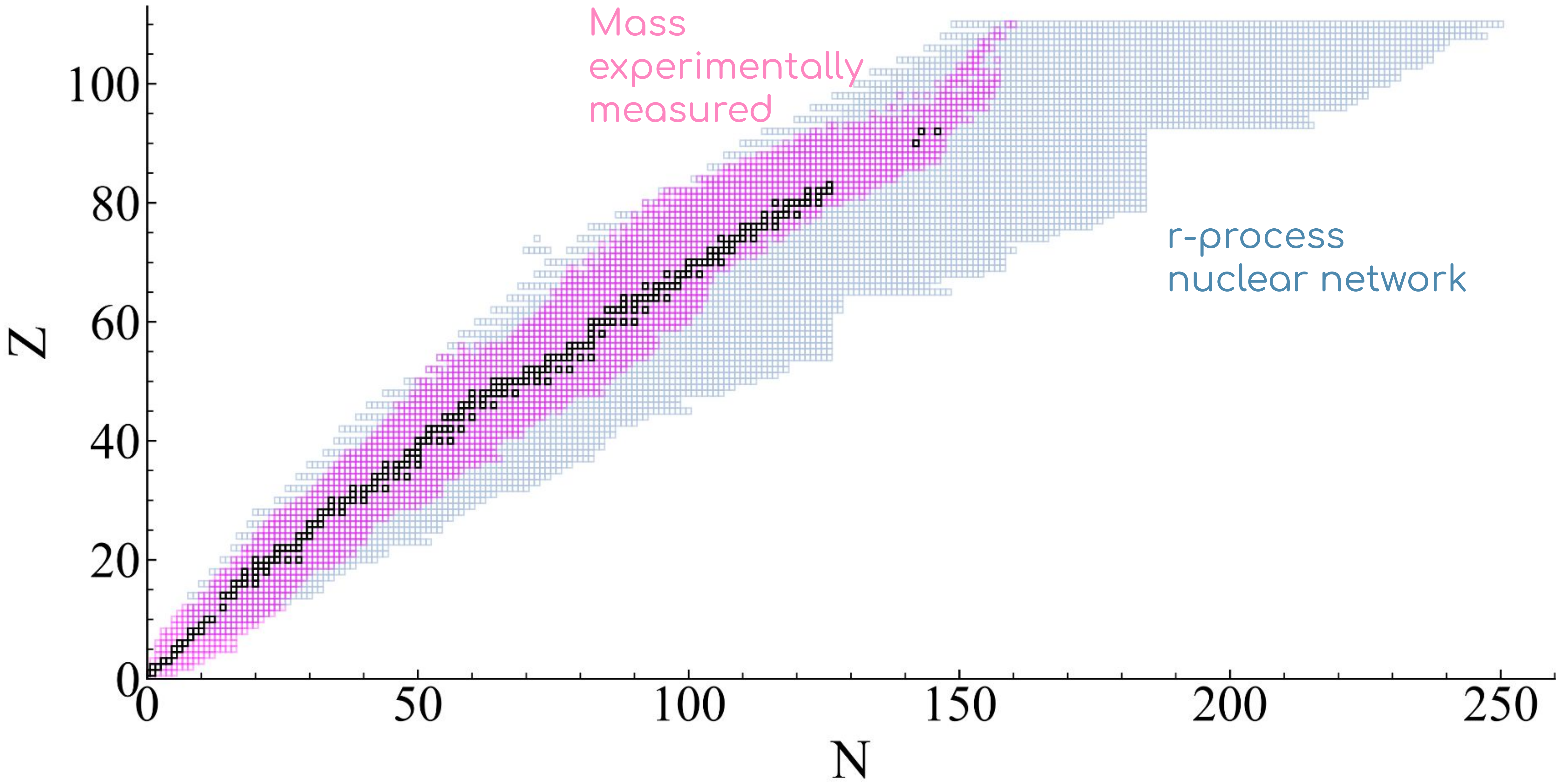

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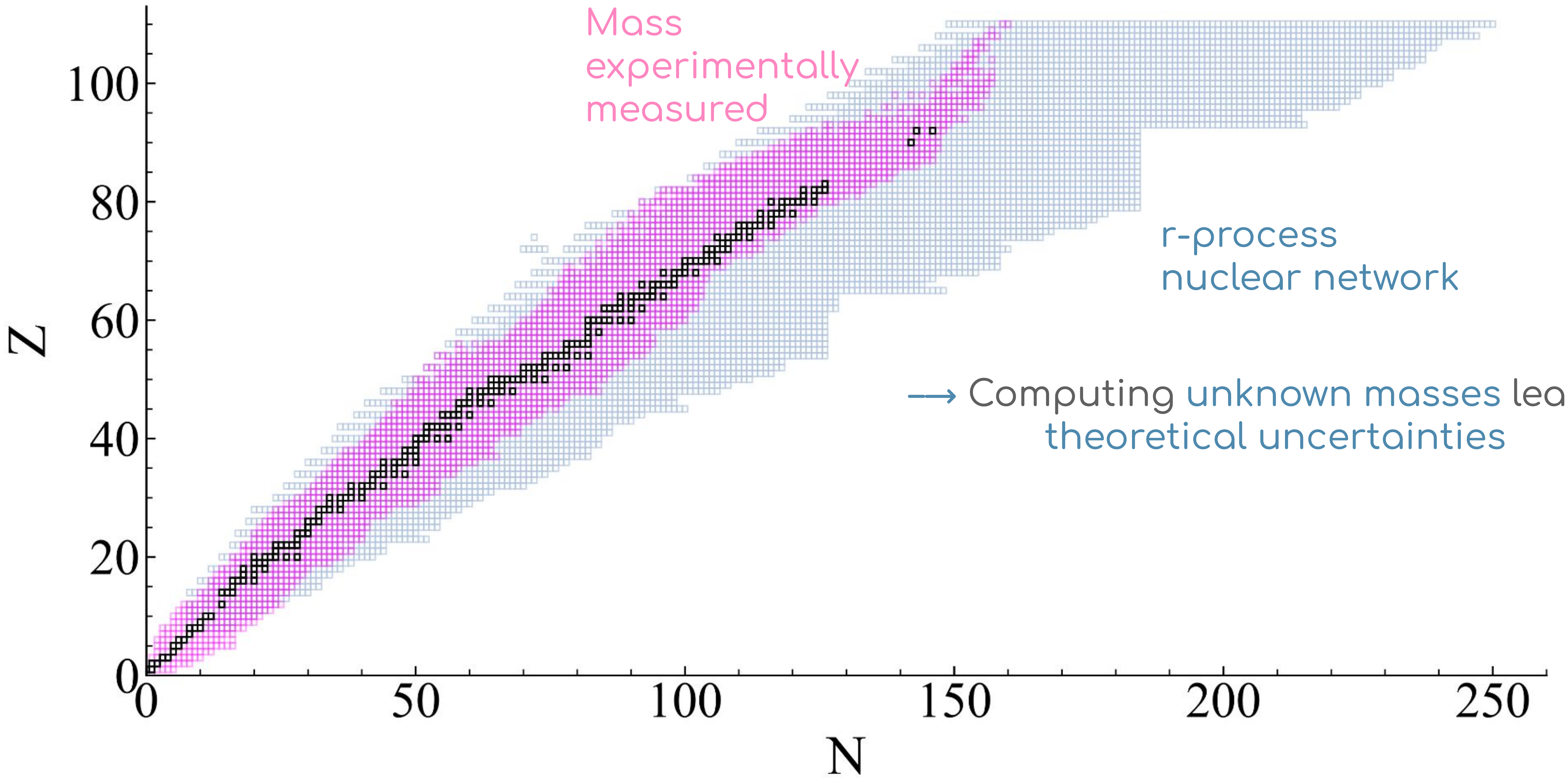

⟶ Computing unknown masses lead to theoretical uncertainties

Estimating Nuclear Uncertainties

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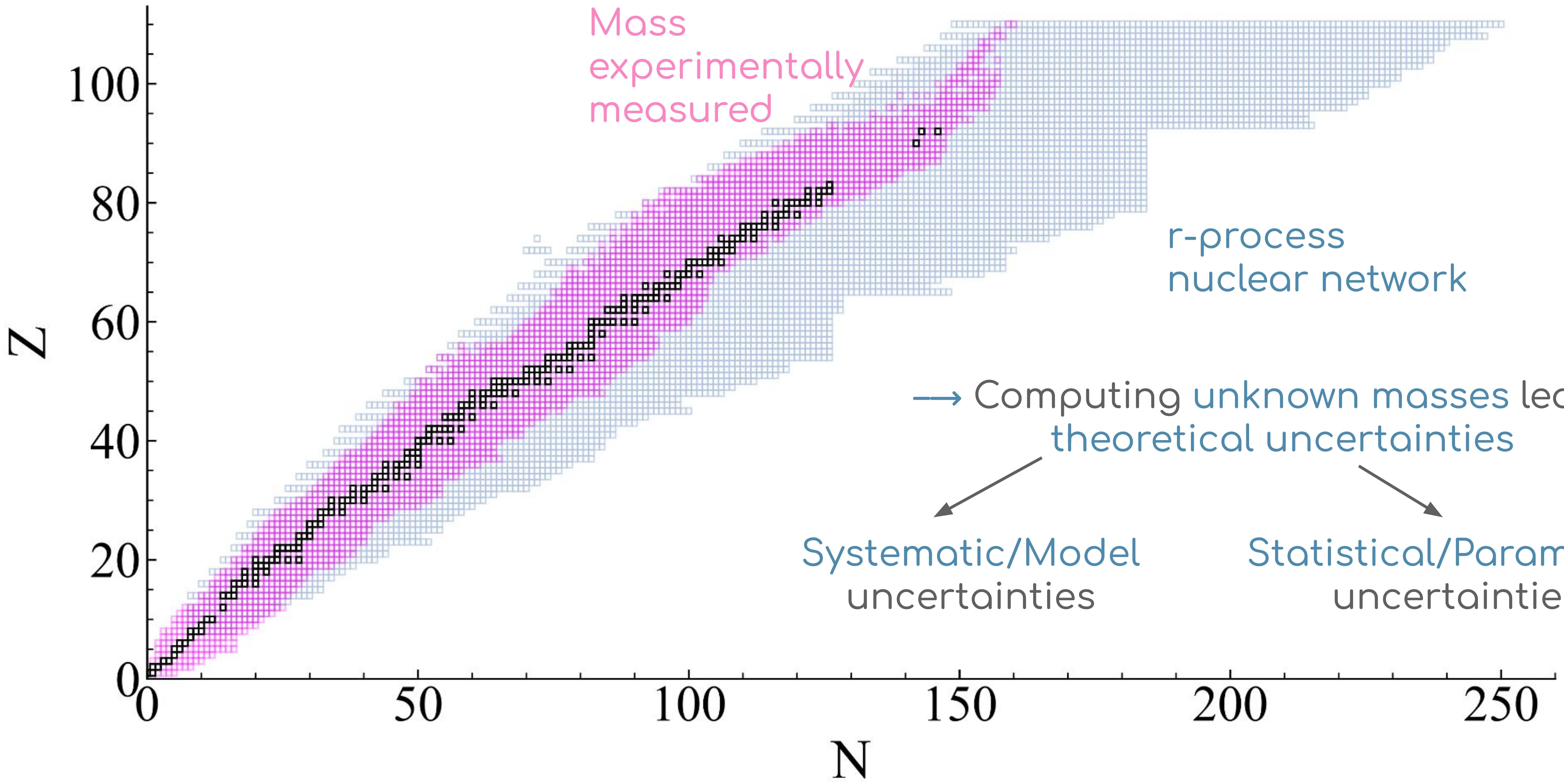


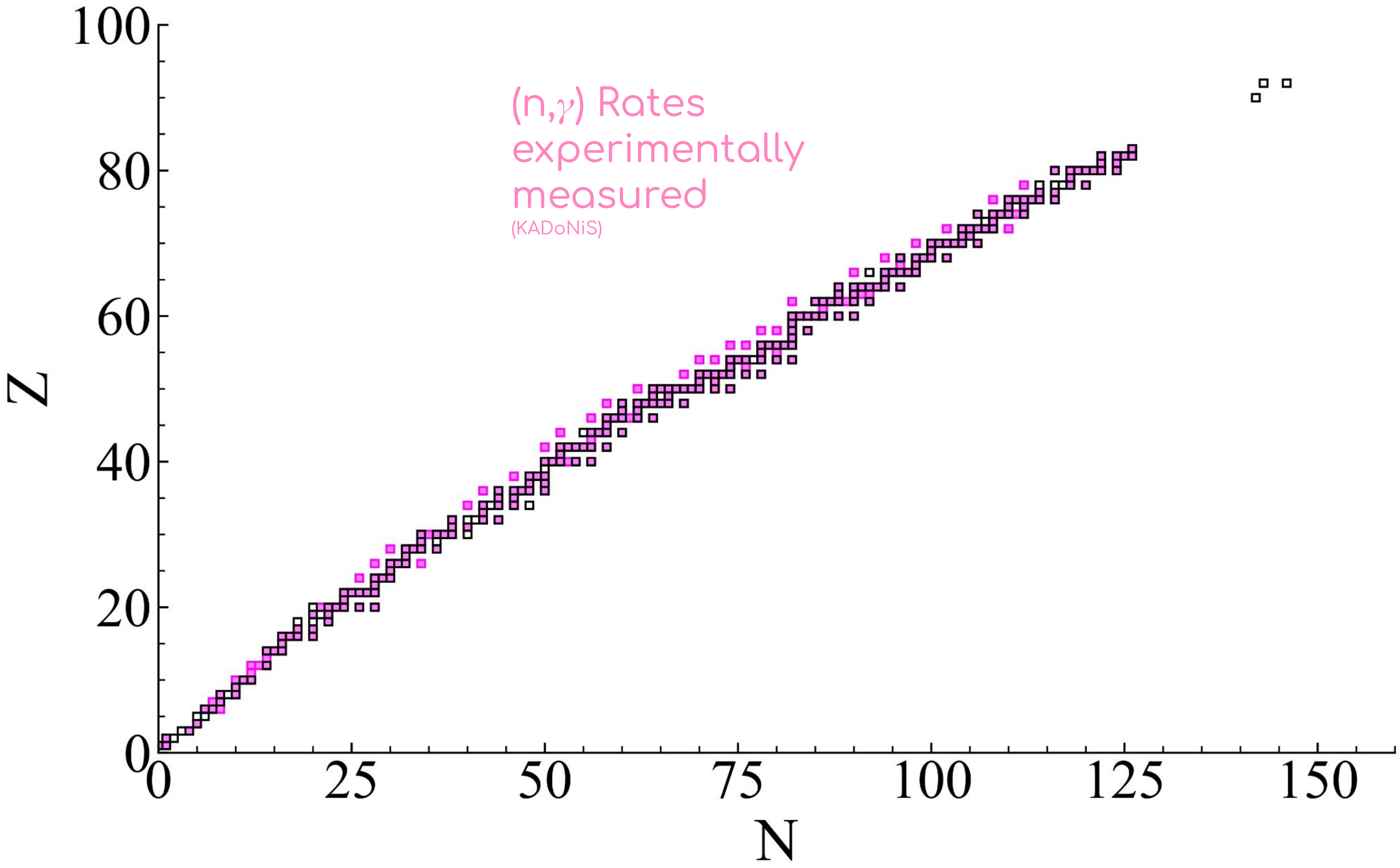
⟶ Computing unknown masses lead to theoretical uncertainties

Systematic/Model uncertainties

Statistical/Parameters uncertainties

Estimating Nuclear Uncertainties

I-process in early AGB phase



Estimating Nuclear Uncertainties

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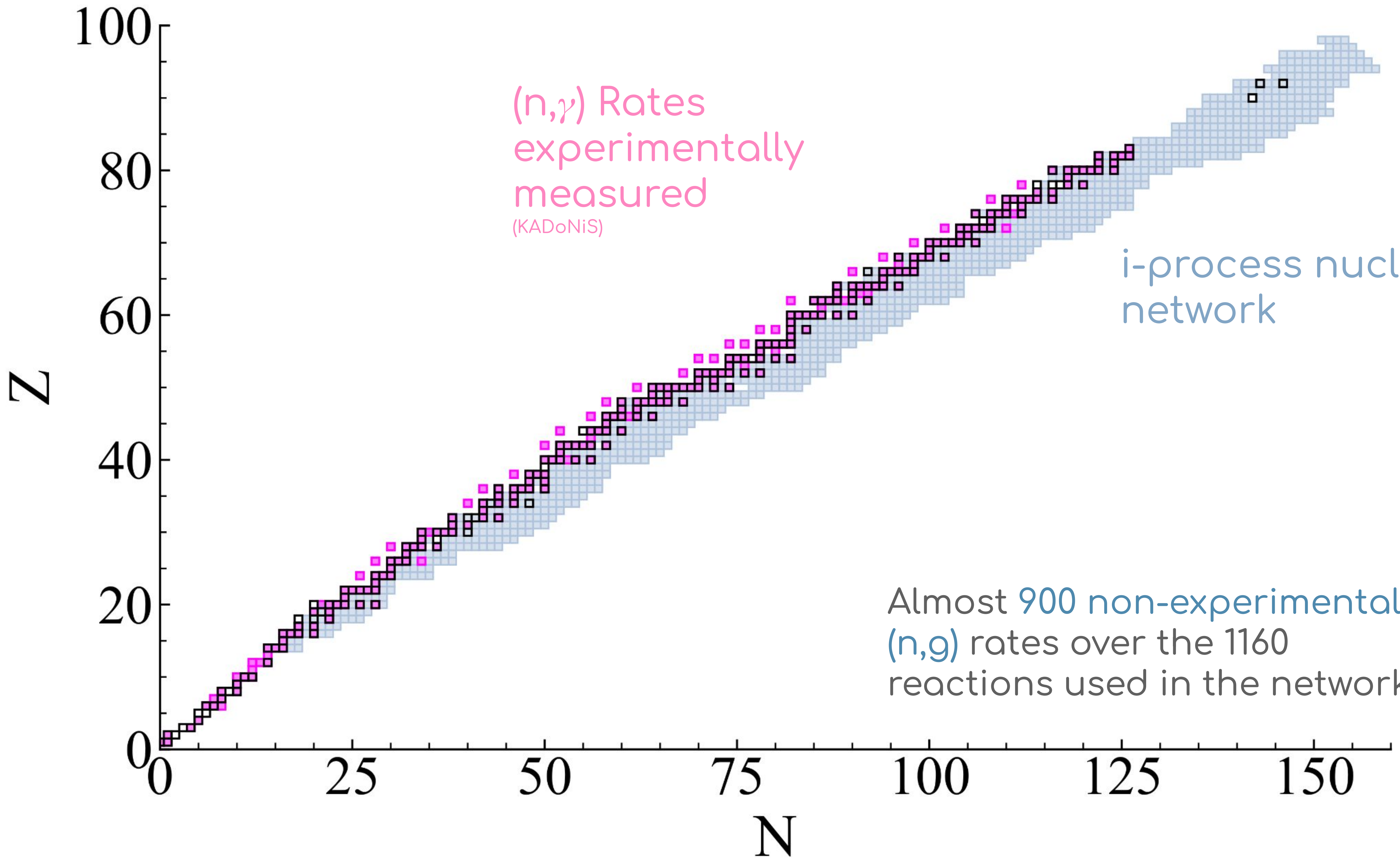
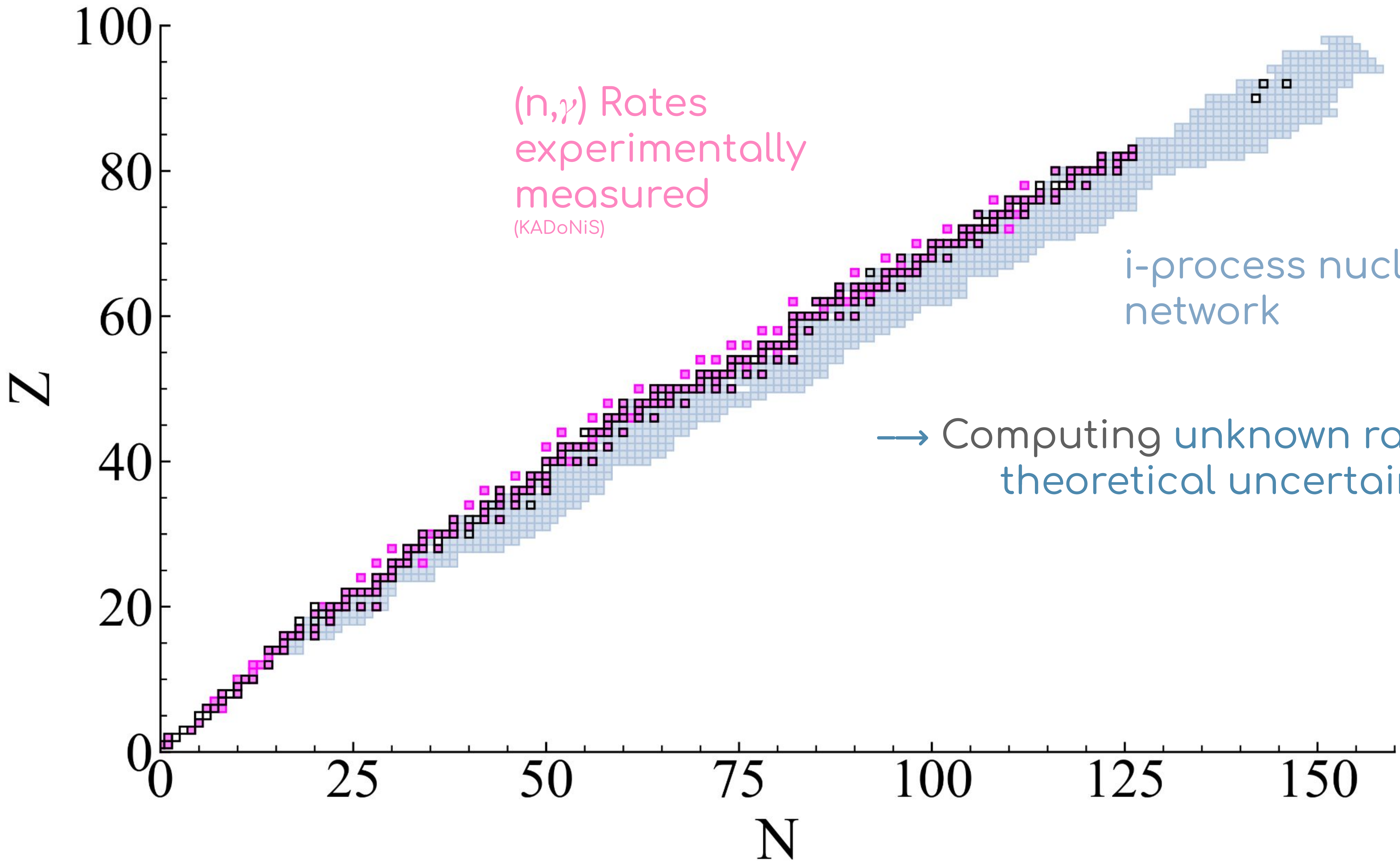


Almost 900 non-experimental (n,g) rates over the 1160 reactions used in the network

Estimating Nuclear Uncertainties

I-process in early AGB phase



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Estimating Nuclear Uncertainties

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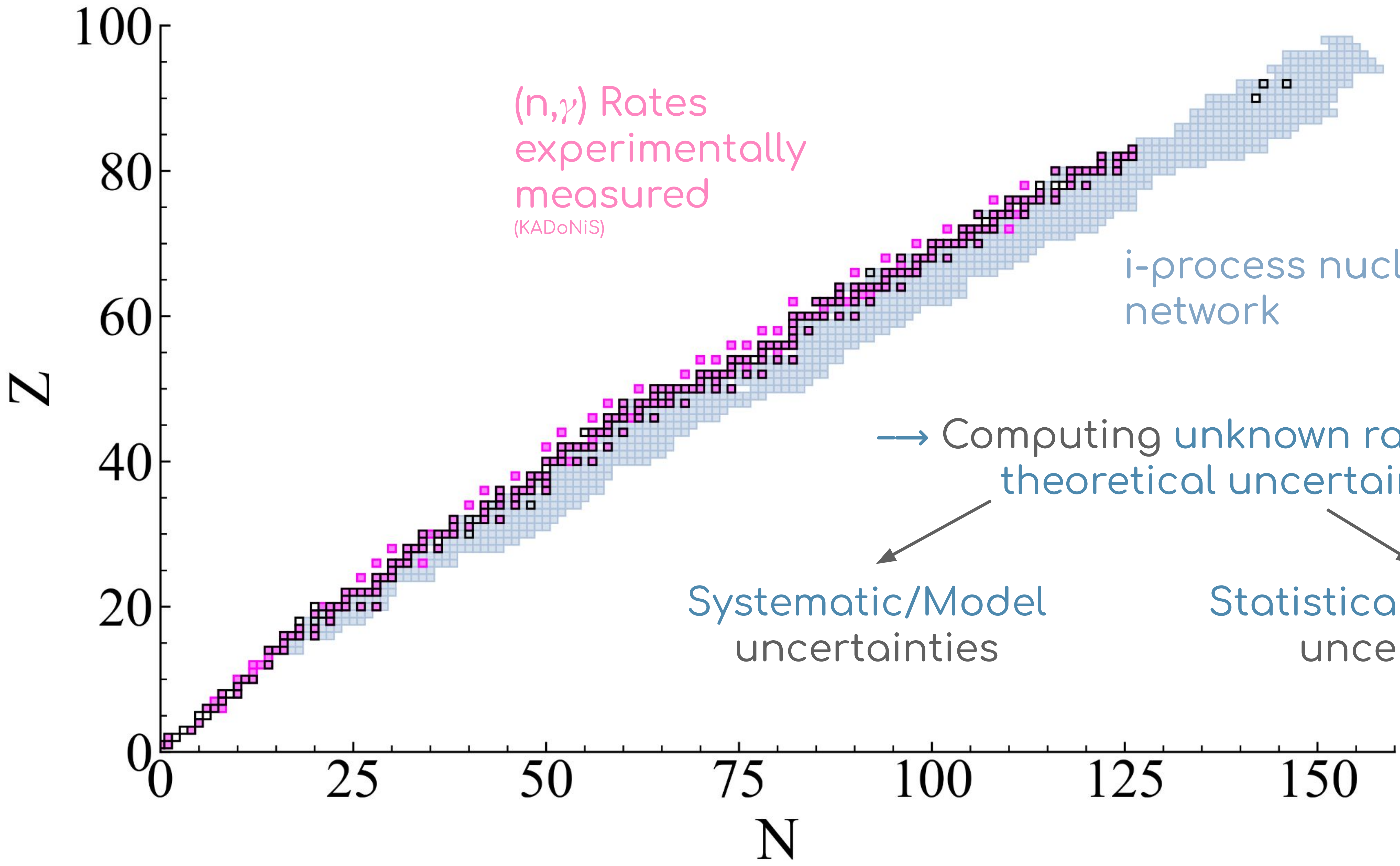


