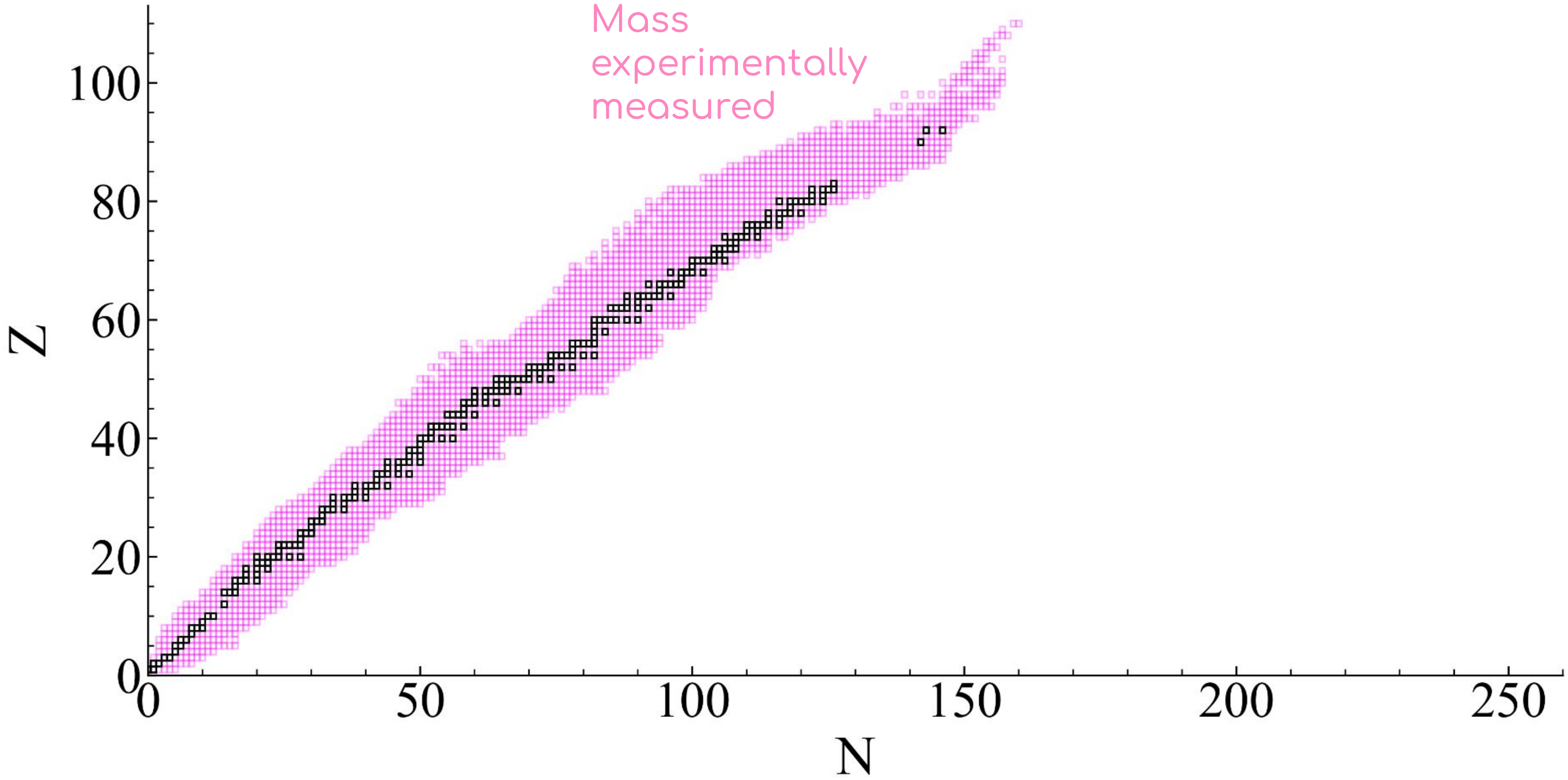
The impact of Systematic and Statistical Nuclear Uncertainties on the R-Process and I-Process Nucleosynthesis

Sébastien Martinet

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

Estimating Nuclear Uncertainties

Experimentally known masses vs r-process network needed



Estimating Nuclear Uncertainties

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