→ Computing unknown rates lead to theoretical uncertainties

Systematic/Model uncertainties

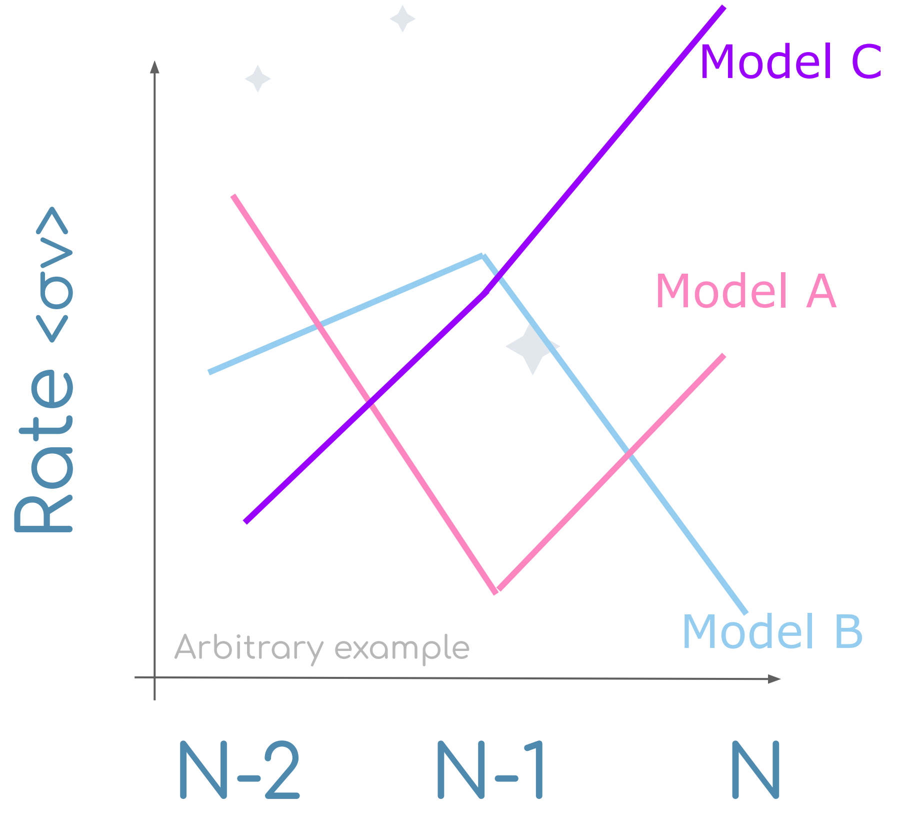
Statistical/Parameters uncertainties

Model Uncertainties vs Parameters Uncertainties

Overestimating uncertainties

Common misuse of model uncertainties:

Z,N-2	Z,N-1	Z,N
$<\sigma v>_{\text{Model A}}$	$<\sigma v>_{\text{Model B}}$	$<\sigma v>_{\text{Model C}}$



Trying to maximize the nuclear reaction rates by using values from different nuclear models leads to physical incompatibilities inside a network

→ Model uncertainties are <u>correlated</u>

Model Uncertainties vs Parameters Uncertainties

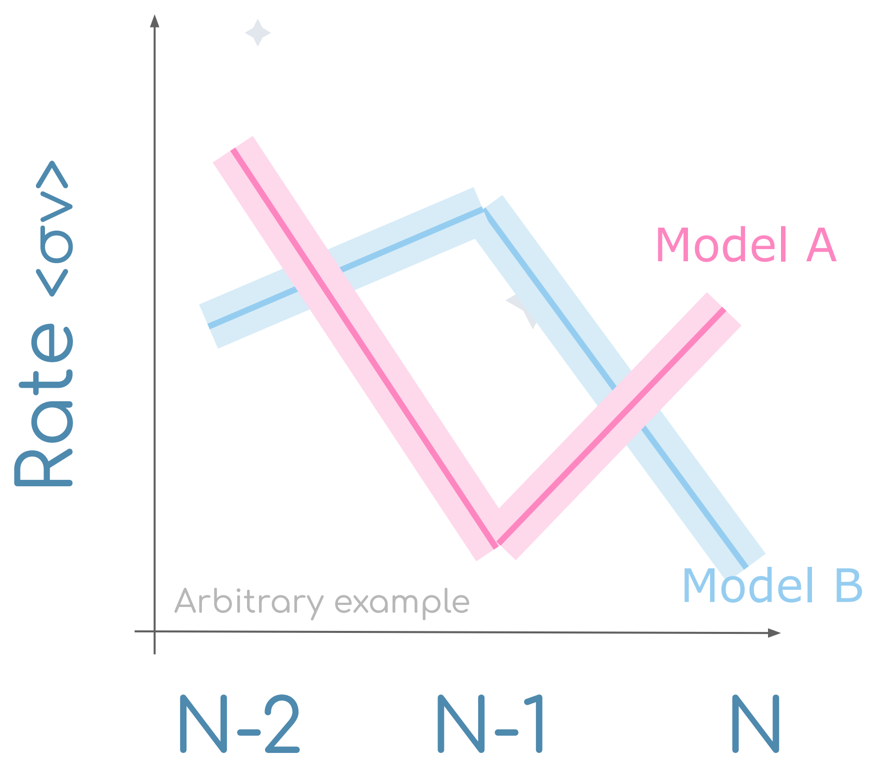
Overestimating uncertainties

Correct use of parameter uncertainties:

Z,N-2	Z,N-1	Z,N
max($<\sigma v>_{\text{Model A}}$)	min($<\sigma v>_{\text{Model A}}$)	mean($<\sigma v>_{\text{Model A}}$)

or

Z,N-2	Z,N-1	Z,N
max($<\sigma v>_{\text{Model B}}$)	random($<\sigma v>_{\text{Model B}}$)	random($<\sigma v>_{\text{Model B}}$)



These are possible combinations to use with the parameter uncertainties. Any value of these uncertainties can be combined for a same nuclear model.

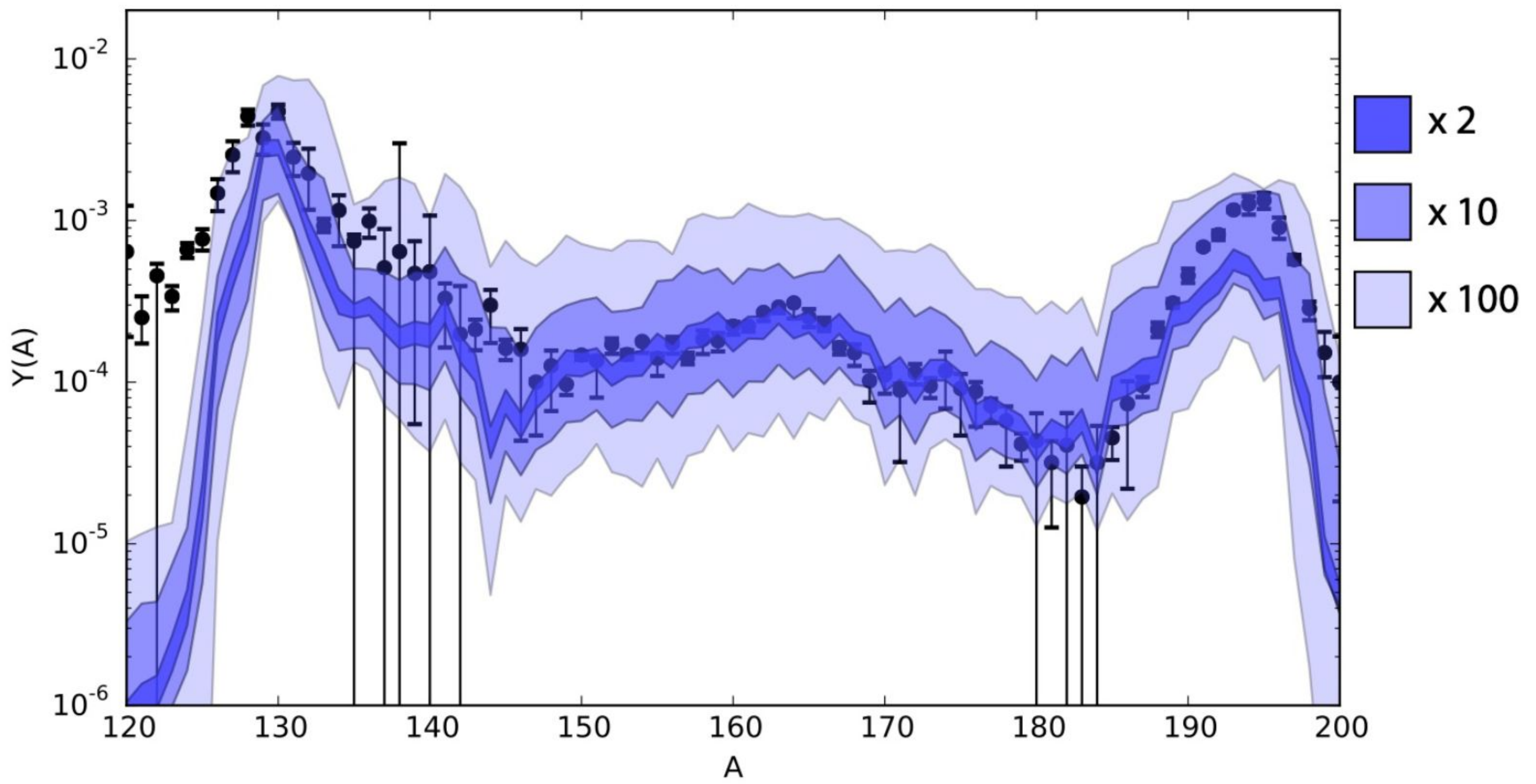
→ Parameter uncertainties are <u>non-correlated</u>

Determining coherently parameter uncertainties

Choosing parameter uncertainties arbitrarily

How to obtain parameter uncertainties ?

Uncorrelated MC approach (Mumpower+2016, Surman+2016, Nikas+2020, Jiang+21)



- Neglect correlations between uncertainties
- Overestimates impact

Choosing arbitrarily an uncertainty for each or all nuclei

The Backward-Forward Monte Carlo approach

Goriely & Capote 2014, Martinet+2025b

Backward Step

1) Generate random parameter sets

Forward Step

The Backward-Forward Monte Carlo approach

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2) Compare to experimental data

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3) Keep only sets that reproduce observables
(e.g., $\text{deviation}_{th} \leq \text{uncert.}_{exp}$)

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Propagation

Forward Step

4) Use constrained parameter sets to calculate the unknown nuclear properties
(reaction rate, masses, …)

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Uncertainty range grounded in real data

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Uncertainty range grounded in real data

One Drawback

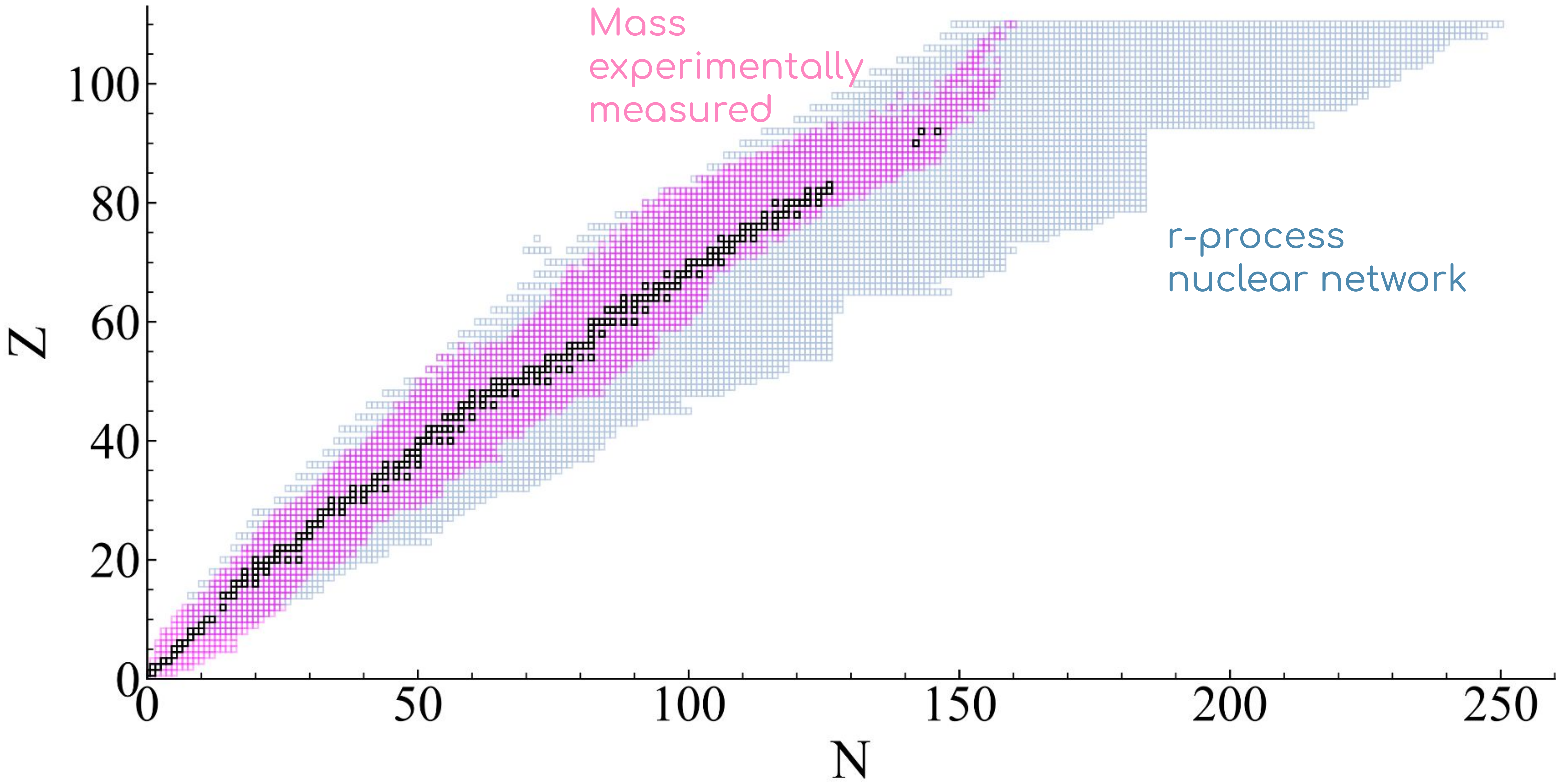
→ Heavy computation

Generating tens of thousands of parameter sets and computing the nuclear properties for 1000-2000 nuclei

(HPC facilities needed)

Determining coherently parameter uncertainties

Parameters uncertainties obtained from the BFMC method



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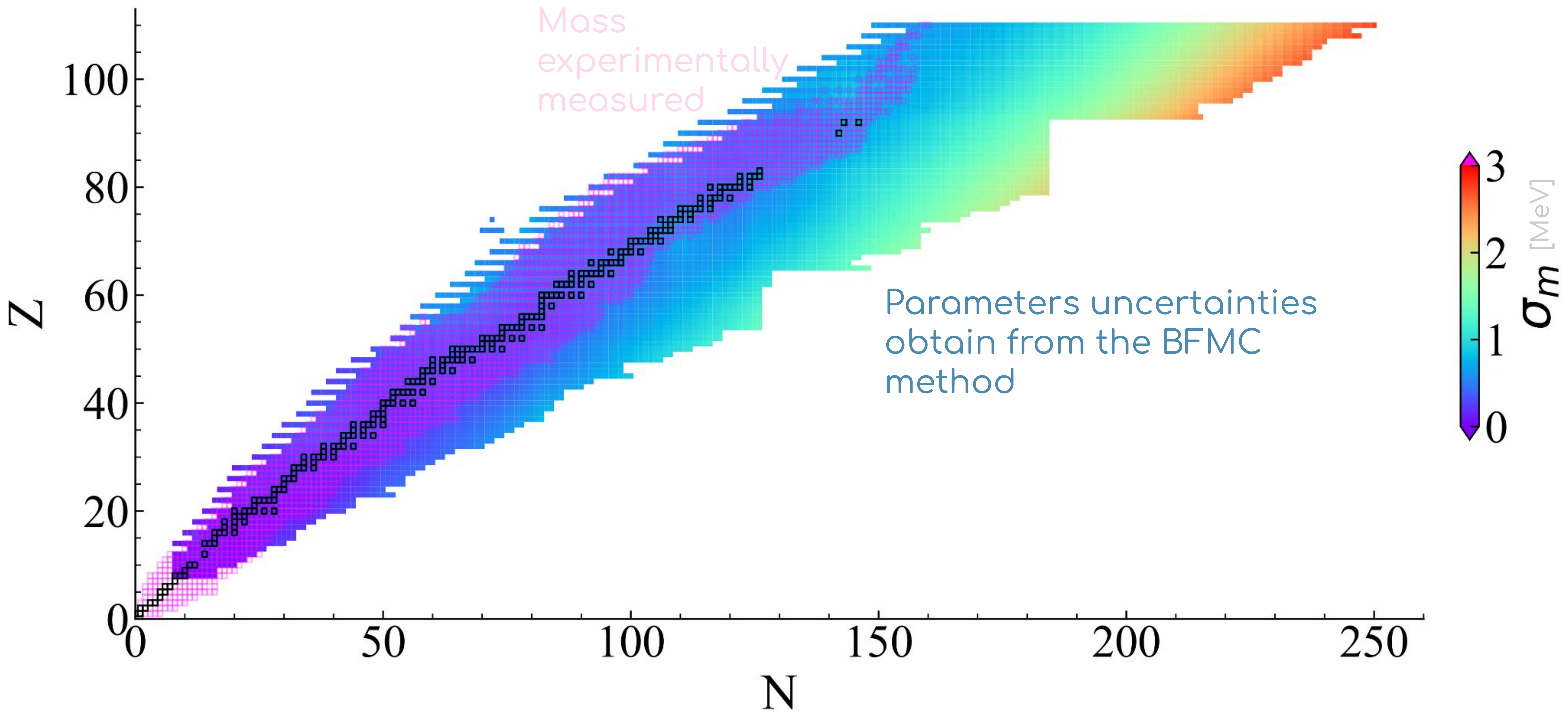
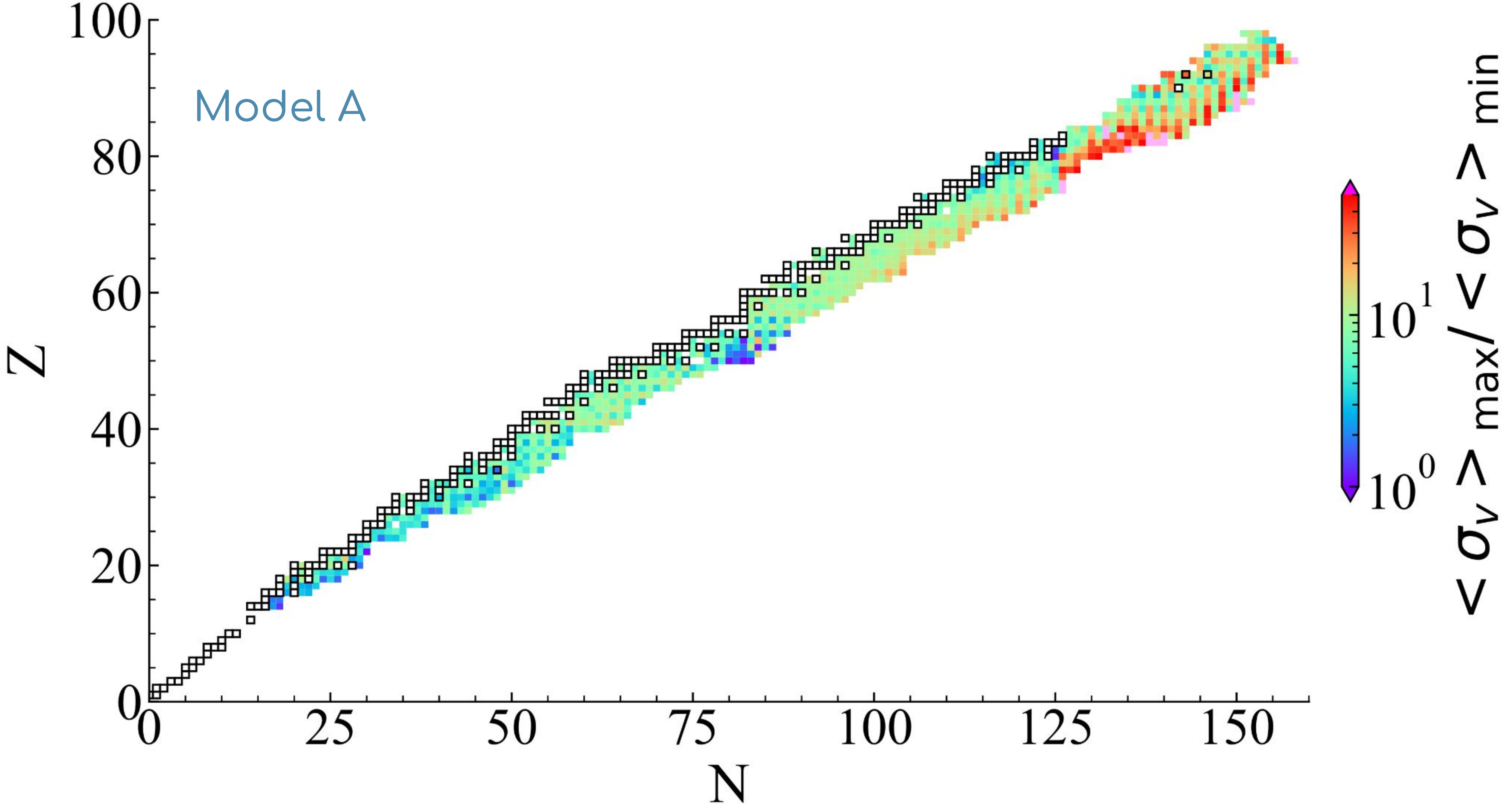


Determining coherently parameter uncertainties

Parameters uncertainties obtained from the BFMC method

(n,g) rates uncertainties for the i-process



Impact of Nuclear Uncertainties on the i-process in AGB Stars

Effect of statistical uncertainties on the surface enrichment of early AGB stars (Martinet+2024a)

Stellar Evolution code

STAREVOL code (Siess et al. 2006)

→ i-process nucleosynthesis

1 Msol at [Fe/H]=-2.5

Proton ingestion event in the early AGB phase

Propagation of the uncertainties

Maximum and minimum (n,g) theoretical rates (862 nuclei)
(with 4-parameter variation s.t. $f_{rms} \leq 2.0$)

→ Random combination of maximum and minimum rates for a large number of stellar models (n>50)

Heavy computations due to the large network (1160 nuclei - 2200 reactions)

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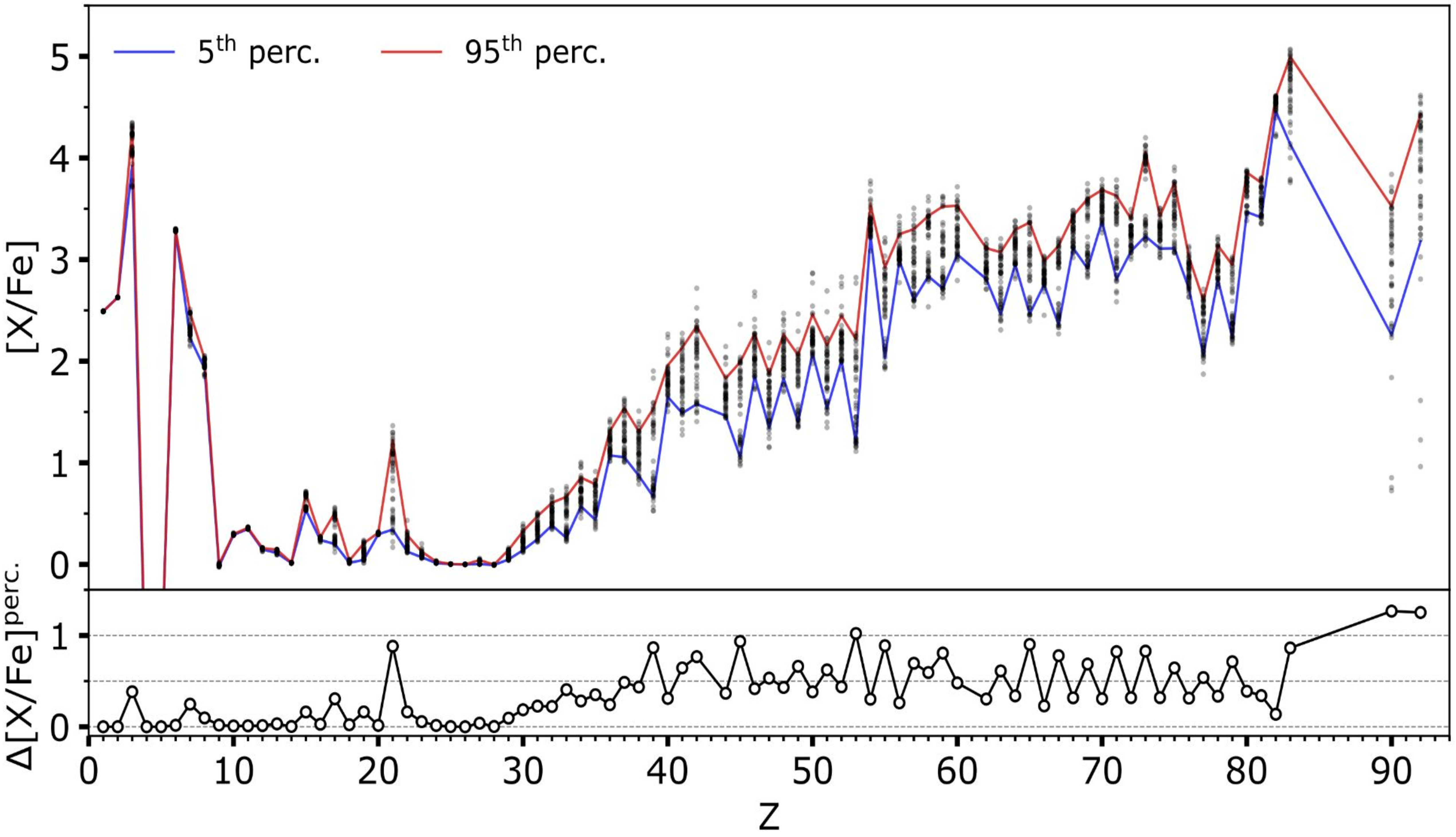
Non-correlated parameter uncertainties



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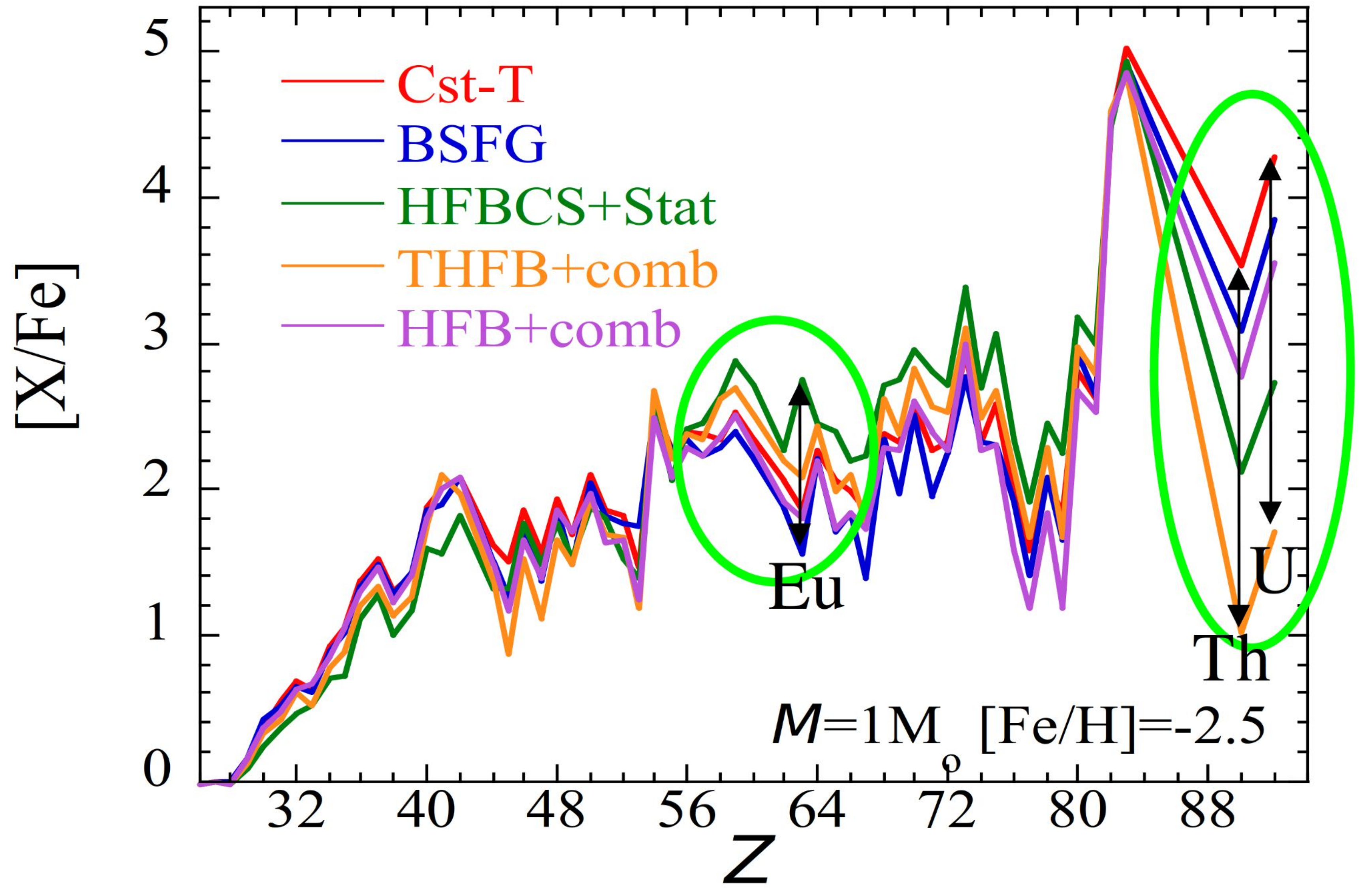
Correlated model uncertainties



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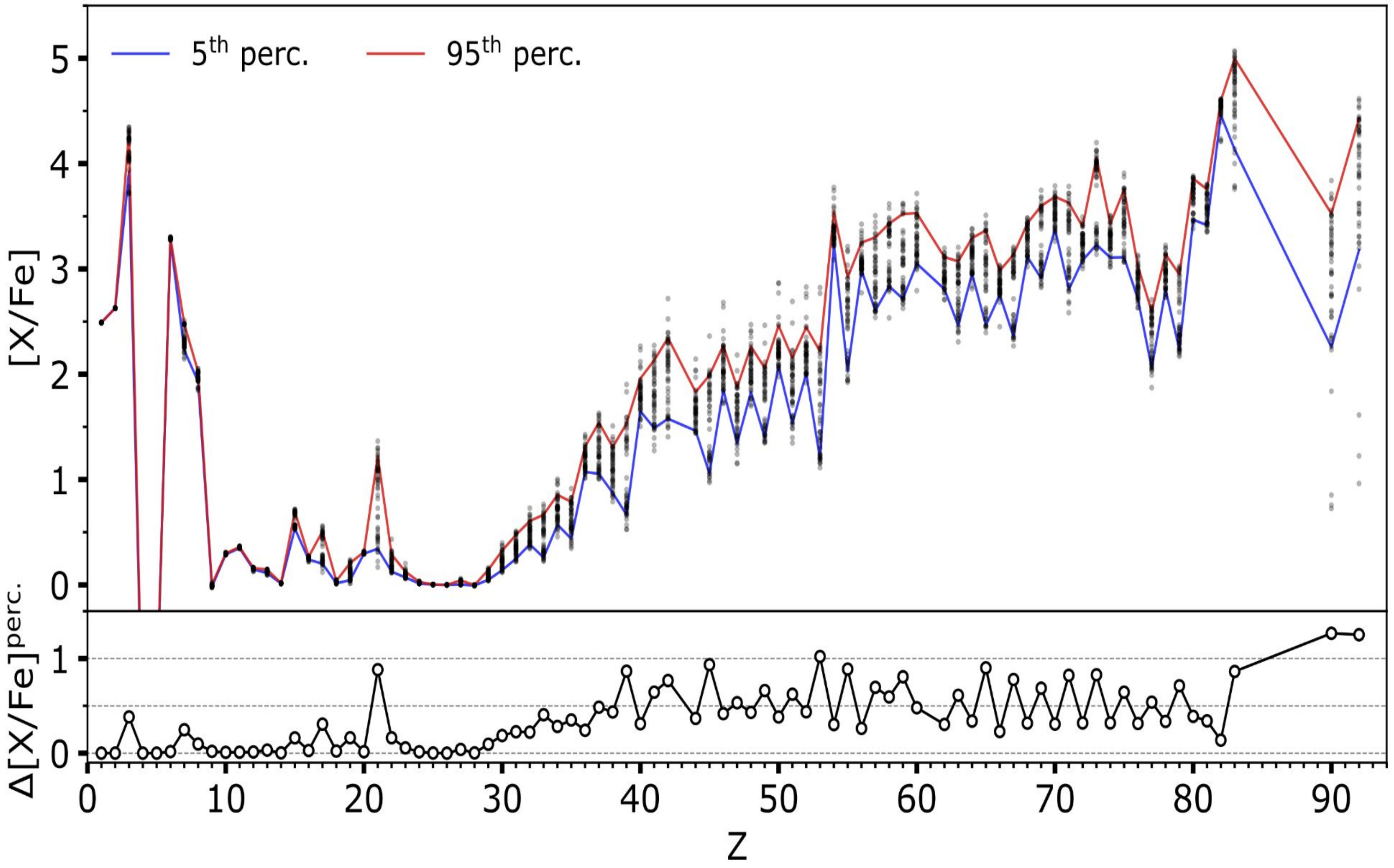
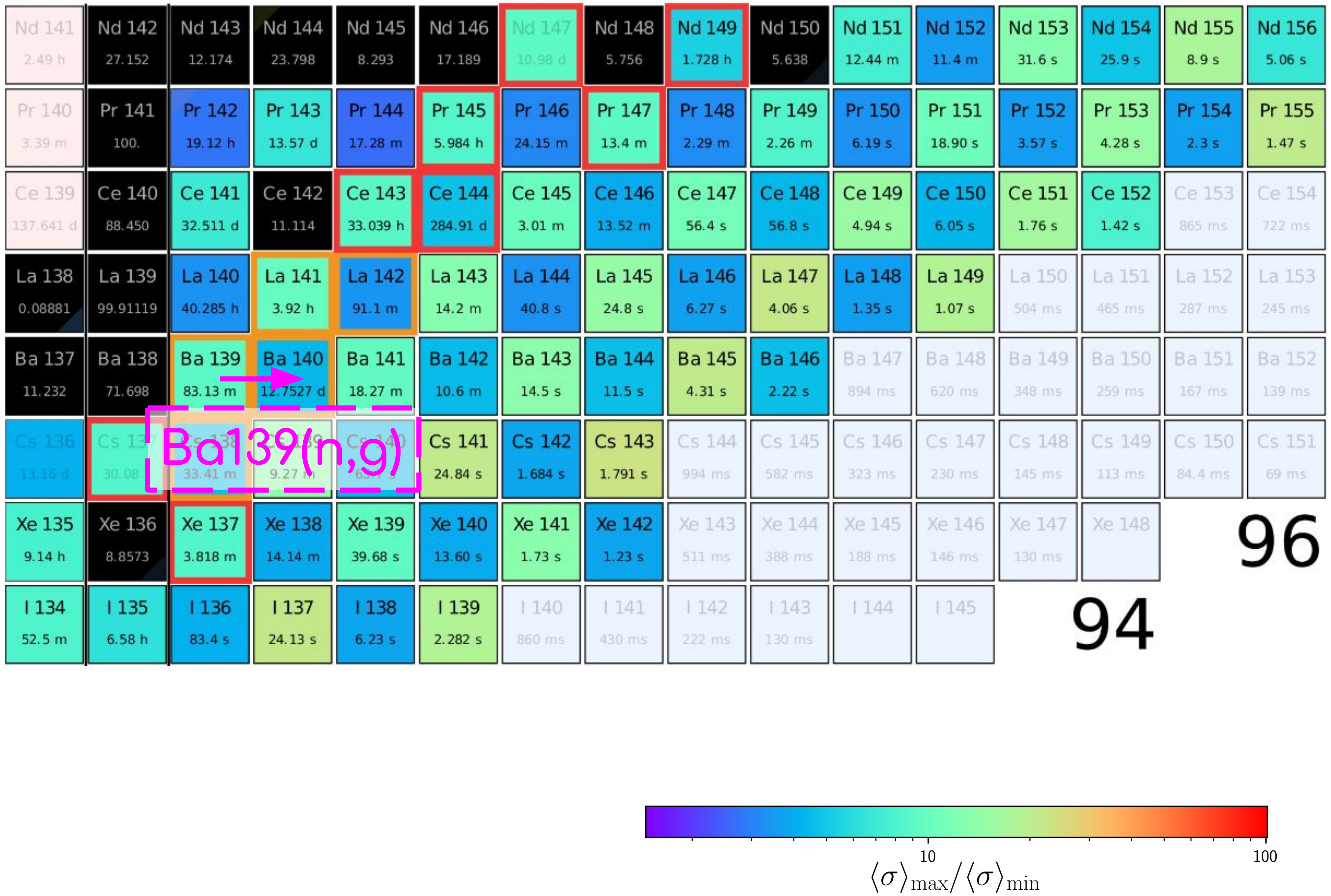


Impact of Nuclear Uncertainties on the i-process in AGB Stars

Identify important (n,g) reactions during the i-process in AGB stars (Martinet+2024a)

Impact of the Ba139(n,g) reaction rate to the La139 abundance



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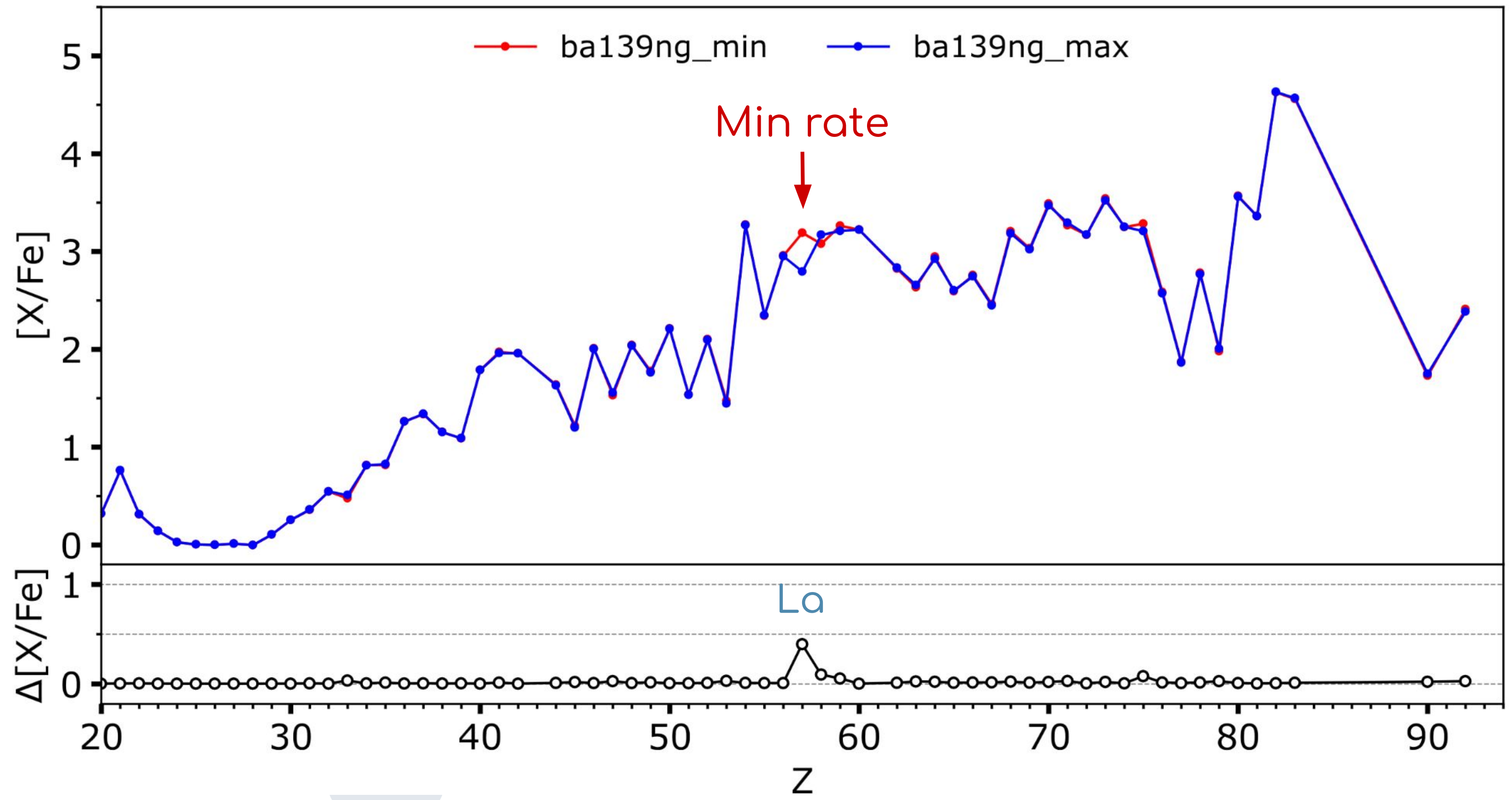

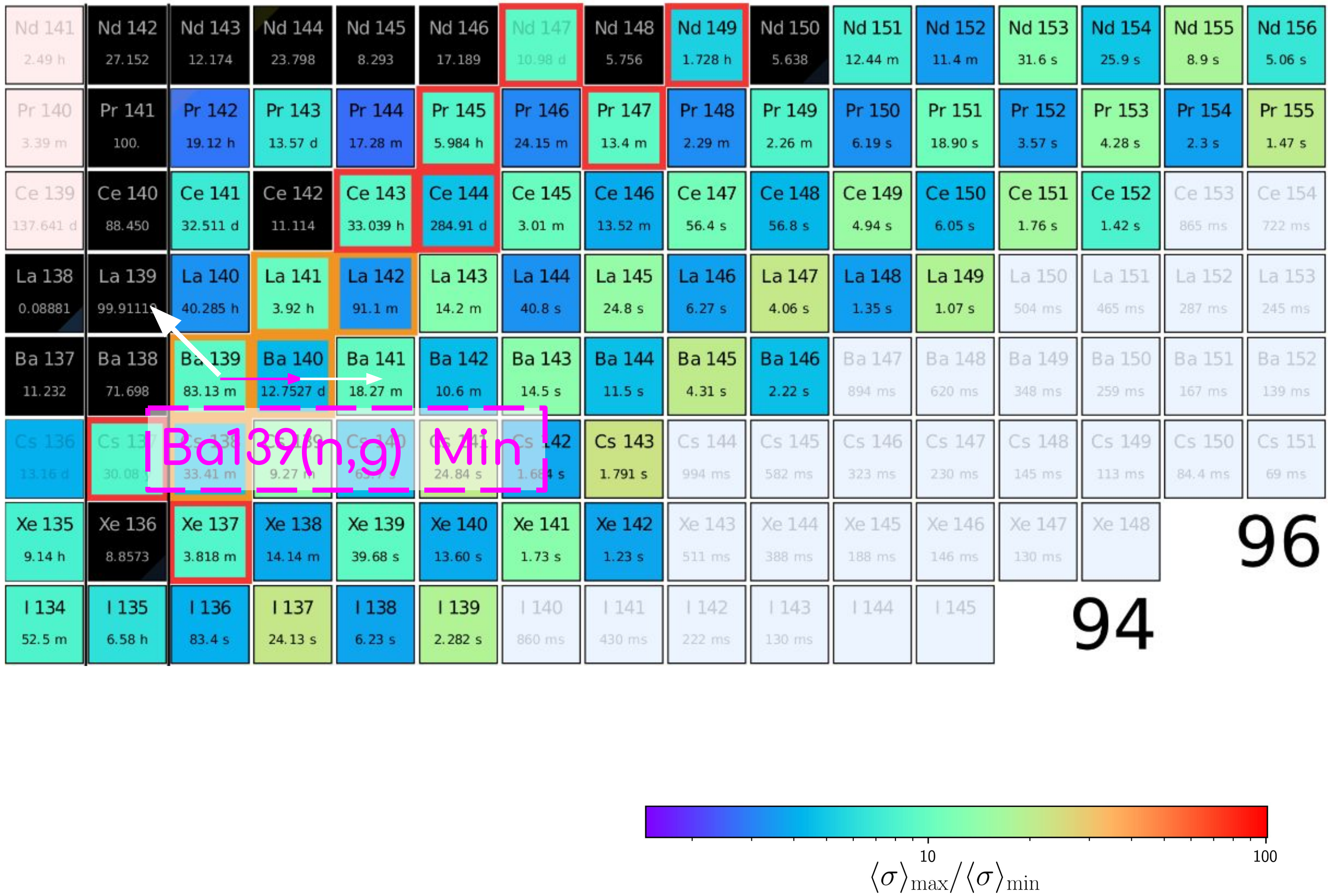

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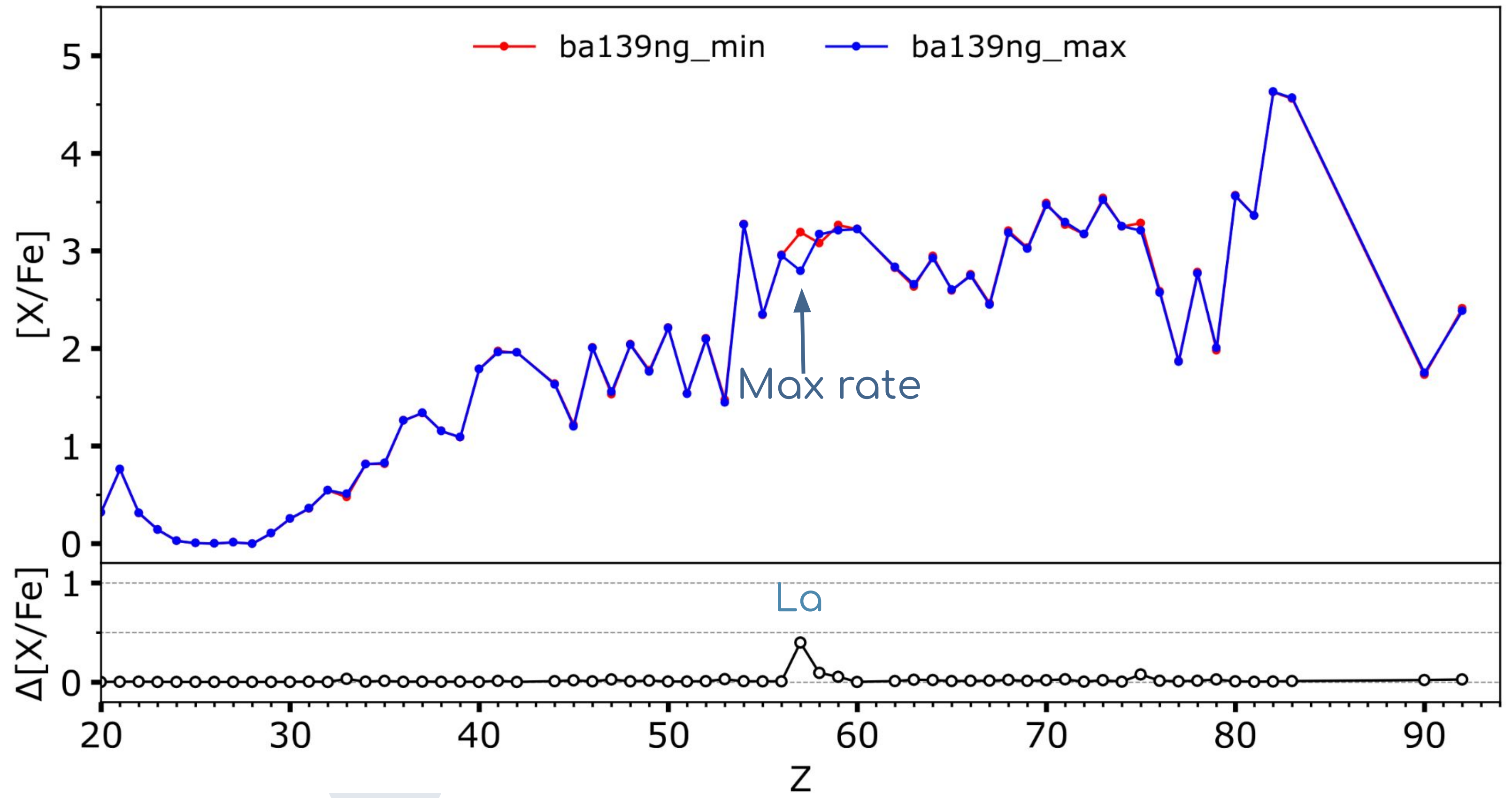

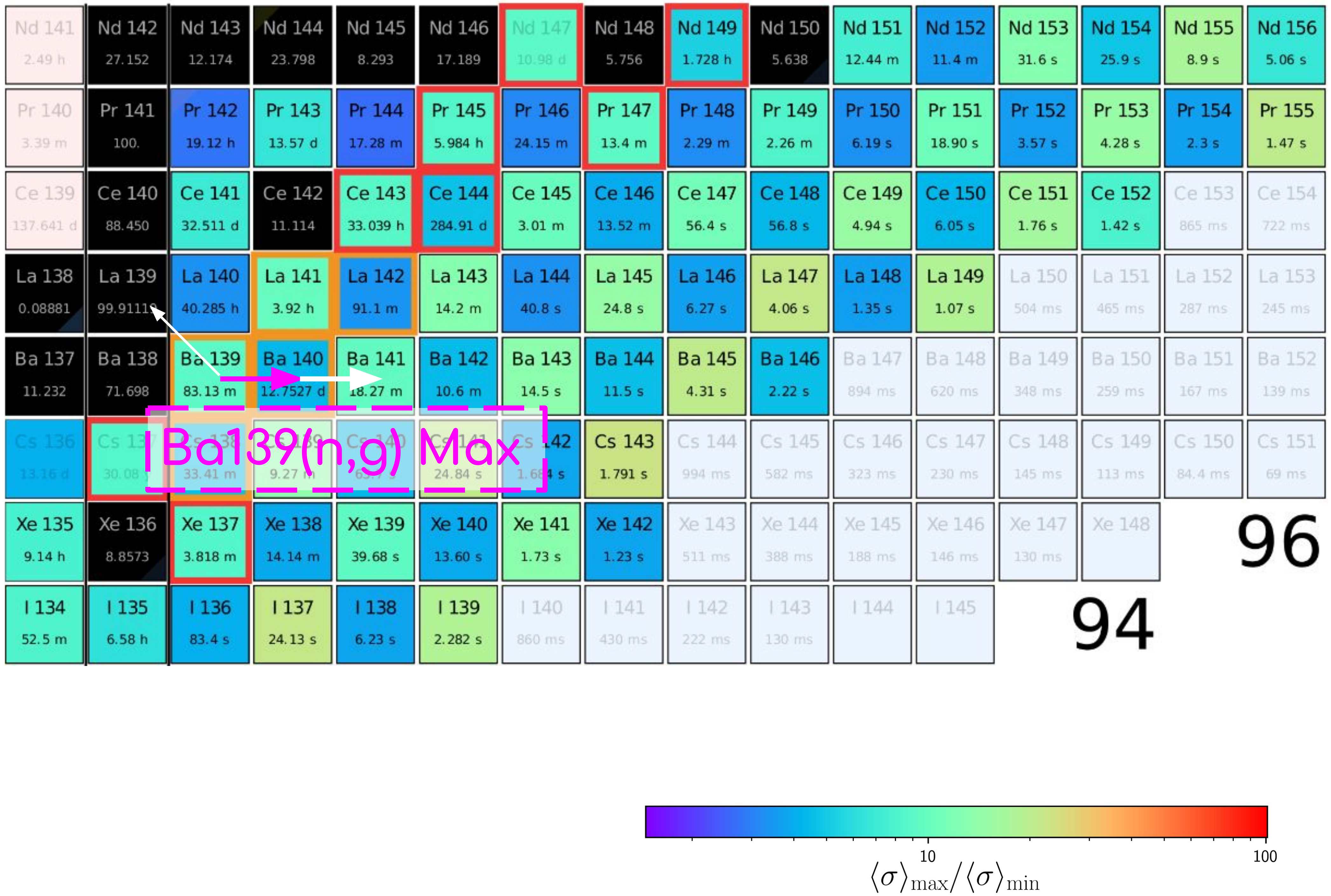

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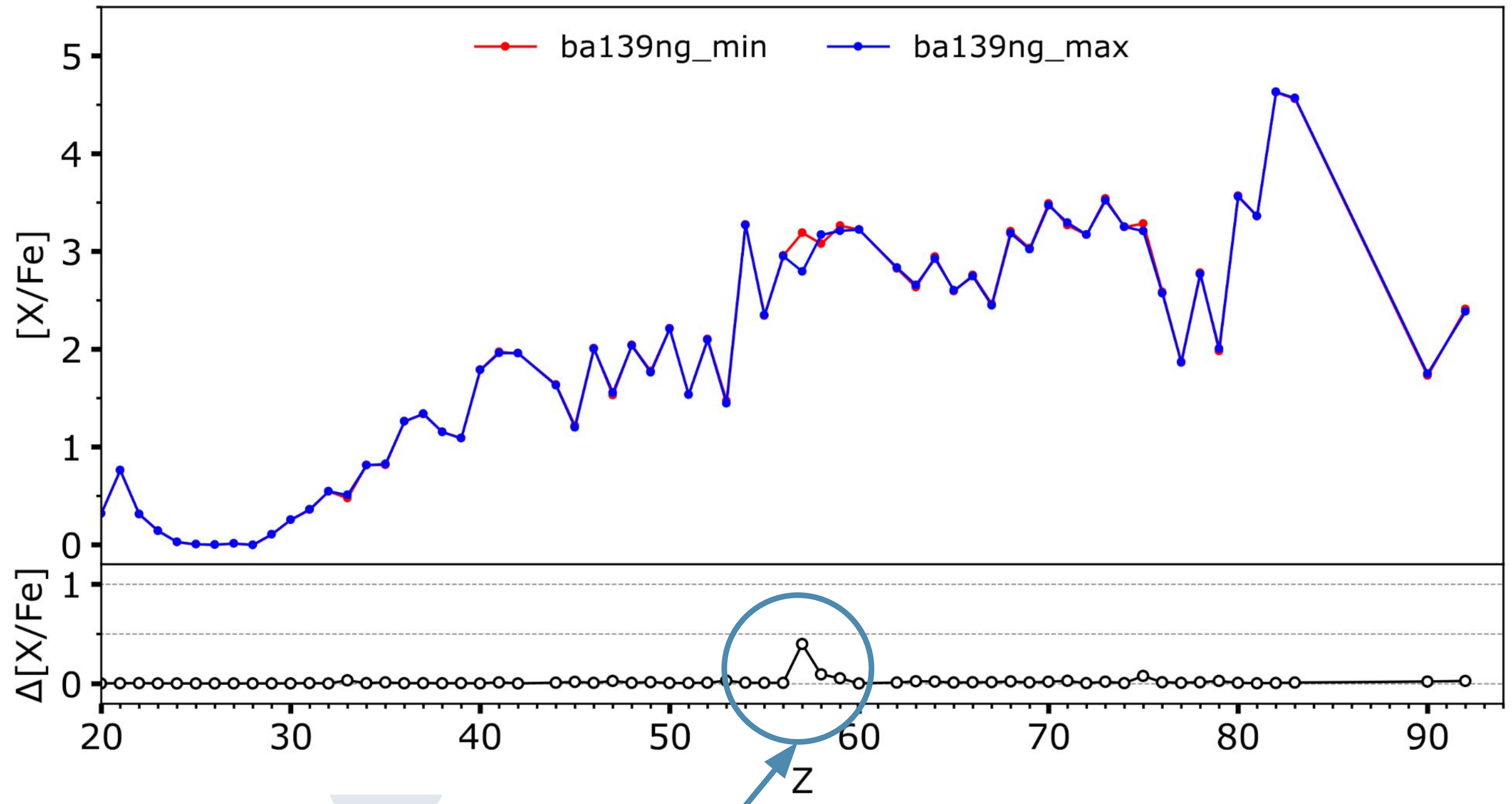

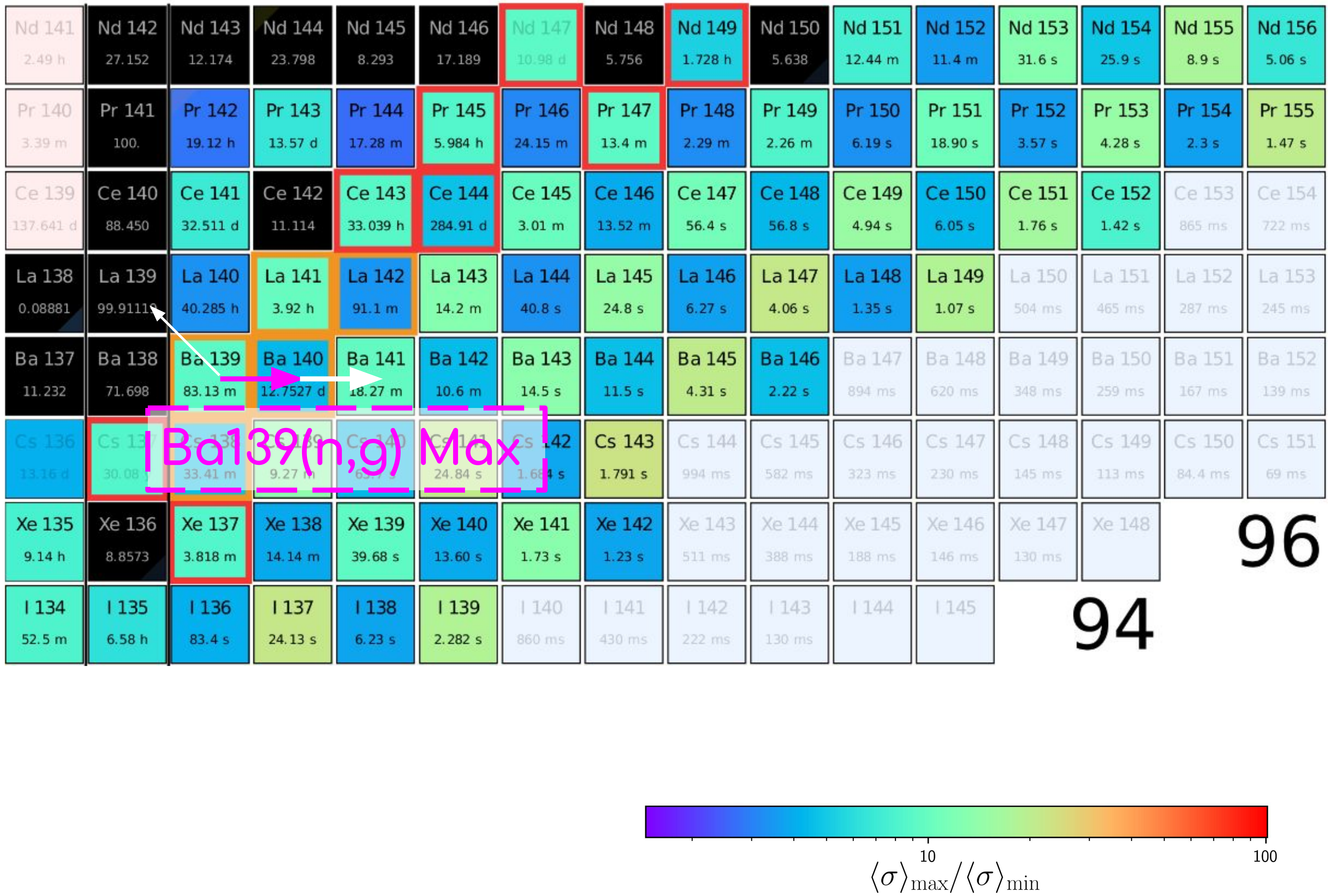

La139 abundance uncertainty: 0.44 dex

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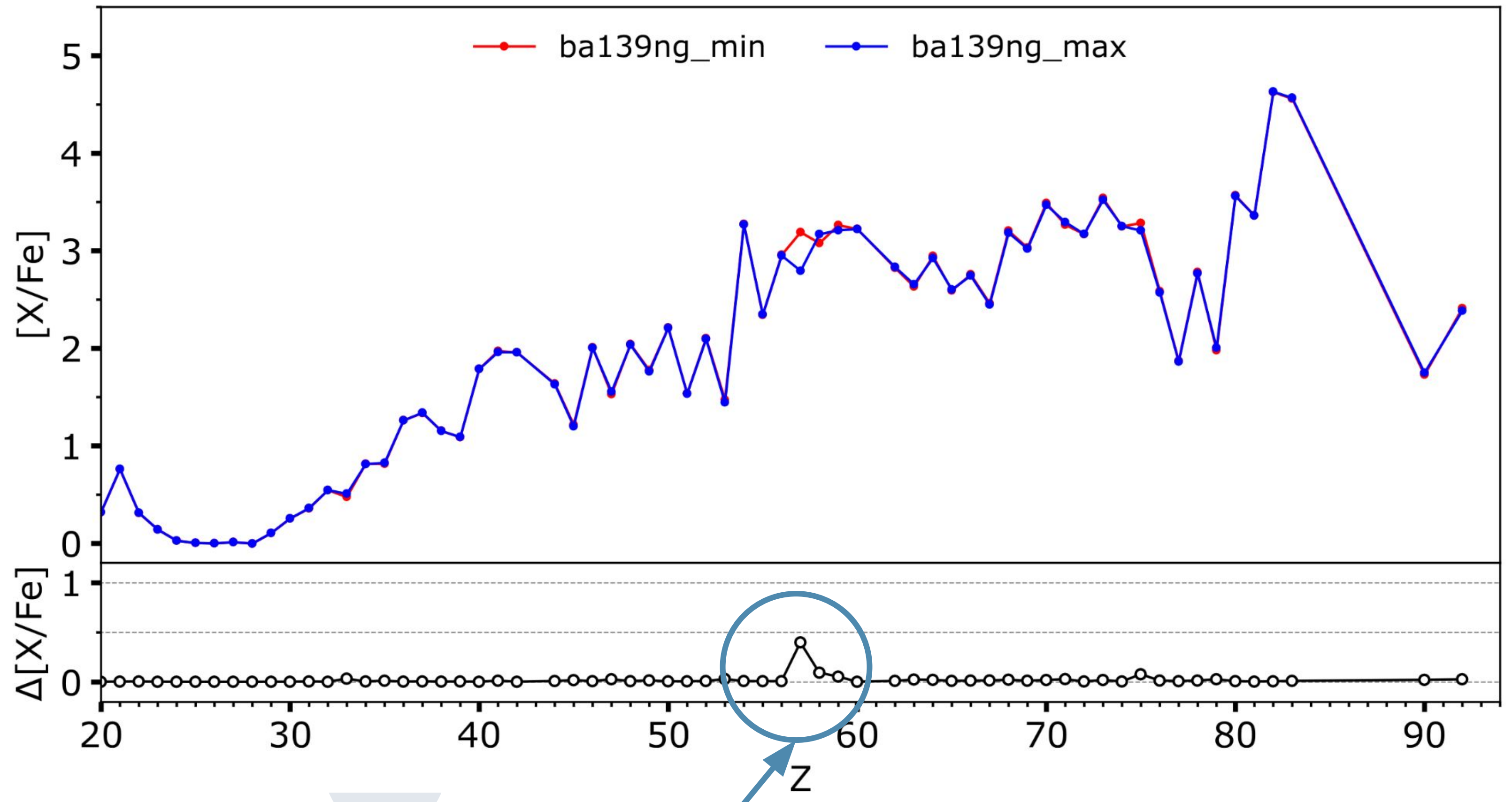

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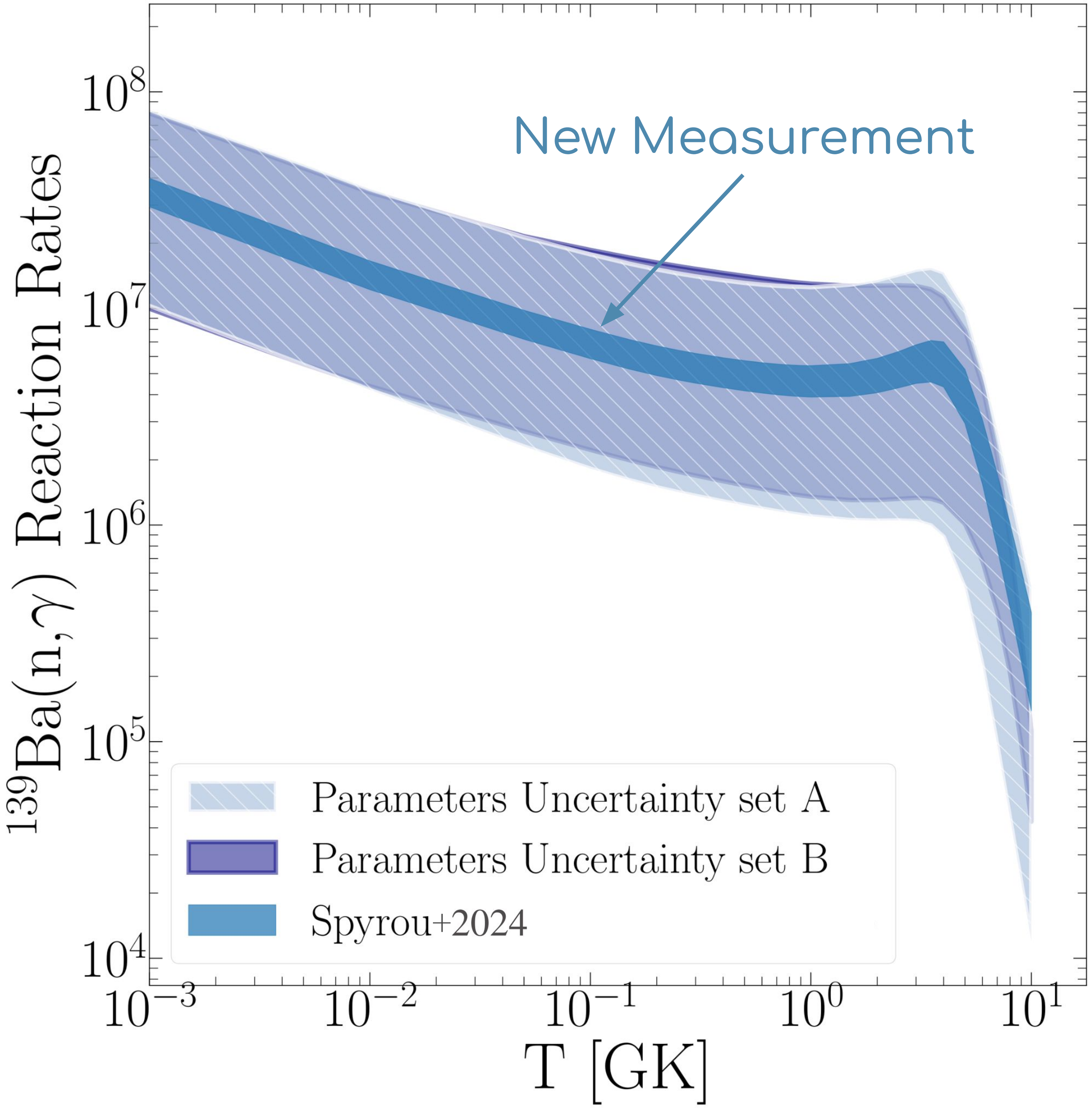

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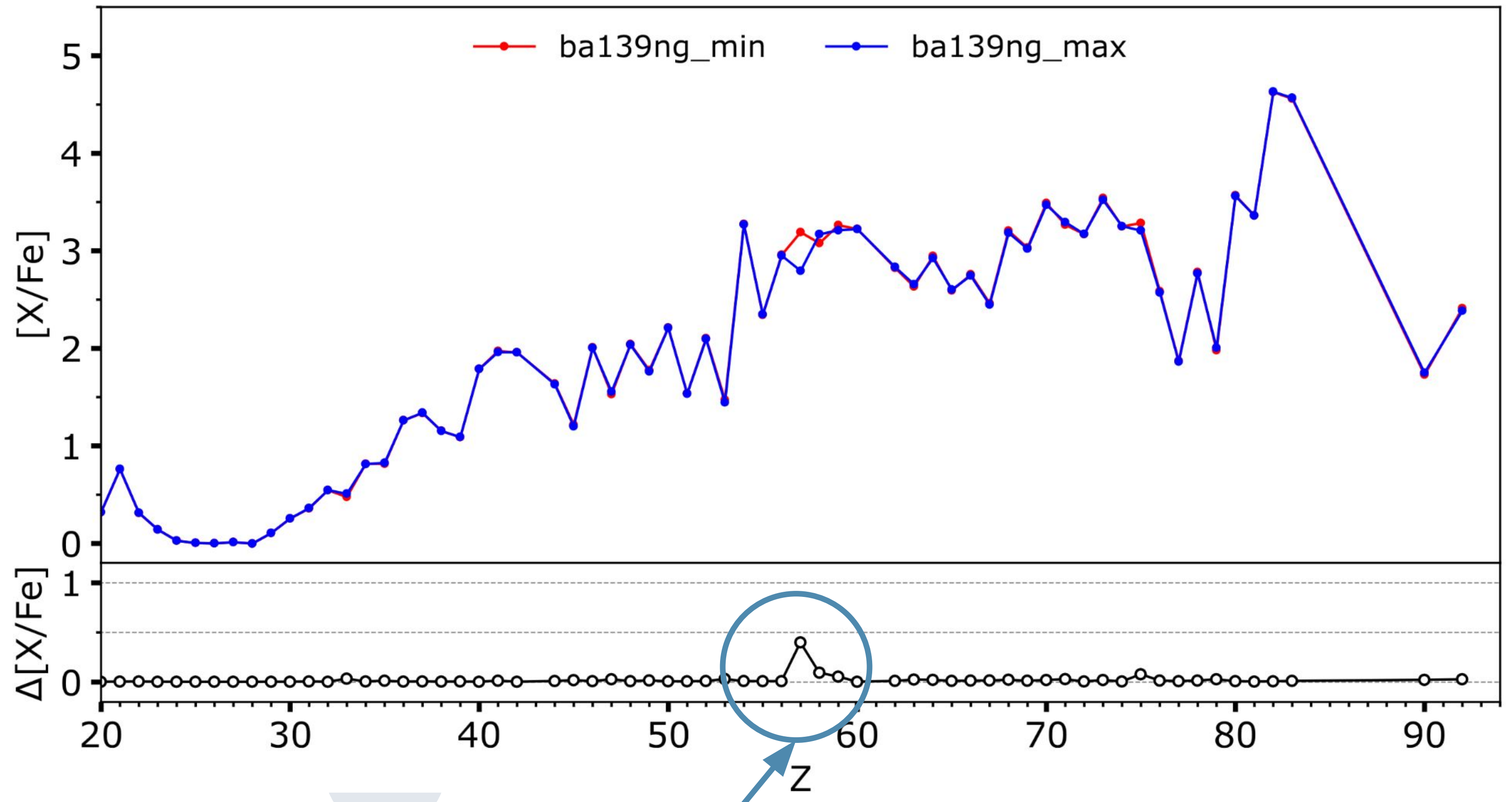
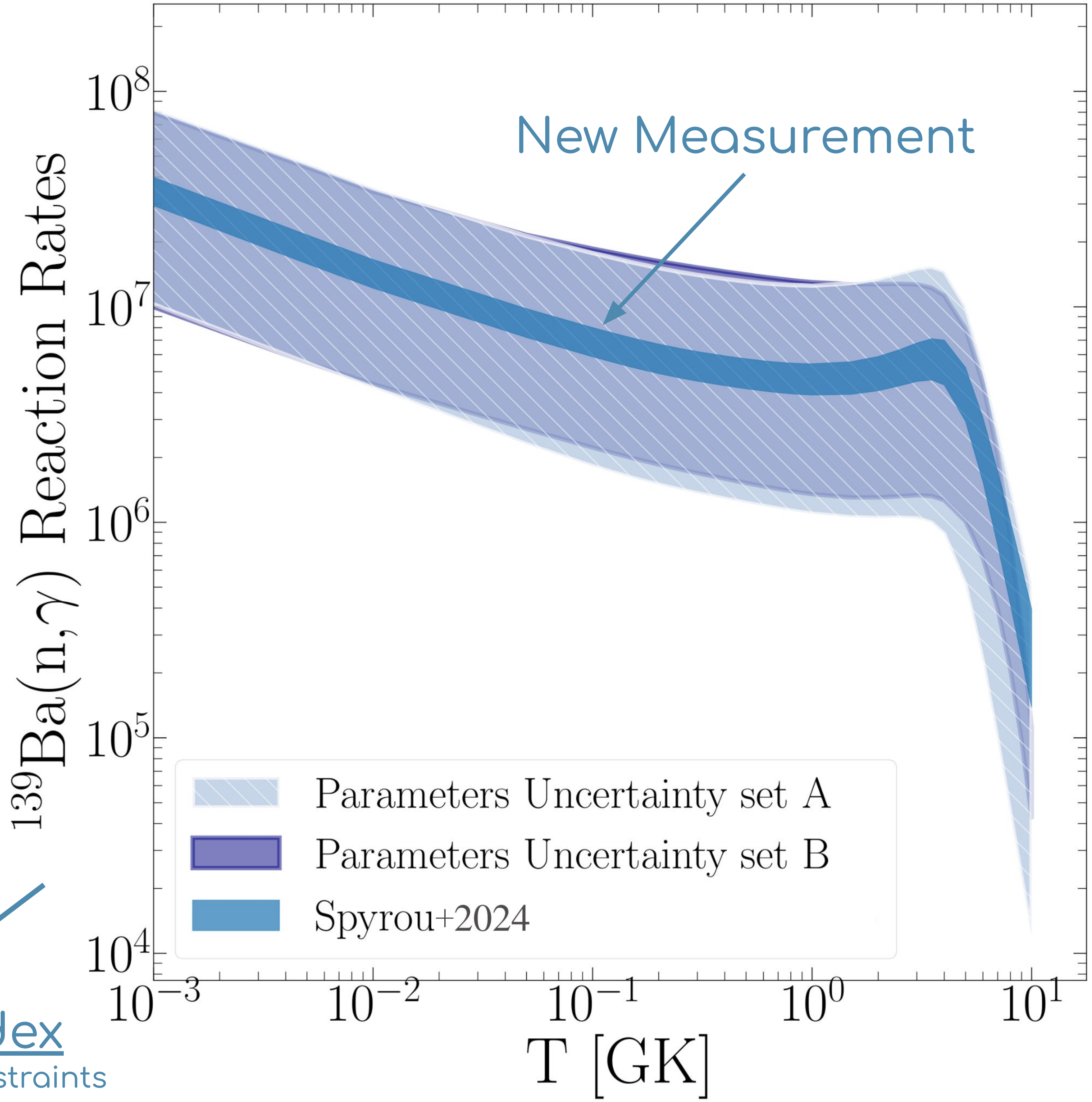


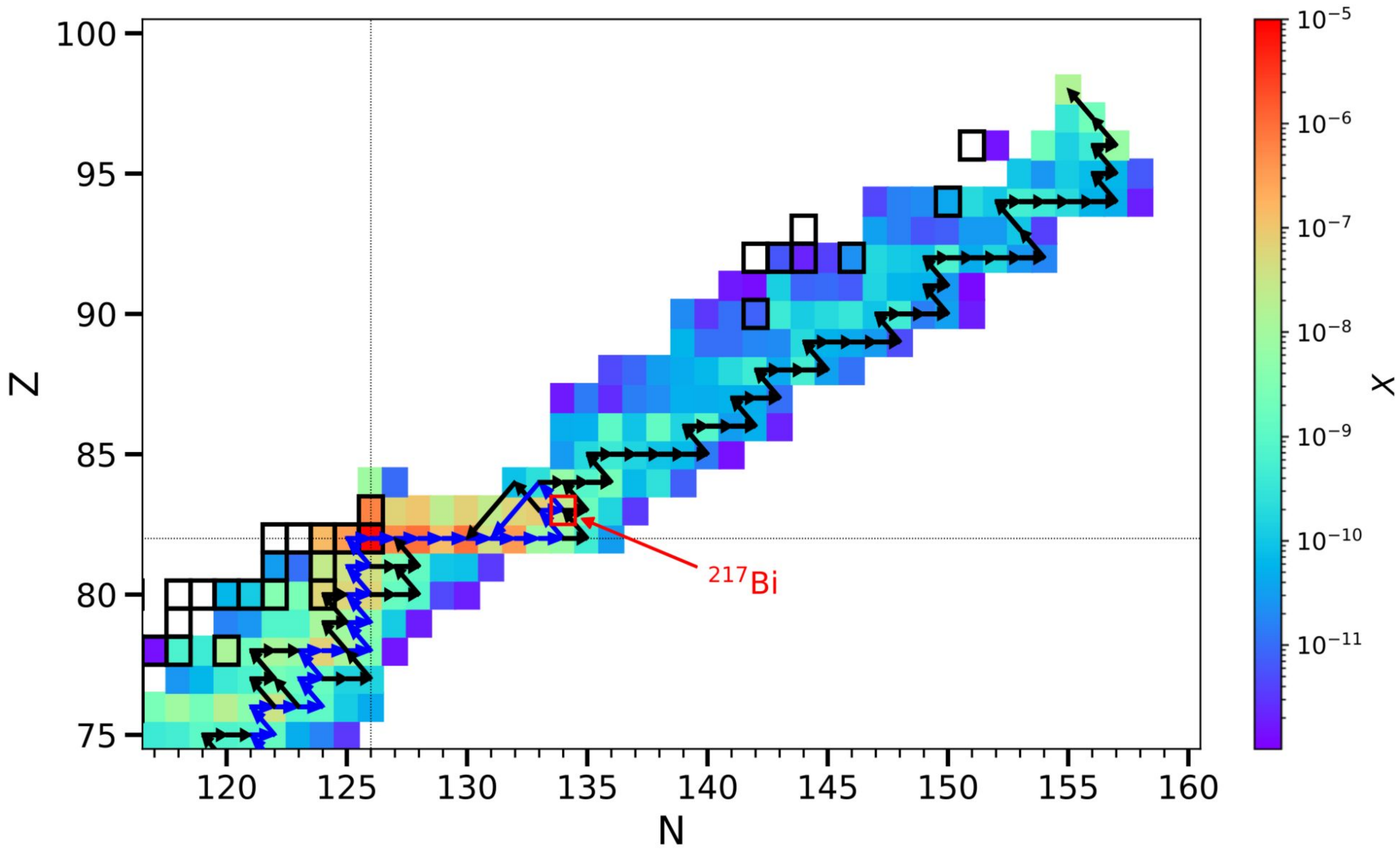


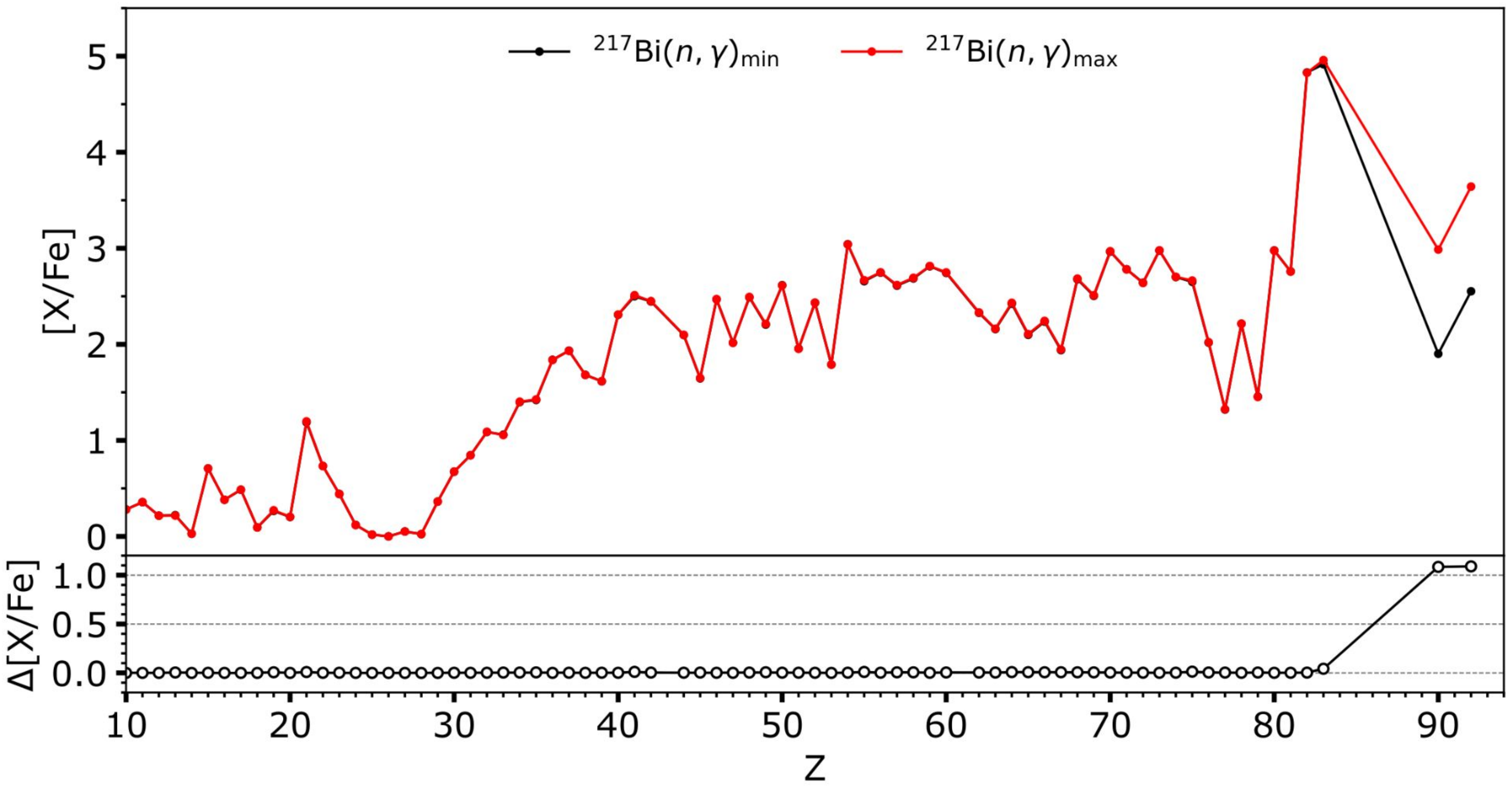
La139 abundance uncertainty: 0.44 dex

Reduced to 0.06 dex
thanks to experimental constraints

Impact of Nuclear Uncertainties on the i-process in AGB Stars

Identify important (n,g) reactions during the i-process in AGB stars (Martinet+2025b)

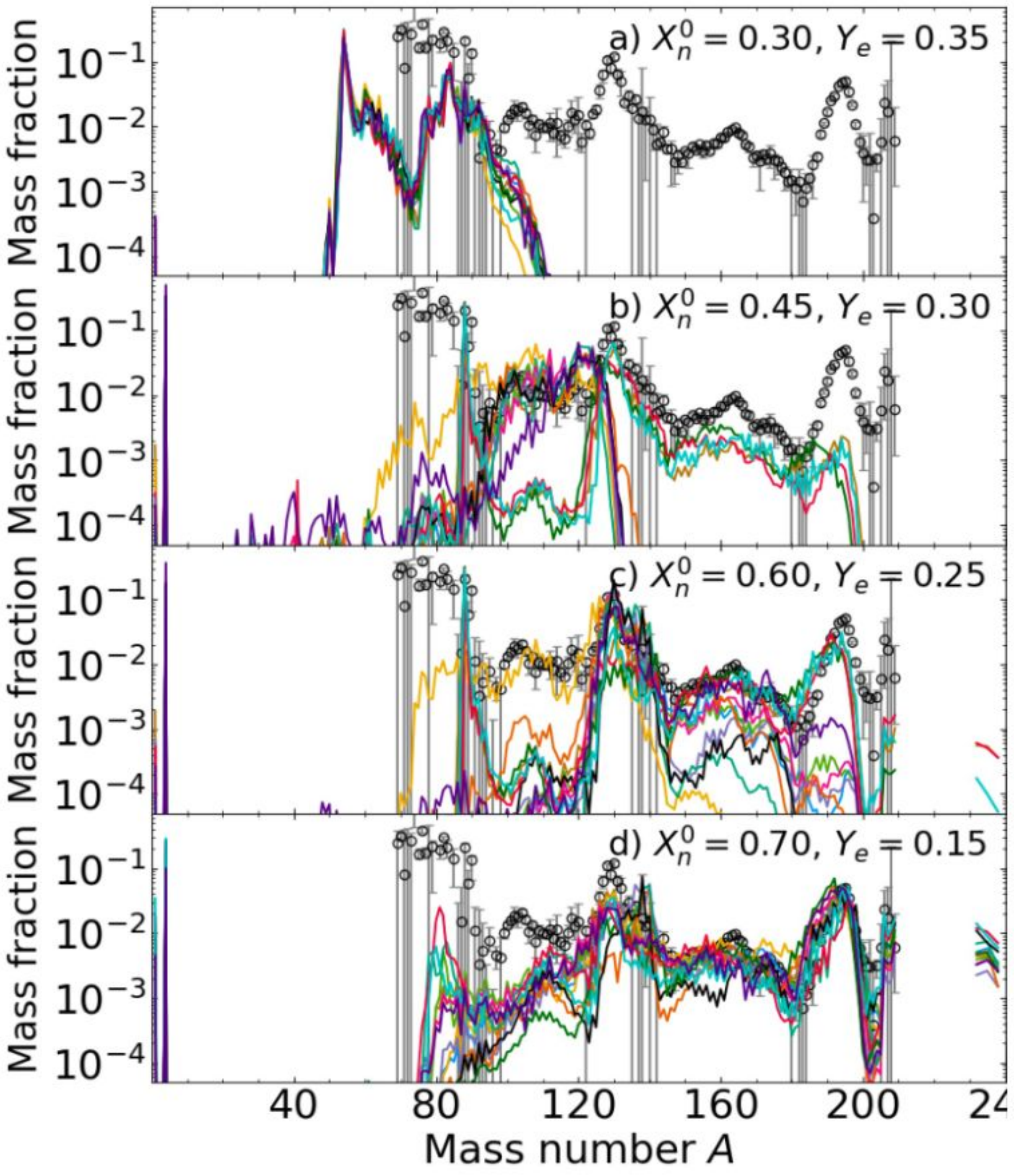




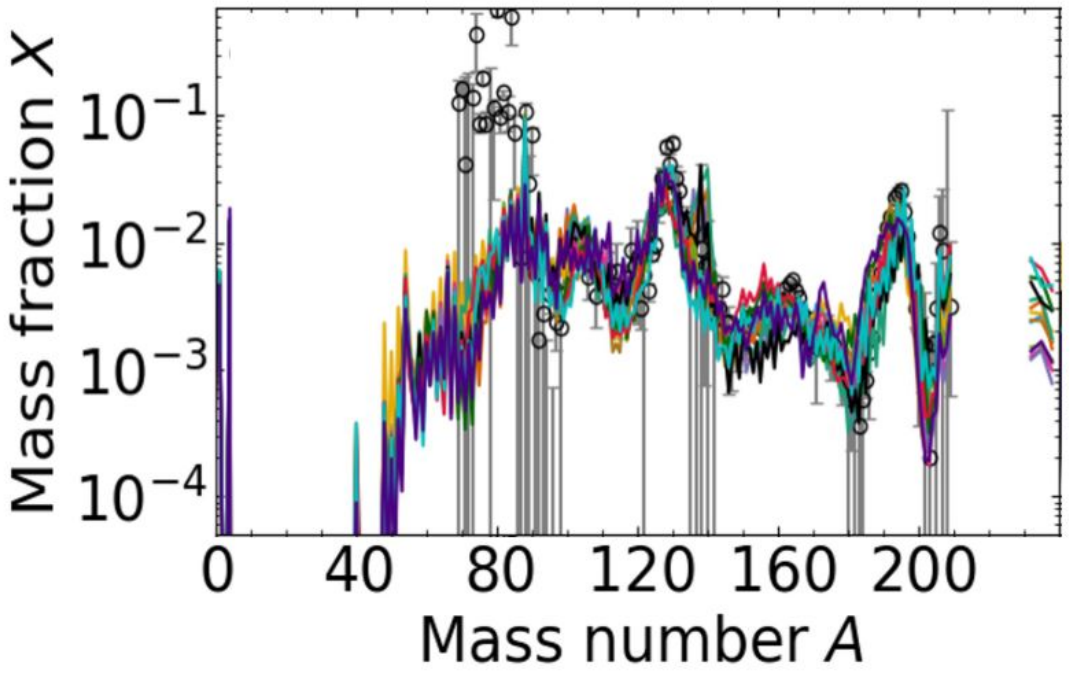
Propagating nuclear uncertainties to r-process simulations

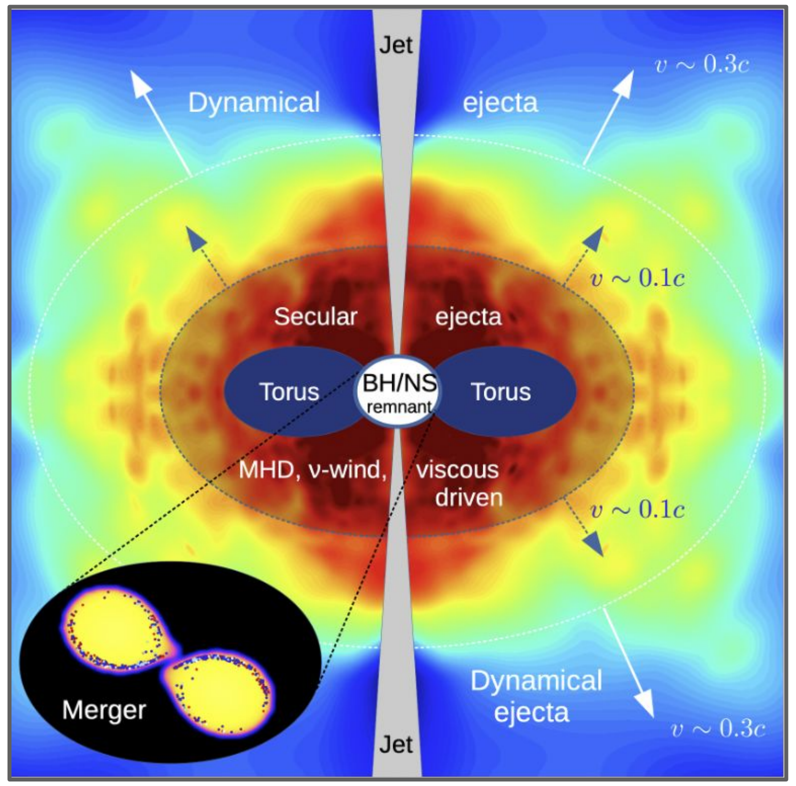
Importance of using multiple trajectories representing the whole NSM event (Martinet & Goriely 2025)

Prompt dynamical ejecta



Multiple trajectories





358 trajectories representing the total ~2500 trajectories

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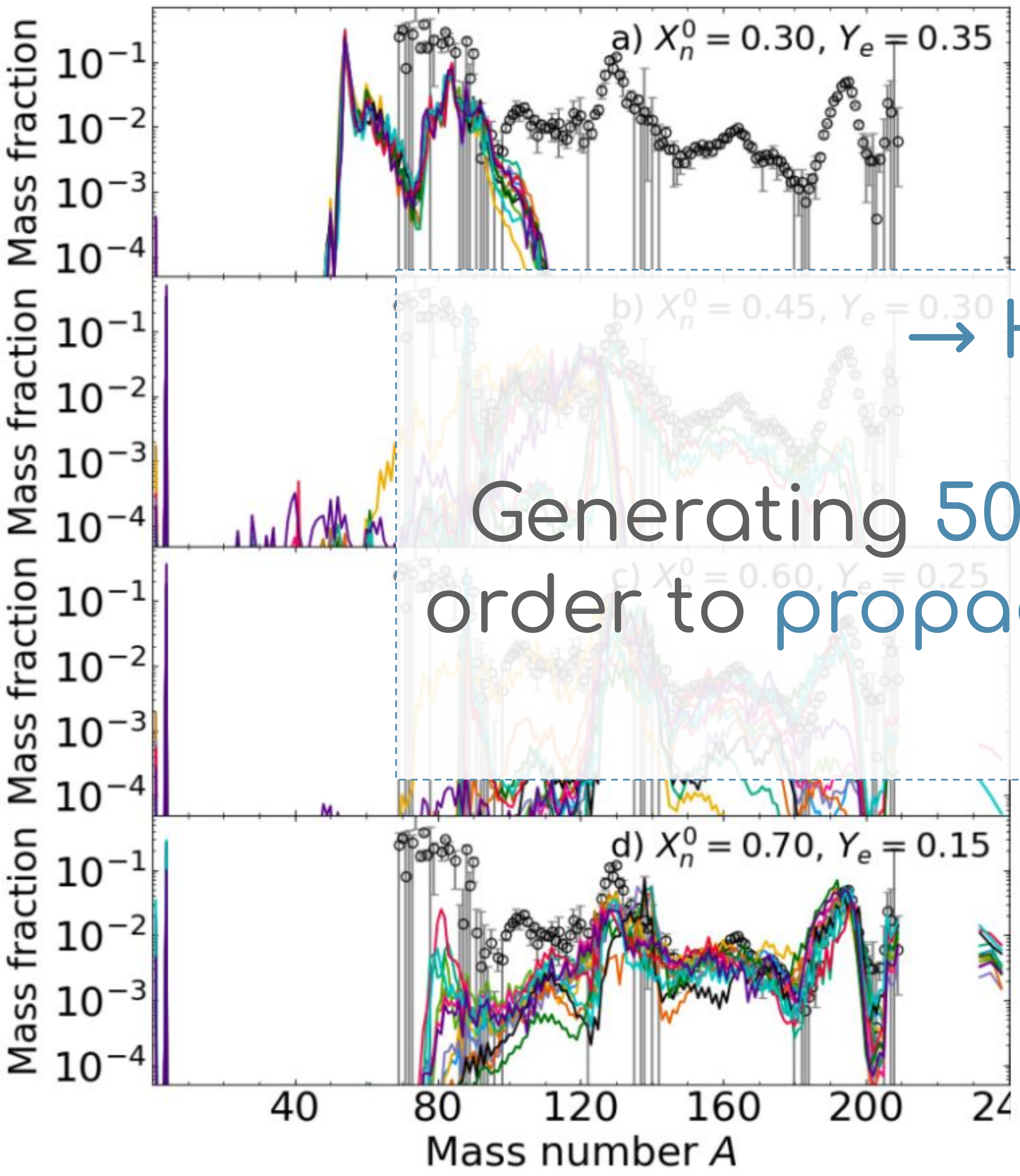

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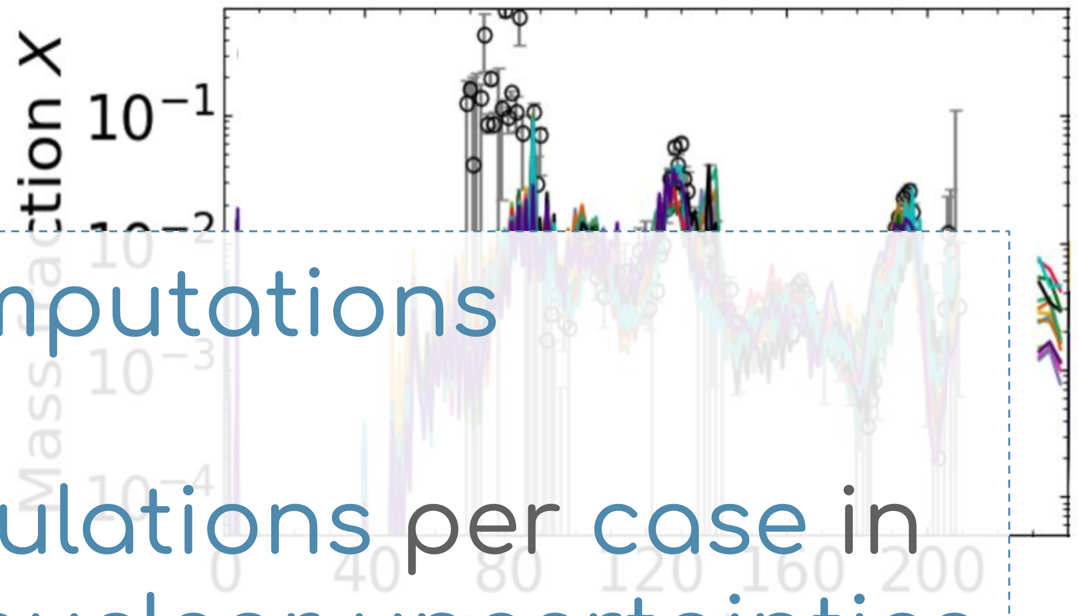
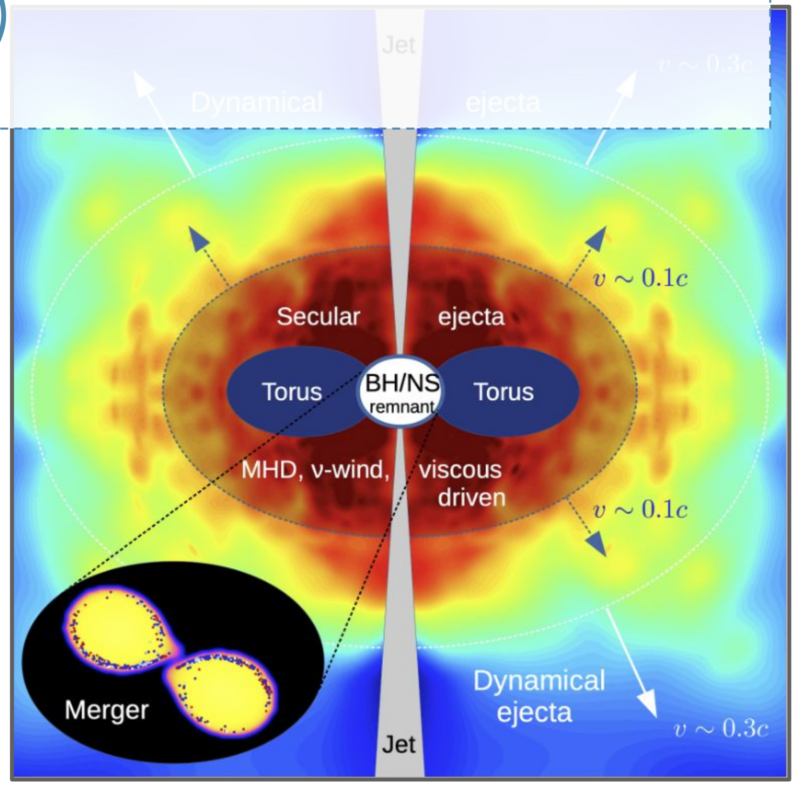


→ Heavy computations

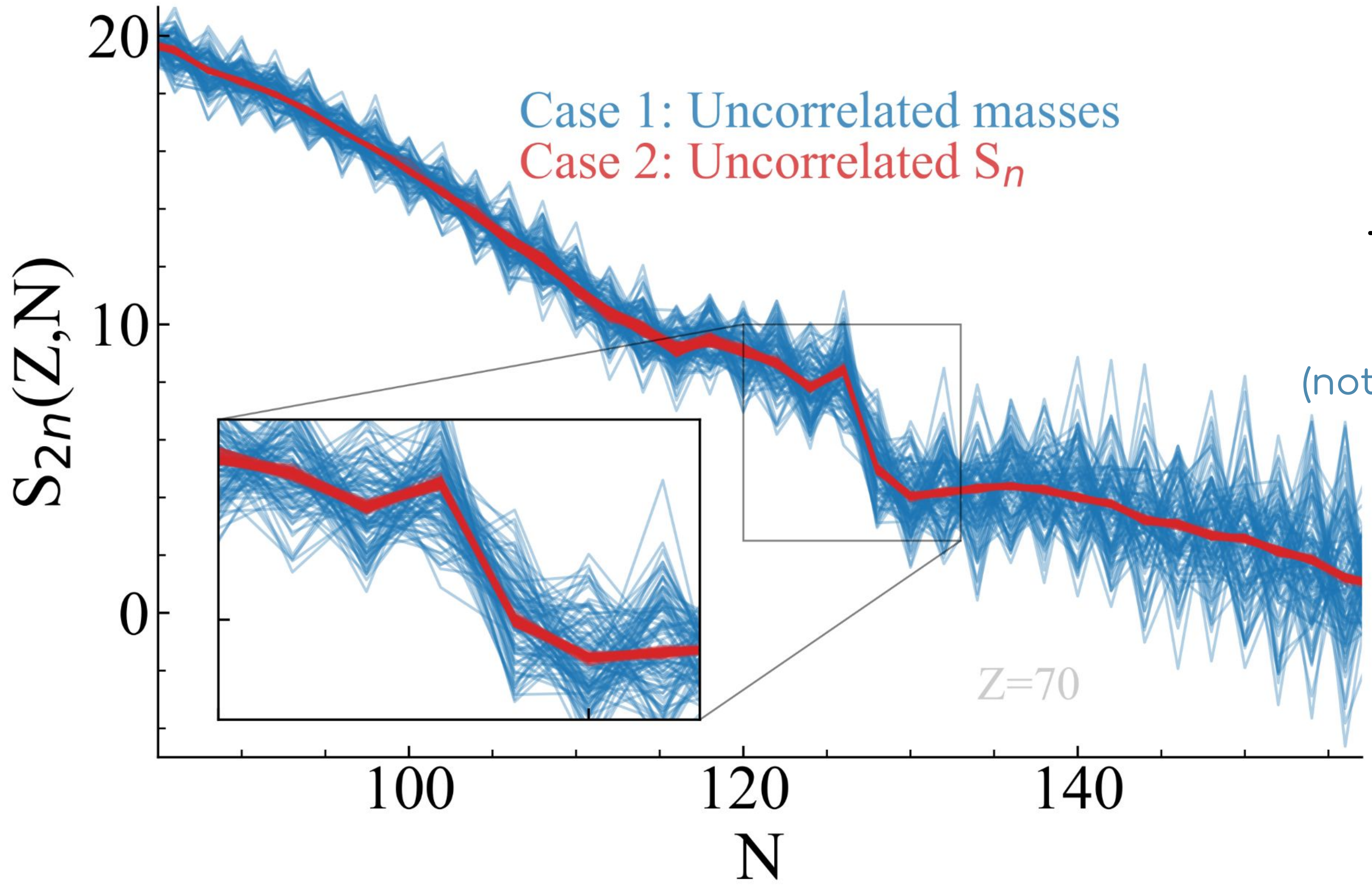
Generating 50 NSM simulations per case in order to propagate the nuclear uncertainties
(HPC facilities needed)



358 trajectories representing the total ~2500 trajectories

Propagating nuclear uncertainties to r-process simulations

Importance of taking correlations between properties themselves into account (Martinet & Goriely 2025)

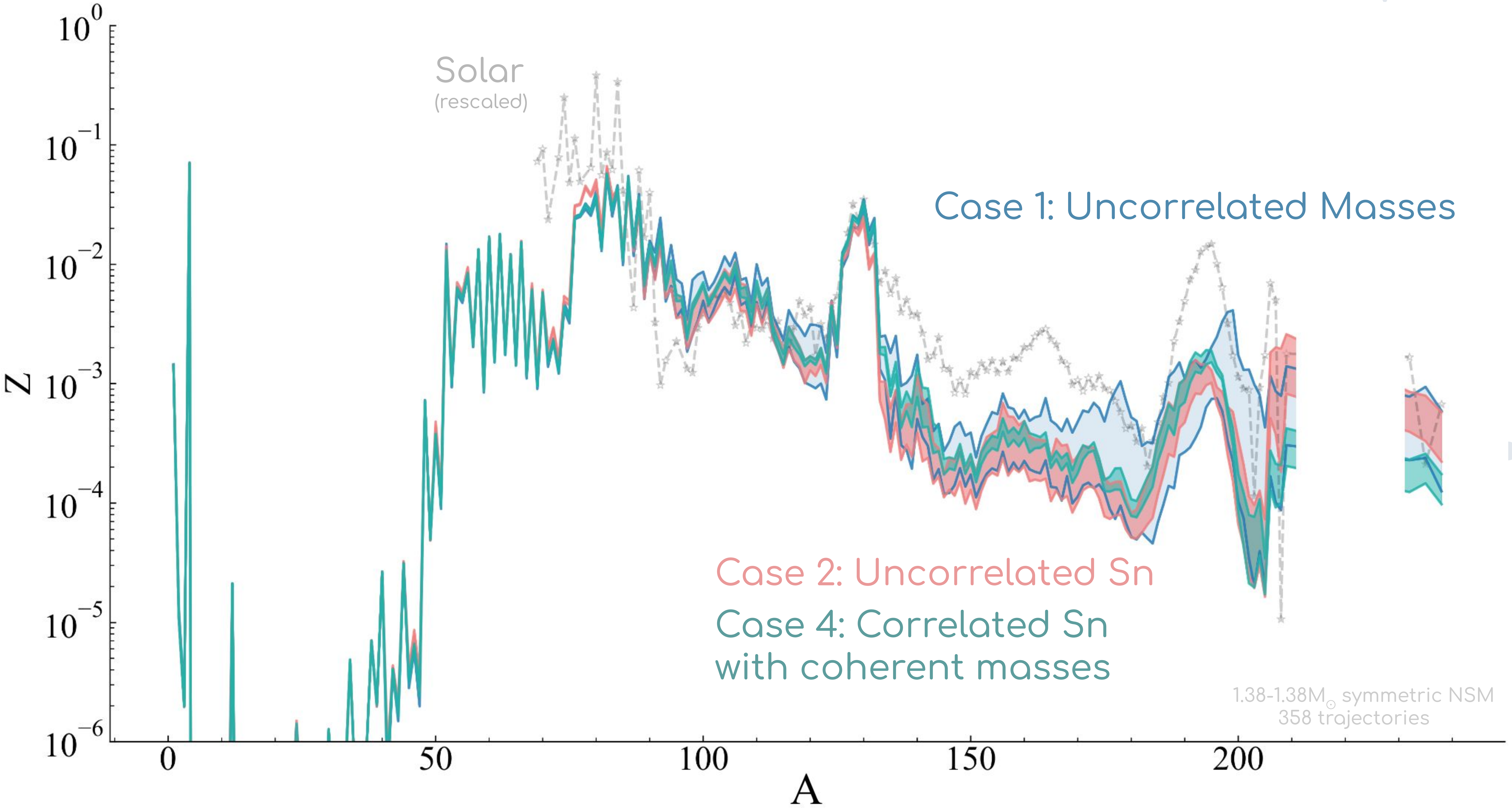


→ Photodissociation reaction rates depend exponentially on the separation energy Sn

(not the actual measured property → care needed for taking into account correlations)

Propagating nuclear uncertainties to r-process simulations

Anti-correlation of Sn and Qb, and coherent masses (Martinet & Goriely 2025)



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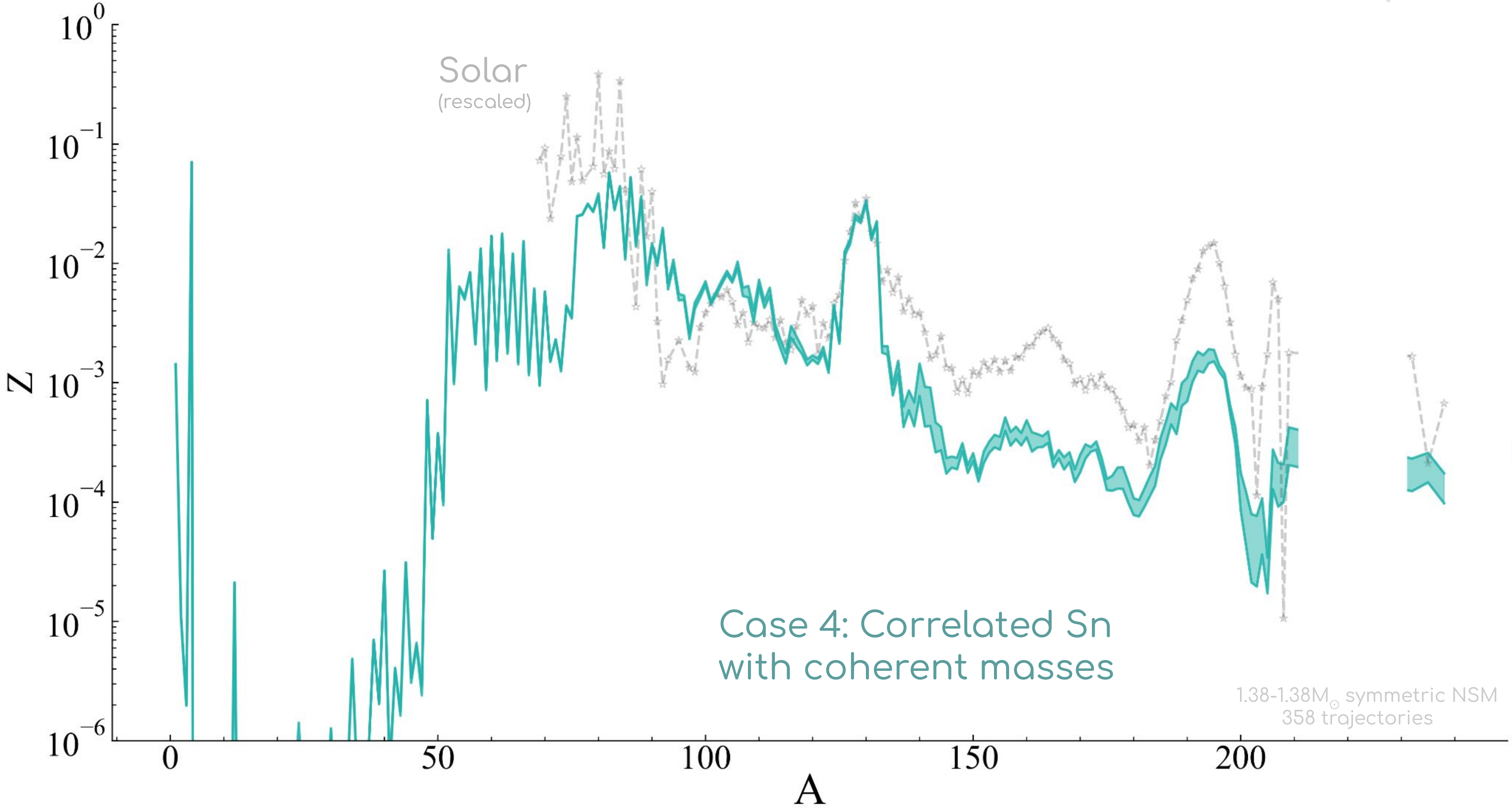
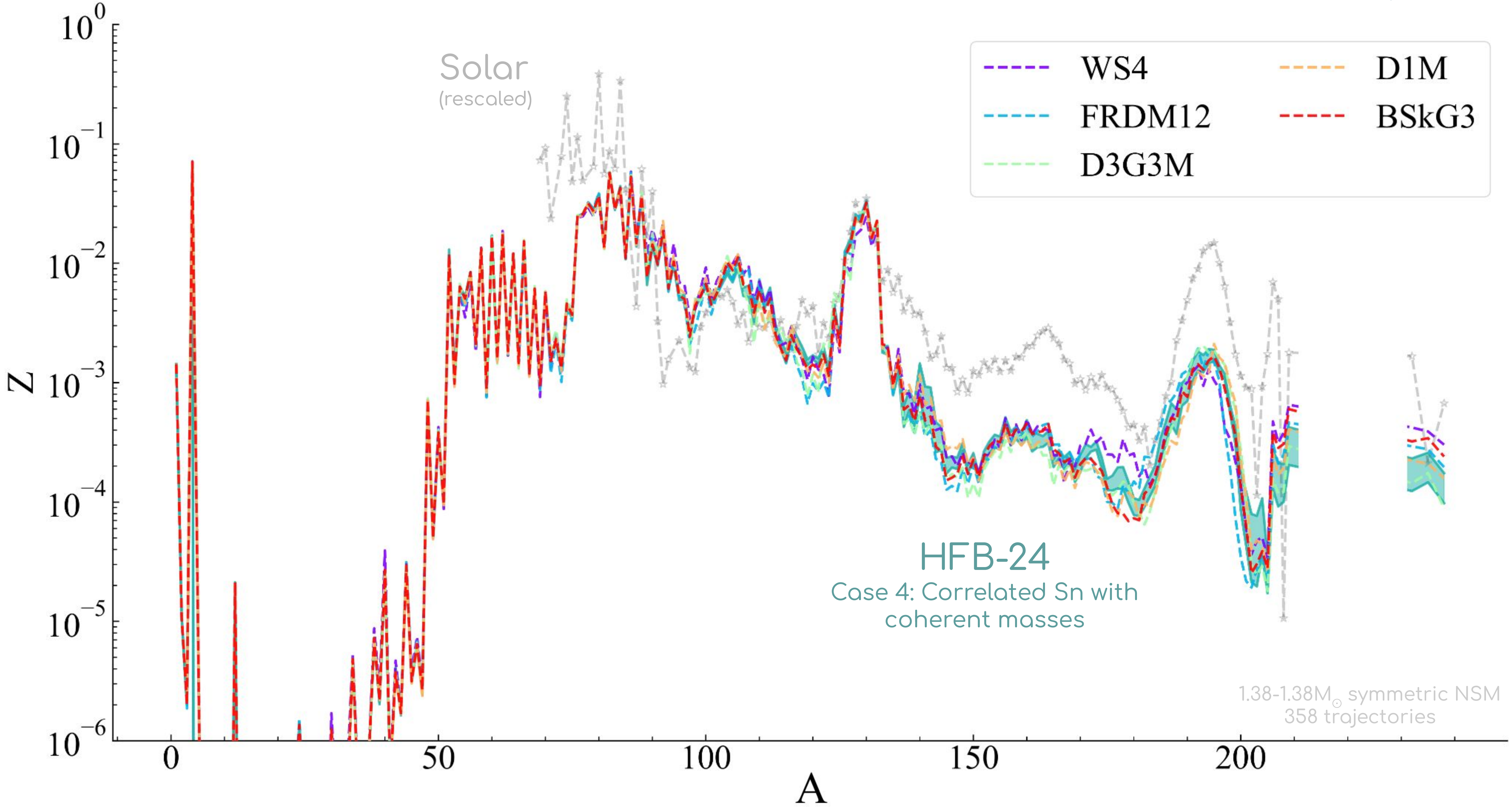


Propagating nuclear uncertainties to r-process simulations

Model uncertainties vs Parameter uncertainties (Martinet & Goriely 2025)



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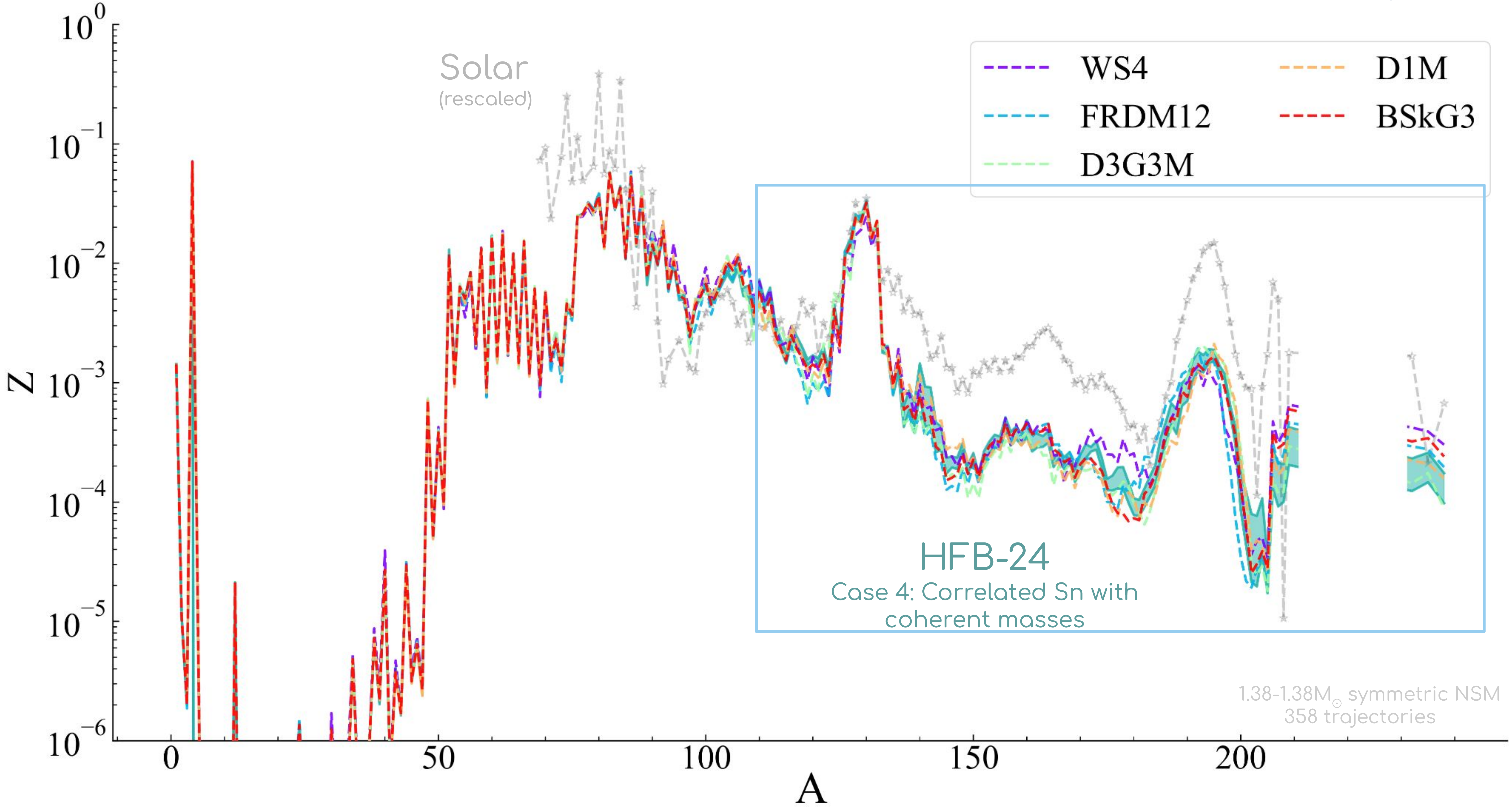

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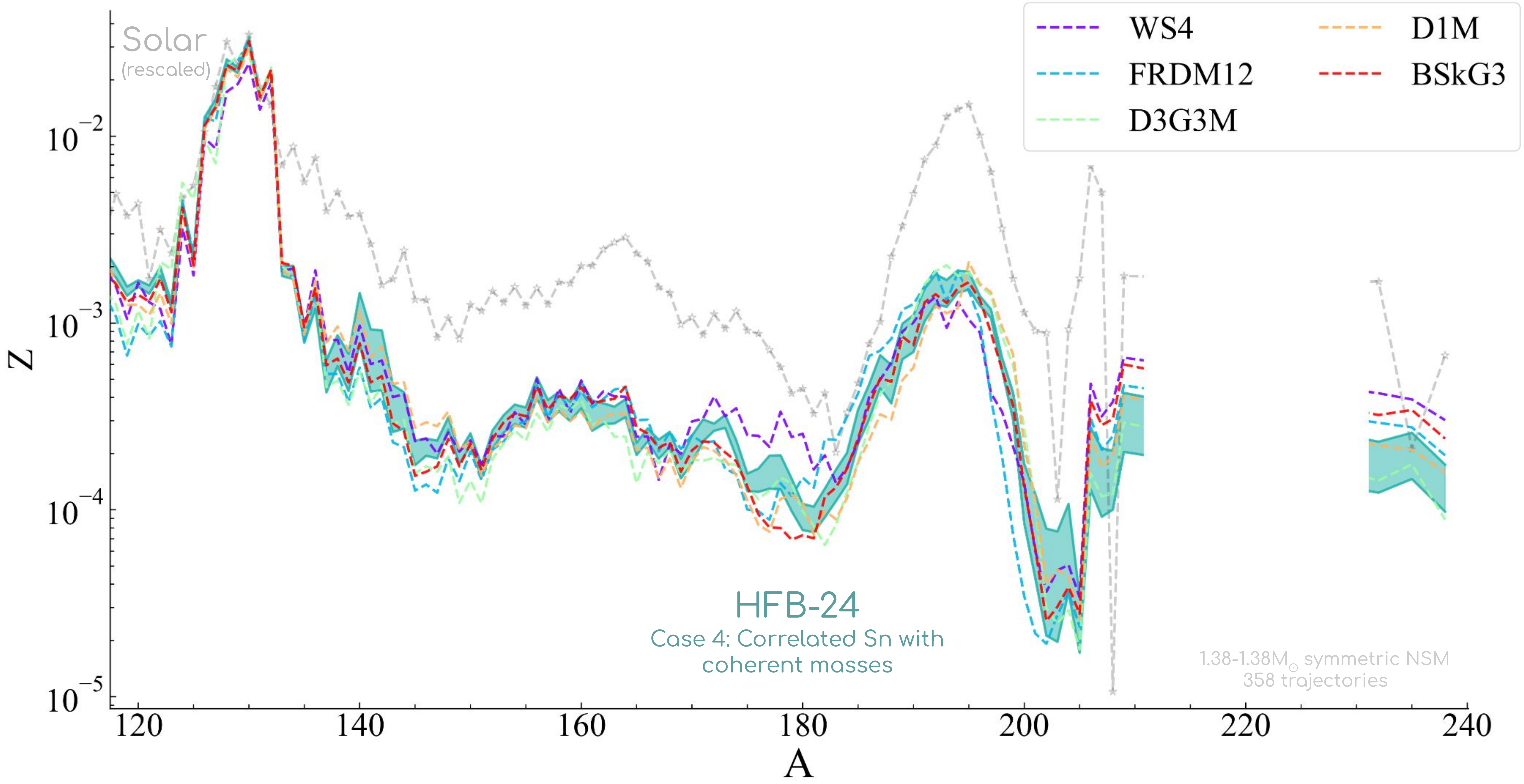

Conclusions

The impact of Systematic and Statistical nuclear uncertainties on the r- and i-process nucleosynthesis

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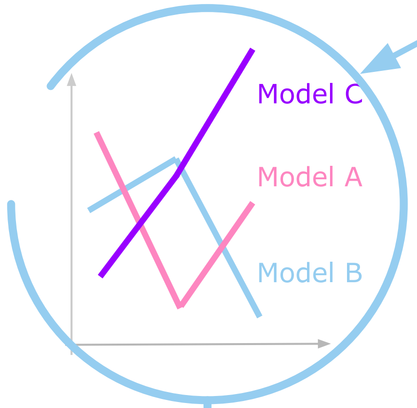

Statistical framework for nuclear parameter uncertainties

The BFMC method provides a robust, data-constrained way to quantify and propagate nuclear parameter uncertainties. This is essential for reliable predictions of nucleosynthesis

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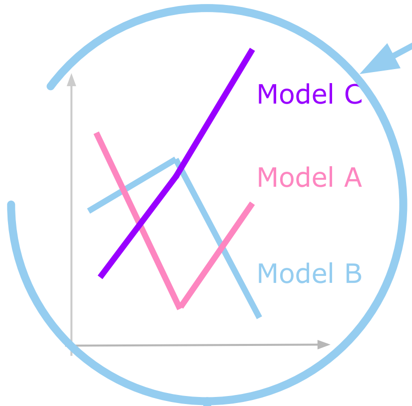
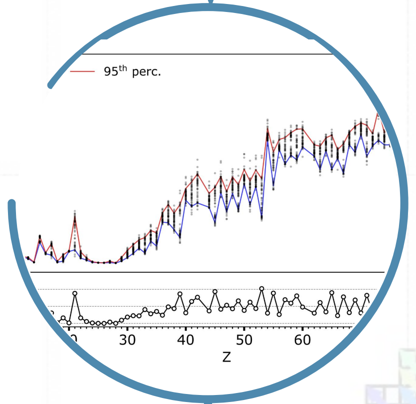
Systematic and Statistical nuclear uncertainties





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Impact on i-process nucleosynthesis in AGB stars

Important impact on the production of observable tracers (surface abundance uncertainties by 1 dex for La, 3 dex for Th/U, 1.2 dex Eu, ...)

Results consistent for different nuclear models

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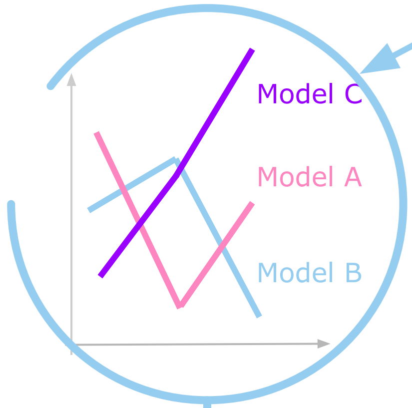
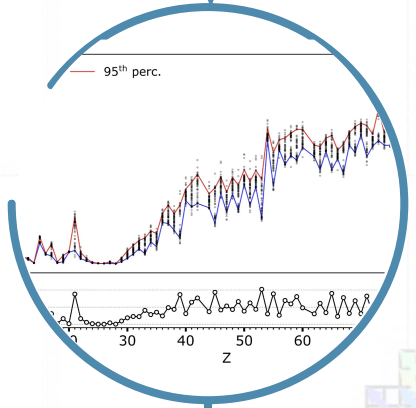
Systematic and Statistical nuclear uncertainties





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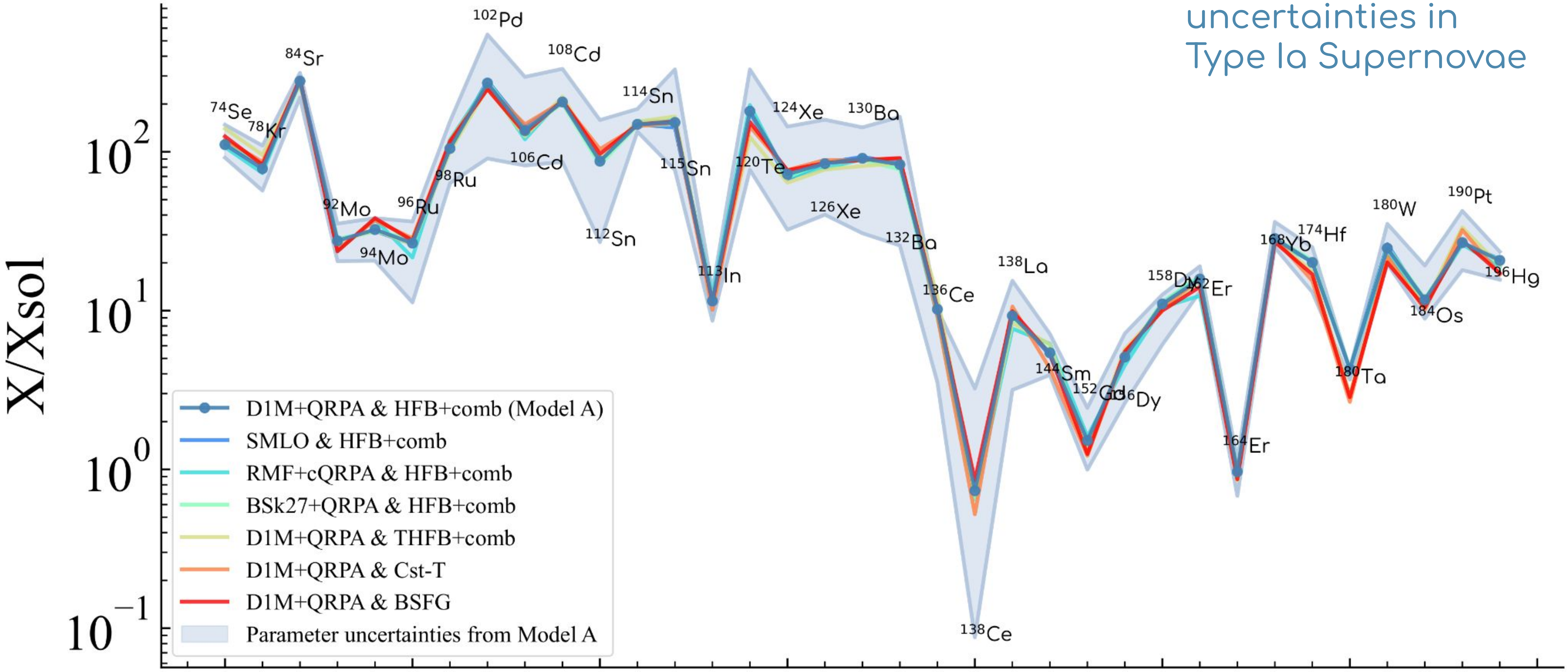
Results consistent for different nuclear models

Impact on r-process nucleosynthesis in Neutron Star Mergers

Multiple trajectories needed to represent the real impact of nuclear uncertainties.

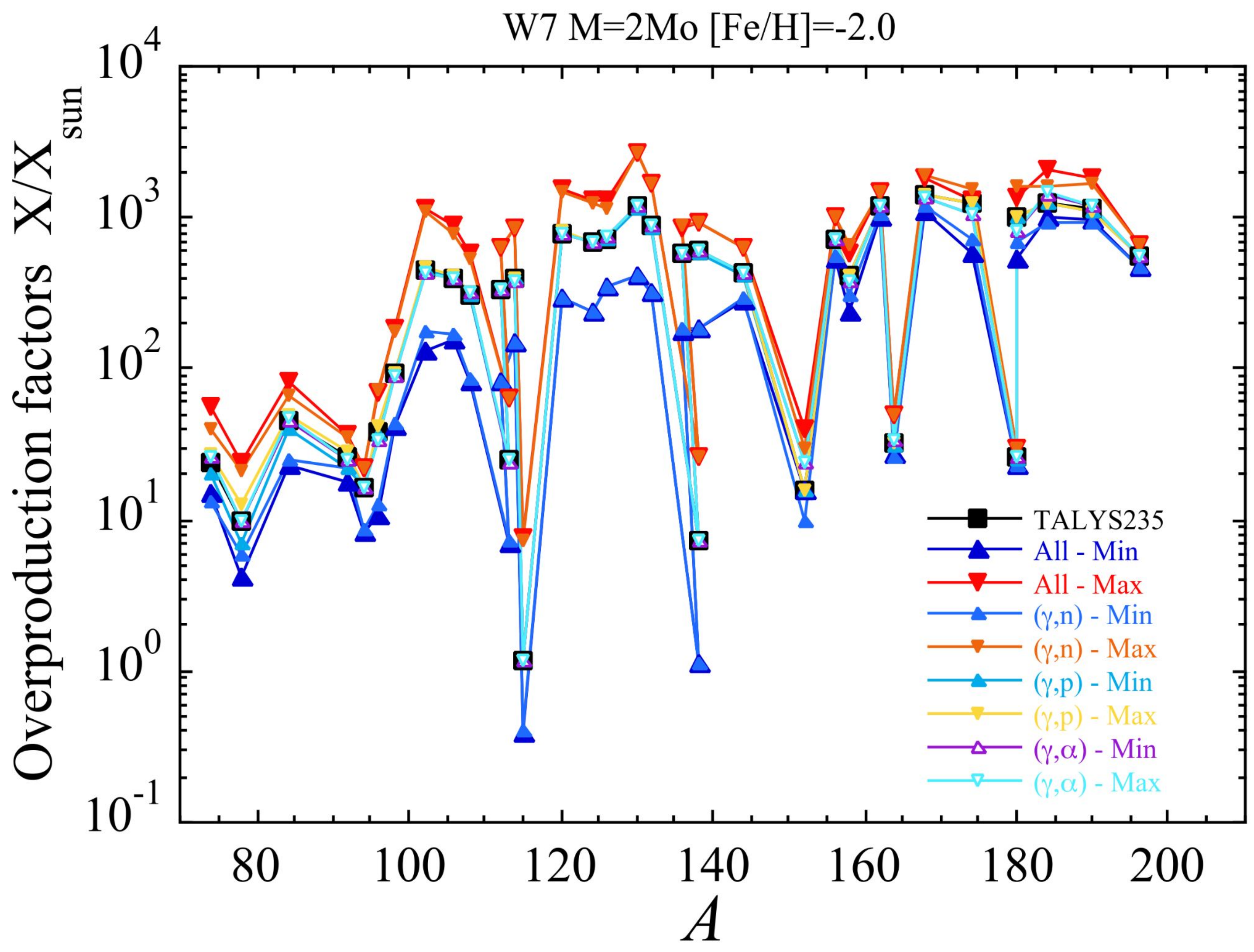
Mostly affects abondances of nuclei with A > 135. Model uncertainties leads to larger uncertainties on abondances than parameter ones

p-process NLD and PSF uncertainties in Type Ia Supernovae



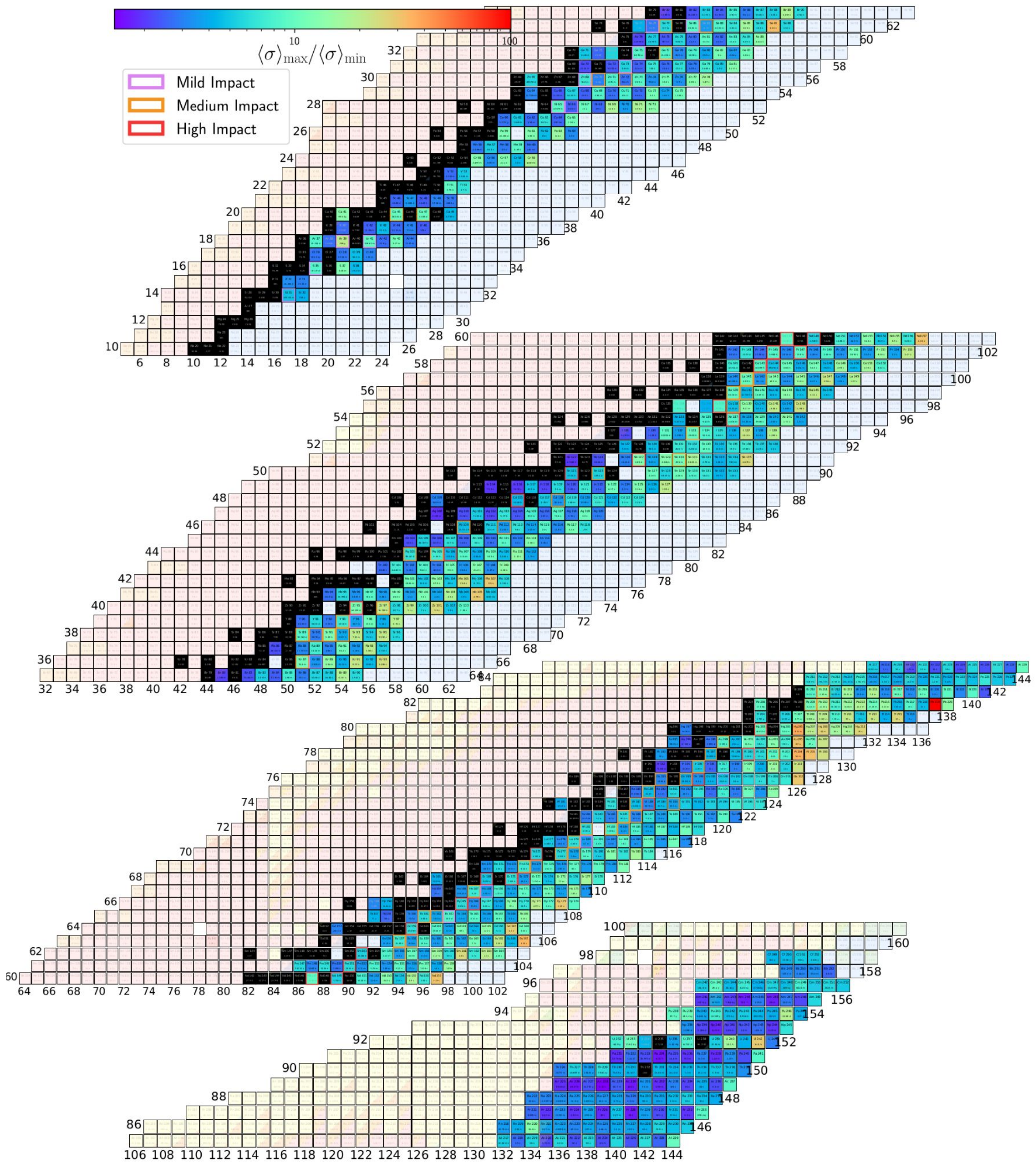
Impact of (p,g) and (a,g)

The impact of Systematic and Statistical nuclear uncertainties on the i-process nucleosynthesis



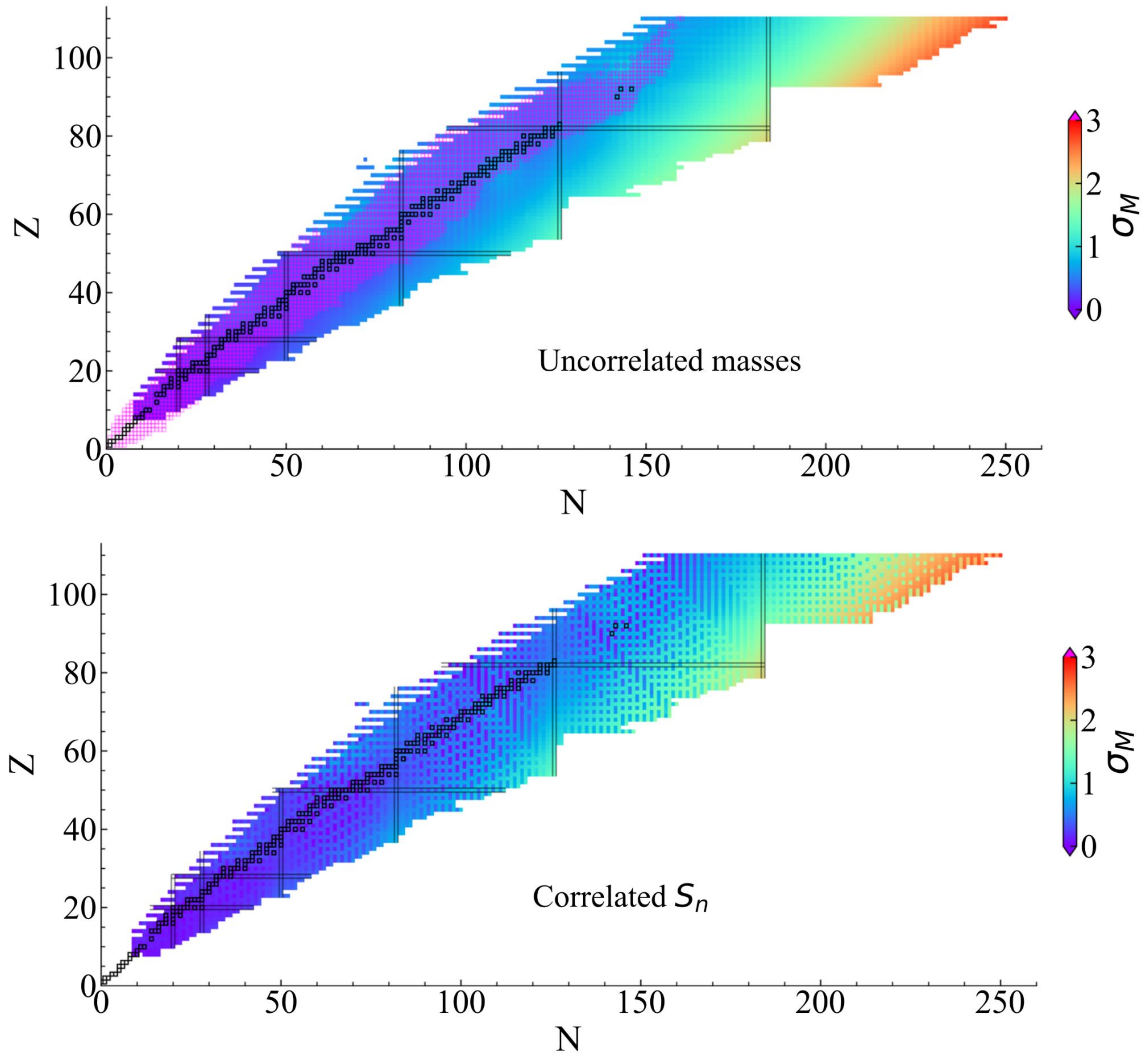
Impact of Nuclear Uncertainties on the i-process in AGB Stars

Identify important (n,g) reactions during the i-process in AGB stars (Martinet+2024a)

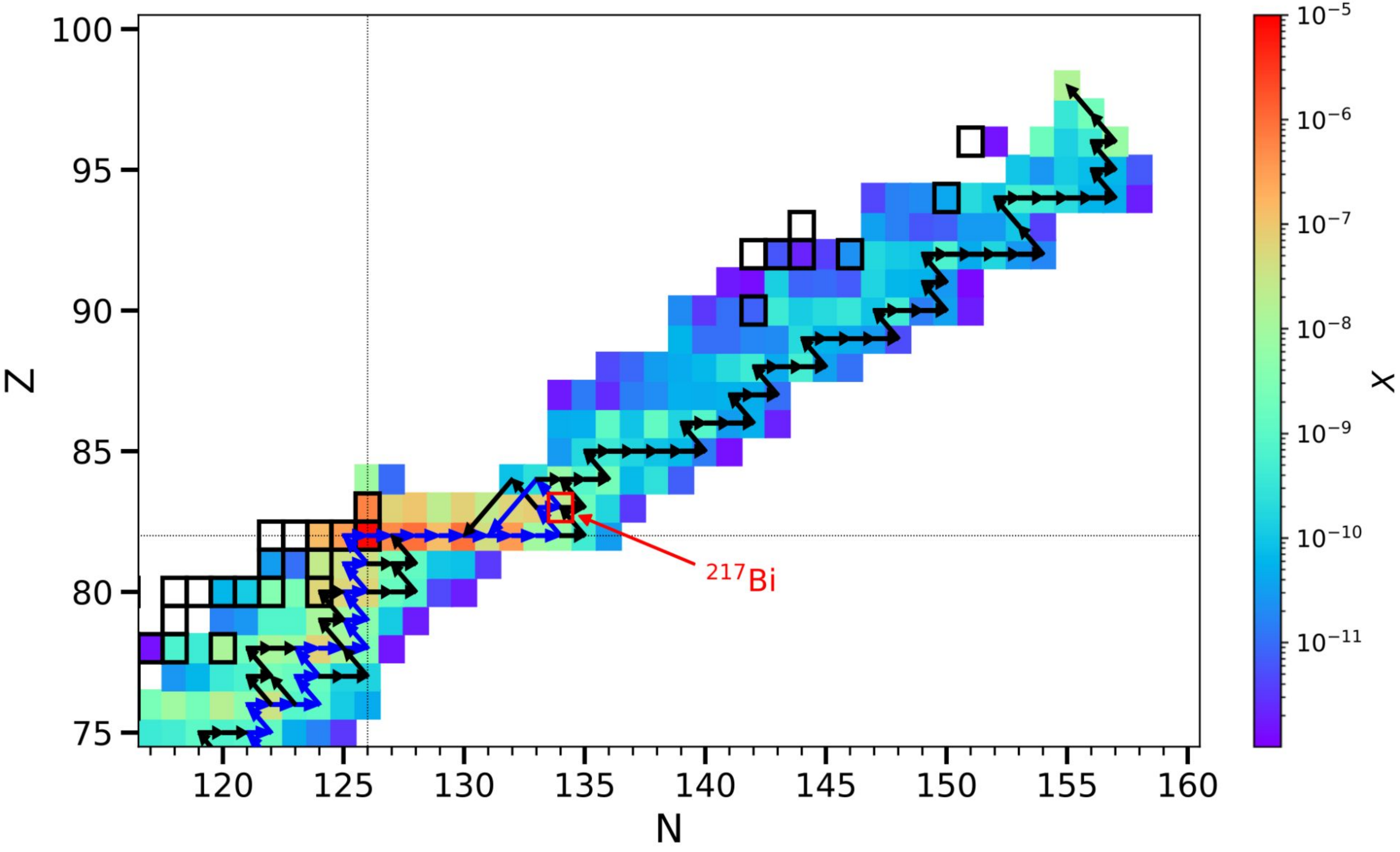


Element	Z	A	Iso. Frac.	Surface abund. uncertainty (in log) set A	set B	Reaction	$\langle\sigma\rangle_{max}$ / $\langle\sigma\rangle_{min}$ set A	set B
Sr	38	86	1-4%	0.49	0.31	^{86}Rb(n,γ)	5.3	2.2
Sr	38	87	0-1%	0.01	0.00	^{86}Rb(n,γ)	5.3	2.2
Sr	38	88	95-99%	0.42	0.45	^{88}Kr(n,γ)	3.4	3.5
Y	39	89	100%	0.92	0.78	^{89}Sr(n,γ)	7.6	8.4
Zr	40	90	10-43%	0.62	0.73	^{90}Sr(n,γ)	2.8	3.0
Zr	40	91	2-28%	0.88	1.12	^{91}Sr(n,γ)	8.2	11.9
Zr	40	92	7-25%	0.61	0.57	^{92}Sr(n,γ)	4.0	3.9
Zr	40	94	8-24%	0.49	0.48	^{94}Y(n,γ)	10.0	3.7
Ba	56	134	<0.5%	0.49	0.55	^{134}Cs(n,γ)	8.0	6.3
Ba	56	136	0-6%	1.17	1.58	^{135}Xe(n,γ)	5.1	7.6
Ba	56	136	0-6%	1.17	1.58	^{136}Cs(n,γ)	6.8	14.2
Ba	56	137	4-85%	1.34	1.95	^{137}Xe(n,γ)	11.6	8.4
Ba	56	137	4-85%	1.34	1.95	^{137}Cs(n,γ)	15.4	78.4
Ba	56	138	9-80%	0.66	0.52	^{138}Cs(n,γ)	7.0	4.8
La	57	139	100%	0.59	0.77	^{139}Ba(n,γ)	10.3	9.0
Ce	58	140	27-90%	0.78	0.86	^{140}Ba(n,γ)	3.2	4.3
Ce	58	142	10-73%	0.54	0.51	^{142}La(n,γ)	7.8	3.4
Pr	59	141	100%	0.97	0.96	^{141}La(n,γ)	11.1	10.0
Nd	60	142	<0.5%	0.68	0.30	^{142}Pr(n,γ)	12.6	3.1
Nd	60	143	2-36%	1.10	0.99	^{143}Ce(n,γ)	12.6	8.9
Nd	60	144	27-79%	1.07	0.85	^{144}Ce(n,γ)	7.2	4.7
Nd	60	145	1-18%	1.05	0.91	^{145}Pr(n,γ)	12.0	8.7
Nd	60	150	3-13%	0.34	0.38	^{149}Nd(n,γ)	7.3	5.4
Sm	62	147	6-51%	1.14	1.17	^{147}Pr(n,γ)	11.9	9.8
Sm	62	147	6-51%	1.14	1.17	^{147}Nd(n,γ)	10.5	9.5
Sm	62	148	<0.5%	1.20	1.01	^{148}Pm(n,γ)	8.9	3.1
Sm	62	148	<0.5%	1.20	1.01	^{147}Nd(n,γ)	10.5	9.5
Sm	62	149	4-30%	1.07	0.84	^{149}Nd(n,γ)	7.3	5.4
Sm	62	150	0-4%	1.31	1.08	^{149}Nd(n,γ)	7.3	5.4
Eu	63	151	18-85%	1.04	0.83	^{151}Pm(n,γ)	8.6	6.1
Eu	63	153	15-82%	1.15	0.88	^{153}Sm(n,γ)	12.5	5.5

Martinet+2024



Uncorrelated masses
Correlated S_n
Z
N
σ_M
0
20
40
60
80
100
50
150
200
250
1
2
3



Z
N
X
217Bi

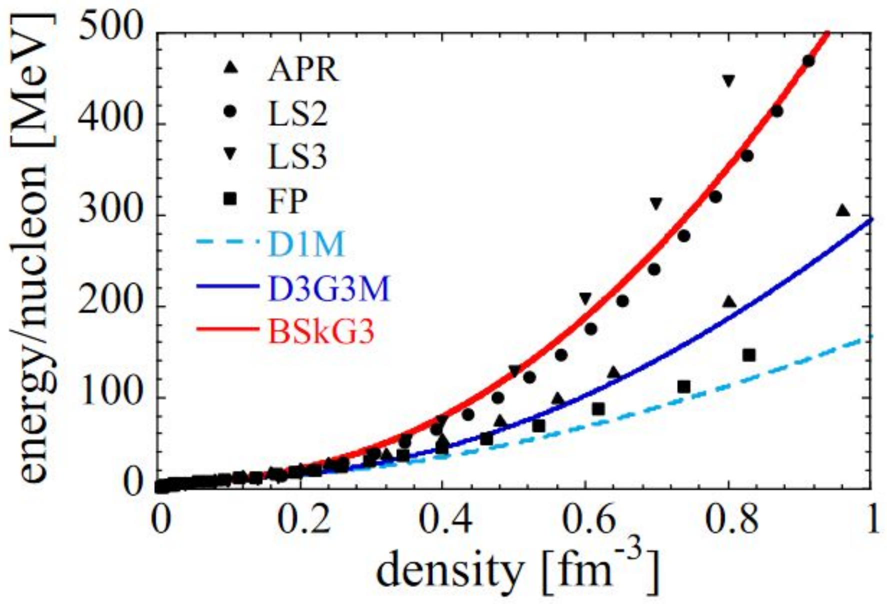
New HFB nuclear mass models

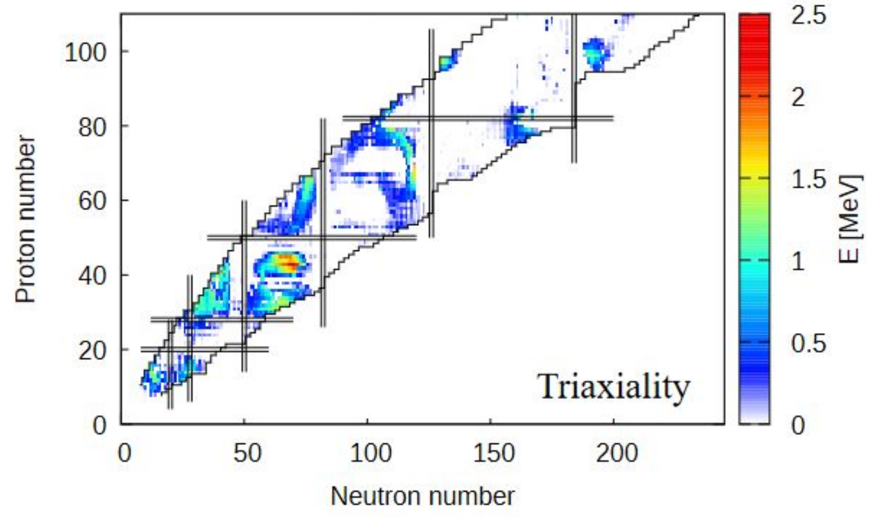
- New Gogny-HFB mass model: D3G3M
  - Gogny interaction with 3 Gaussians
  - Stiffer EoS than D1M
  - Accurate masses: σ(2457*M*)=0.87MeV

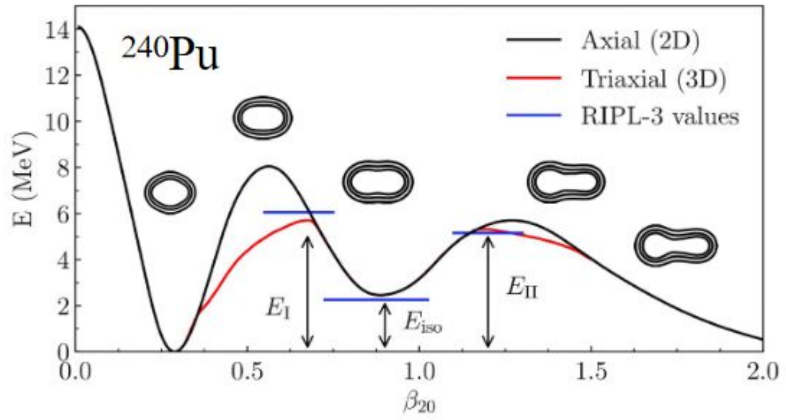
Batail et al. (2024)

- New Syrme-HFB mass model: BSkG3
  - Triaxiality, time-reversal symmetry breaking & octupole GS deformation
  - Microscopic pairing from "realistic" calculations
  - Stiff EoS
  - Accurate masses: σ(2457*M*)=0.63MeV
  - Accurate fission barriers σ(45B_f)=0.33MeV including triaxial & octupole deformations simultaneously

Grams et al. (2023)

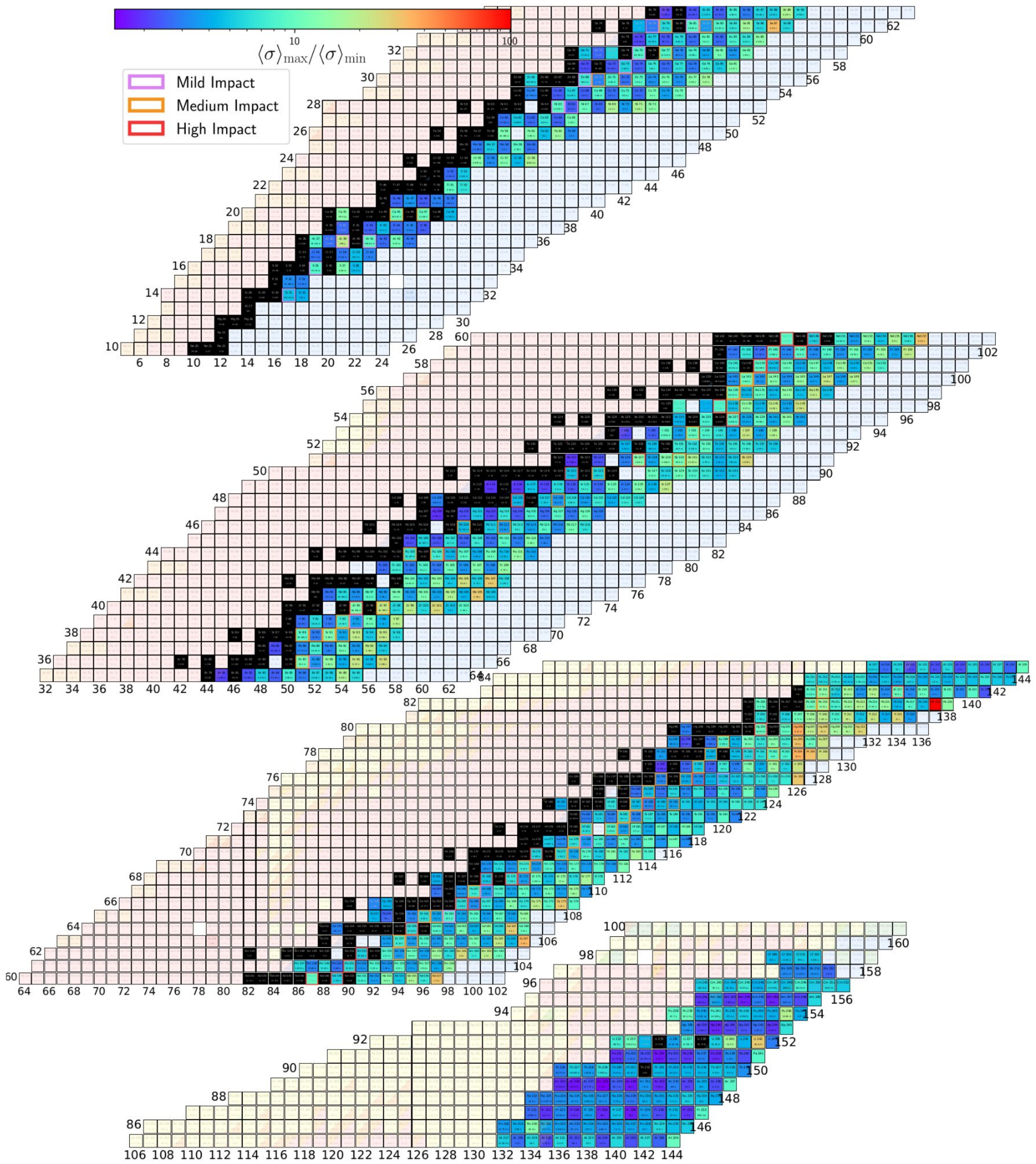






Impact of Nuclear Uncertainties on the i-process in AGB Stars

Identify important (n,g) reactions during the i-process in AGB stars (Martinet+2024a)

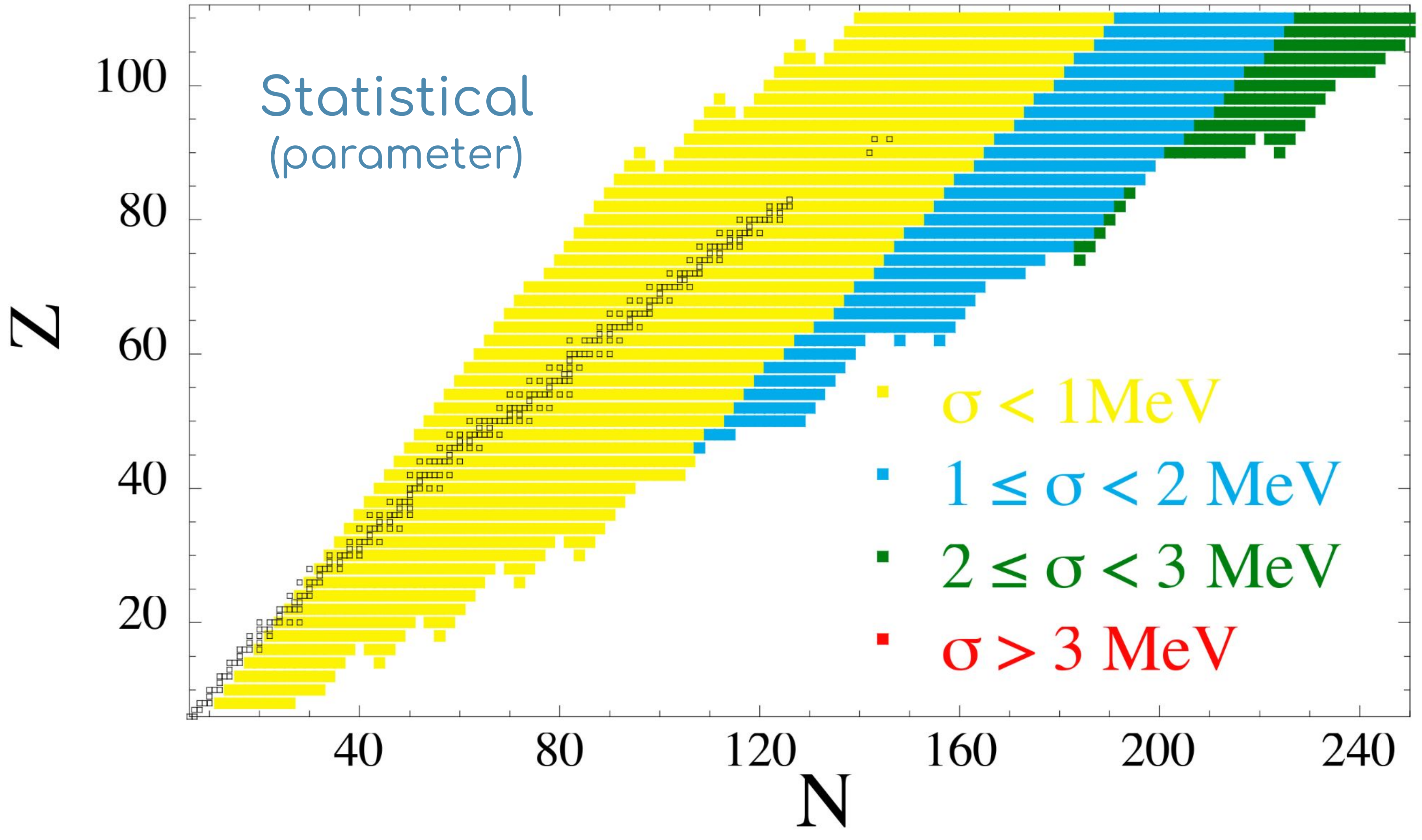


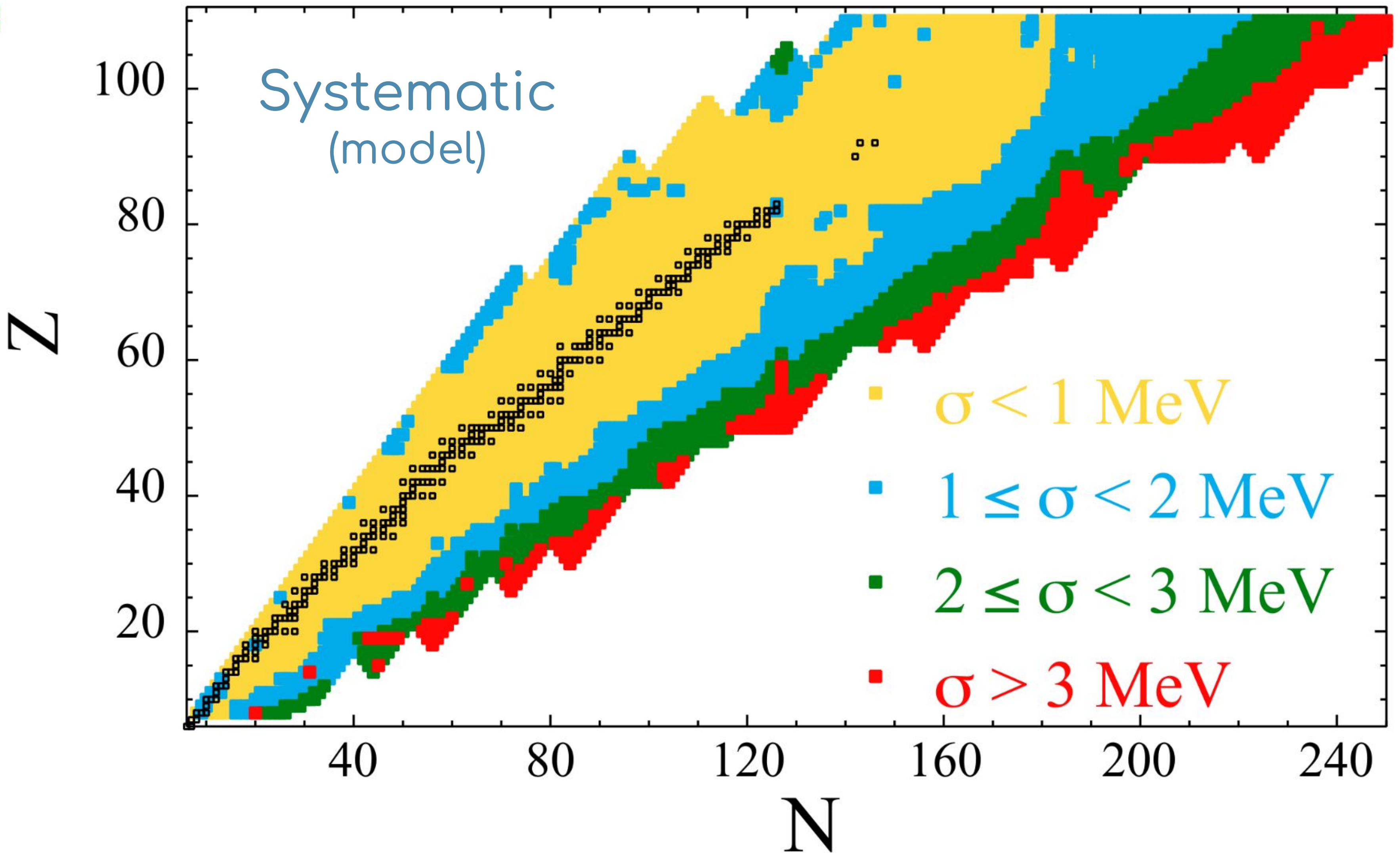
Element	Z	A	Iso. Frac.	Surf. abund. uncertainty (in log) set A	set B	Reaction	$\langle\sigma\rangle_{max}$ / $\langle\sigma\rangle_{min}$ set A	set B
U	92	235	8-51%	2.90	1.37	^{217}Bi(n,γ)	57.2	10.0
U	92	238	49-92%	2.87	1.80	^{217}Bi(n,γ)	57.2	10.0
Th	90	232	100%	2.75	1.36	^{217}Bi(n,γ)	57.2	10.0
Dy	66	160	0-1%	1.66	0.91	^{160}Tb(n,γ)	7.5	3.2
Dy	66	160	0-1%	1.66	0.91	^{159}Gd(n,γ)	12.0	6.5
Gd	64	154	<0.5%	1.39	1.02	^{153}Sm(n,γ)	12.5	5.5
Ba	56	137	4-85%	1.34	1.95	^{137}Xe(n,γ)	11.6	8.4
Ba	56	137	4-85%	1.34	1.95	^{137}Cs(n,γ)	15.4	78.4
Pb	82	204	<0.5%	1.31	1.55	^{203}Hg(n,γ)	6.3	9.8
Sm	62	150	0-4%	1.31	1.08	^{149}Nd(n,γ)	7.3	5.4
Xe	54	130	<0.5%	1.30	0.78	^{130}I(n,γ)	8.6	2.7
Sb	51	121	10-72%	1.24	0.95	^{121}Sn(n,γ)	9.4	4.5
Sm	62	148	<0.5%	1.20	1.01	^{148}Pm(n,γ)	8.9	3.1
Sm	62	148	<0.5%	1.20	1.01	^{147}Nd(n,γ)	10.5	9.5
Mo	42	95	2-66%	1.18	1.19	^{95}Zr(n,γ)	11.5	11.8
Os	76	188	30-68%	1.17	0.62	^{188}W(n,γ)	8.6	3.2
Ba	56	136	0-6%	1.17	1.58	^{135}Xe(n,γ)	5.1	7.6
Ba	56	136	0-6%	1.17	1.58	^{136}Cs(n,γ)	6.8	14.2
Eu	63	153	15-82%	1.15	0.88	^{153}Sm(n,γ)	12.5	5.5
Sm	62	147	6-51%	1.14	1.17	^{147}Pr(n,γ)	11.9	9.8
Sm	62	147	6-51%	1.14	1.17	^{147}Nd(n,γ)	10.5	9.5
Cd	48	111	2-12%	1.10	0.71	^{111}Pd(n,γ)	6.8	5.1
I	53	127	100%	1.10	1.18	^{127}Sb(n,γ)	10.7	12.4
Nd	60	143	2-36%	1.10	0.99	^{143}Ce(n,γ)	12.6	8.9
Nd	60	144	27-79%	1.07	0.85	^{144}Ce(n,γ)	7.2	4.7
Lu	71	175	100%	1.07	0.81	^{175}Yb(n,γ)	8.7	5.6
Hg	80	200	9-46%	1.07	0.84	^{200}Pt(n,γ)	11.3	5.6
Sm	62	149	4-30%	1.07	0.84	^{149}Nd(n,γ)	7.3	5.4
Pd	46	106	27-75%	1.07	0.93	^{106}Ru(n,γ)	8.0	4.3
Nd	60	145	1-18%	1.05	0.91	^{145}Pr(n,γ)	12.0	8.7
Pt	78	194	26-63%	1.04	0.68	^{194}Os(n,γ)	8.7	3.4

Martinet+2024

Estimating Nuclear Uncertainties

Overestimating uncertainties





The Backward-Forward Monte Carlo approach

Goriely & Capote 2014

1st Step: Computing masses for random sets of parameters for one nuclear model (HFB-24)

6424 nuclei

Z	N	A	1	2	3	4	…	11014	11015	11016	11019	11020	11021	11022
8	10	18	0.88	0.95	0.93	0.94	…	0.88	0.86	0.97	0.83	0.90	1.00	0.94
8	11	19	5.14	5.14	5.22	5.24	…	5.07	5.16	5.20	5.11	5.15	5.21	5.20
8	12	20	3.23	3.29	3.24	3.27	…	3.18	3.16	3.36	3.16	3.23	3.33	3.21
8	13	21	9.11	9.11	9.15	9.17	…	9.01	9.08	9.15	9.12	9.09	9.19	9.08
8	14	22	9.45	9.48	9.46	9.48	…	9.37	9.36	9.46	9.46	9.39	9.55	9.37
…	…	…	…	…	…	…	…	…	…	…	…	…	…	…
110	246	356	533.09	534.80	532.17	530.81	…	532.92	529.74	531.01	533.00	527.89	533.04	530.81
110	247	357	540.31	542.02	539.73	538.48	…	539.98	537.68	538.38	540.28	535.53	540.06	538.67
110	248	358	548.11	549.85	547.17	545.78	…	547.96	544.72	545.94	548.04	542.80	548.04	545.79
110	249	359	555.79	557.52	555.18	553.90	…	555.49	553.08	553.74	555.79	550.88	555.53	554.09
110	250	360	564.04	565.79	563.09	561.66	…	563.91	560.61	561.80	564.00	558.63	563.94	561.69

11022 random combinations

The Backward-Forward Monte Carlo approach

Goriely & Capote 2014

1st Step: Computing masses for random sets of parameters for one nuclear model (HFB-24)

6424 nuclei

Z	N	A	1	2	3	4	...	11014	11015	11016	11019	11020	11021	11022
8	10	18	0.88	0.95	0.93	0.94	...	0.88	0.86	0.97	0.83	0.90	1.00	0.94
8	11	19	5.14	5.14	5.22	5.24	...	5.07	5.16	5.20	5.11	5.15	5.21	5.20
8	12	20	3.23	3.29	3.24	3.27	...	3.18	3.16	3.36	3.16	3.23	3.33	3.21
8	13	21	9.11	9.11	9.15	9.17	...	9.01	9.08	9.15	9.12	9.09	9.19	9.08
8	14	22	9.45	9.48	9.46	9.48	...	9.37	9.36	9.46	9.46	9.39	9.55	9.37
...	...	...	...	...	...	...	...	...	...	...	...	...	...	...
110	246	356	533.09	534.80	532.17	530.81	...	532.92	529.74	531.01	533.00	527.89	533.04	530.81
110	247	357	540.31	542.02	539.73	538.48	...	539.98	537.68	538.38	540.28	535.53	540.06	538.67
110	248	358	548.11	549.85	547.17	545.78	...	547.96	544.72	545.94	548.04	542.80	548.04	545.79
110	249	359	555.79	557.52	555.18	553.90	...	555.49	553.08	553.74	555.79	550.88	555.53	554.09
110	250	360	564.04	565.79	563.09	561.66	...	563.91	560.61	561.80	564.00	558.63	563.94	561.69

2nd Step: Checking if each parameter set as a rms for the known nuclei compatible with the experimental rms and discard the rest

↔

Anchor values to experimental uncertainties

The Backward-Forward Monte Carlo approach

Goriely & Capote 2014

1st Step: Computing masses for random sets of parameters for one nuclear model (HFB-24)

6424 nuclei

Z	N	A	1	2	3	4	...	11014	11015	11016	11019	11020	11021	11022
8	10	18	0.88	0.95	0.93	0.94	...	0.88	0.86	0.97	0.83	0.90	1.00	0.94
8	11	19	5.14	5.14	5.22	5.24	...	5.07	5.16	5.20	5.11	5.15	5.21	5.20
8	12	20	3.23	3.29	3.24	3.27	...	3.18	3.16	3.36	3.16	3.23	3.33	3.21
8	13	21	9.11	9.11	9.15	9.17	...	9.01	9.08	9.15	9.12	9.09	9.19	9.08
8	14	22	9.45	9.48	9.46	9.48	...	9.37	9.36	9.46	9.46	9.39	9.55	9.37
...	...	...	...	...	...	...	...	...	...	...	...	...	...	...
110	246	356	533.09	534.80	532.17	530.81	...	532.92	529.74	531.01	533.00	527.89	533.04	530.81
110	247	357	540.31	542.02	539.73	538.48	...	539.98	537.68	538.38	540.28	535.53	540.06	538.67
110	248	358	548.11	549.85	547.17	545.78	...	547.96	544.72	545.94	548.04	542.80	548.04	545.79
110	249	359	555.79	557.52	555.18	553.90	...	555.49	553.08	553.74	555.79	550.88	555.53	554.09
110	250	360	564.04	565.79	563.09	561.66	...	563.91	560.61	561.80	564.00	558.63	563.94	561.69

2nd Step: Checking if each parameter set as a rms for the known nuclei compatible with the experimental rms and discard the rest

↔ Anchor values to experimental uncertainties

→ Using the remaining sets of parameters compatible with experiments to obtain the uncertainties on unknown masses

Estimating Nuclear Uncertainties

Radiative Neutron Capture Rates

Using TALYS reaction code (Koning et al. 2023)

↓

2 Nuclear physic models

Systematic/Model Uncertainties
(Correlated)

Model A: based on micro-physics
HFB+comb &
D1M+QRPA

Model B: based on phenomenological models
Cst-T + SMLO

Estimating Nuclear Uncertainties

Radiative Neutron Capture Rates

Using TALYS reaction code (Koning et al. 2023)

2 Nuclear physic models

Systematic/Model Uncertainties
(Correlated)

Model A: based on micro-physics
HFB+comb &
D1M+QRPA

Model B: based on phenomenological models
Cst-T + SMLO

4 parameters

4 parameters

Statistical/Parameter Uncertainties
(Non-correlated)

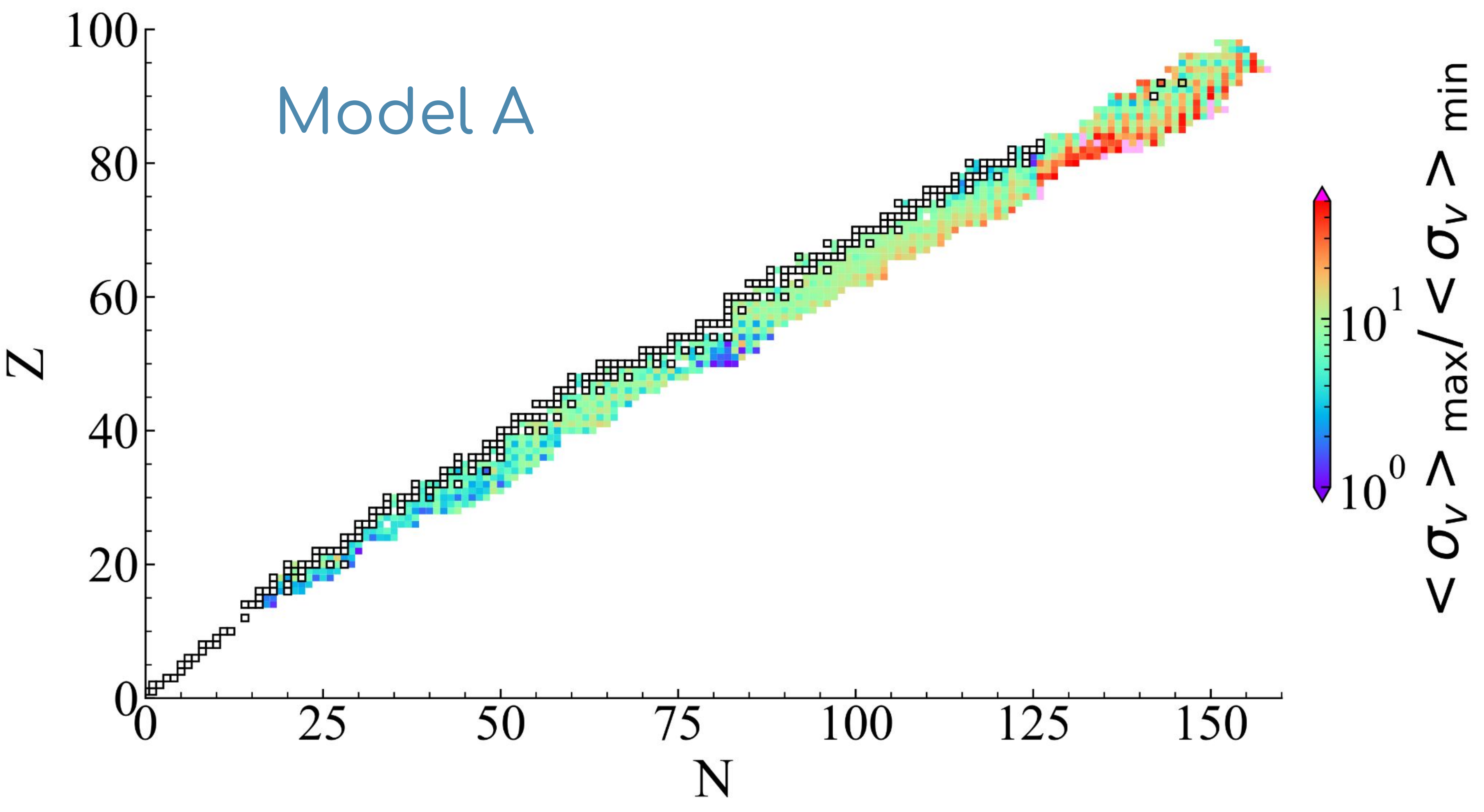
2 parameters affecting nuclear level densities

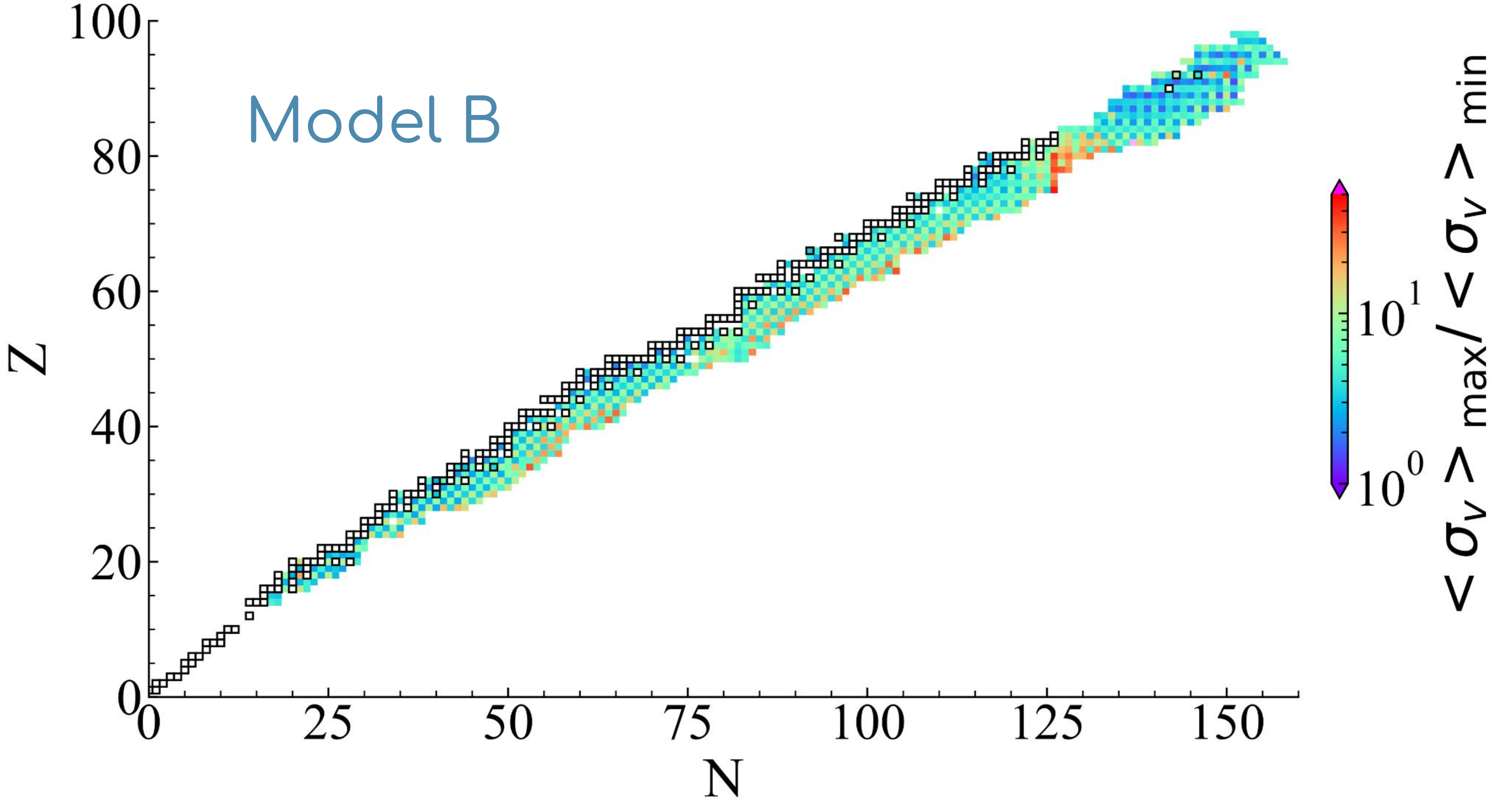
2 parameters affecting the photon strength function

Determining coherently parameter uncertainties

Parameters uncertainties obtained from the BFMC method

(n,g) rates uncertainties for the i-process





Impact of Nuclear Uncertainties on the i-process in AGB Stars

Effect of statistical uncertainties on the surface enrichment of early AGB stars (Martinet+2024a)

STAREVOL code (Siess et al. 2006)

→ i-process nucleosynthesis

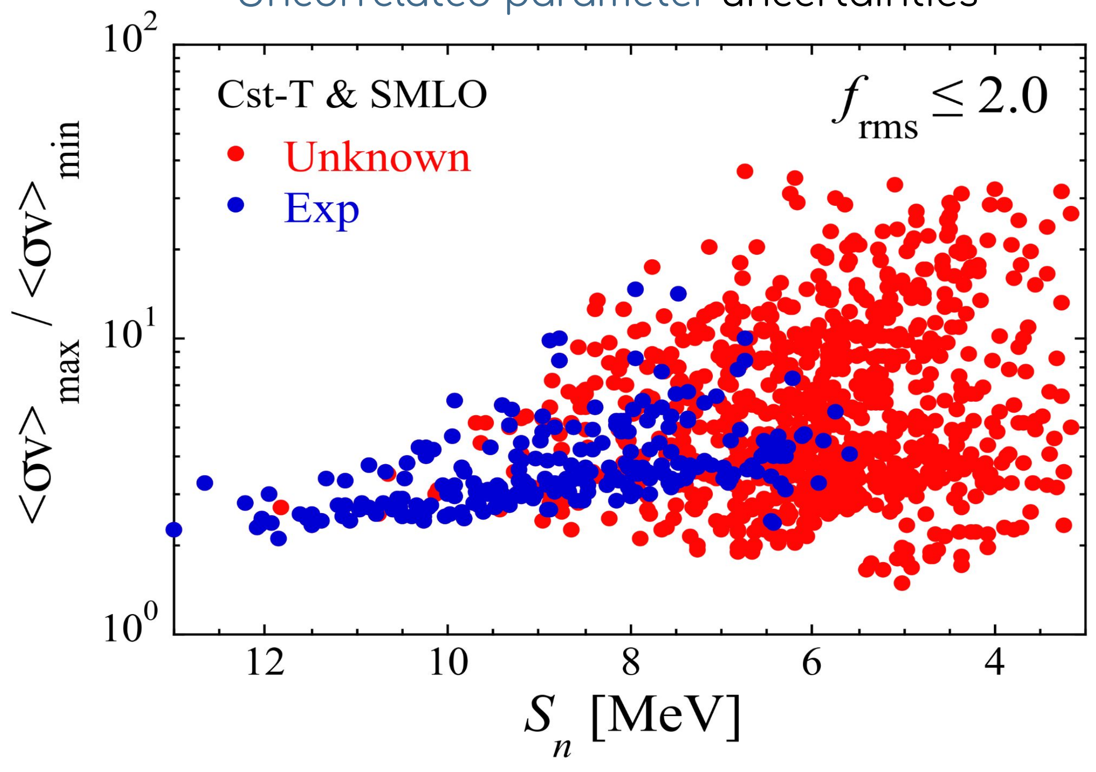
1 Msol at [Fe/H]=-2.5

Proton ingestion event in the early AGB phase

Maximum and minimum (n,g) theoretical rates (862 nuclei)
(with 4-parameter variation s.t. $f_{rms} \leq 2.0$)

→ Random combination of maximum and minimum rates for a large number of stellar models (n>50)

Uncorrelated parameter uncertainties



	1)	2)	3)		862)
	Si31(n,g)	P32(n,g)	Si32(n,g)		Pu252(n,g)
Stellar Model 1	Max	Max	Min	....	Min
Stellar Model 2	Min	Max	Min	....	Max
Stellar Model 3	Min	Min	Min	....	Max
.....	....	....	....	....	....
Stellar Model 50	Min	Min	Max	....	Min

Impact of Nuclear Uncertainties on the i-process in AGB Stars

Effect of statistical uncertainties on the surface enrichment of early AGB stars (Martinet+2024a)

Non-correlated parameter uncertainties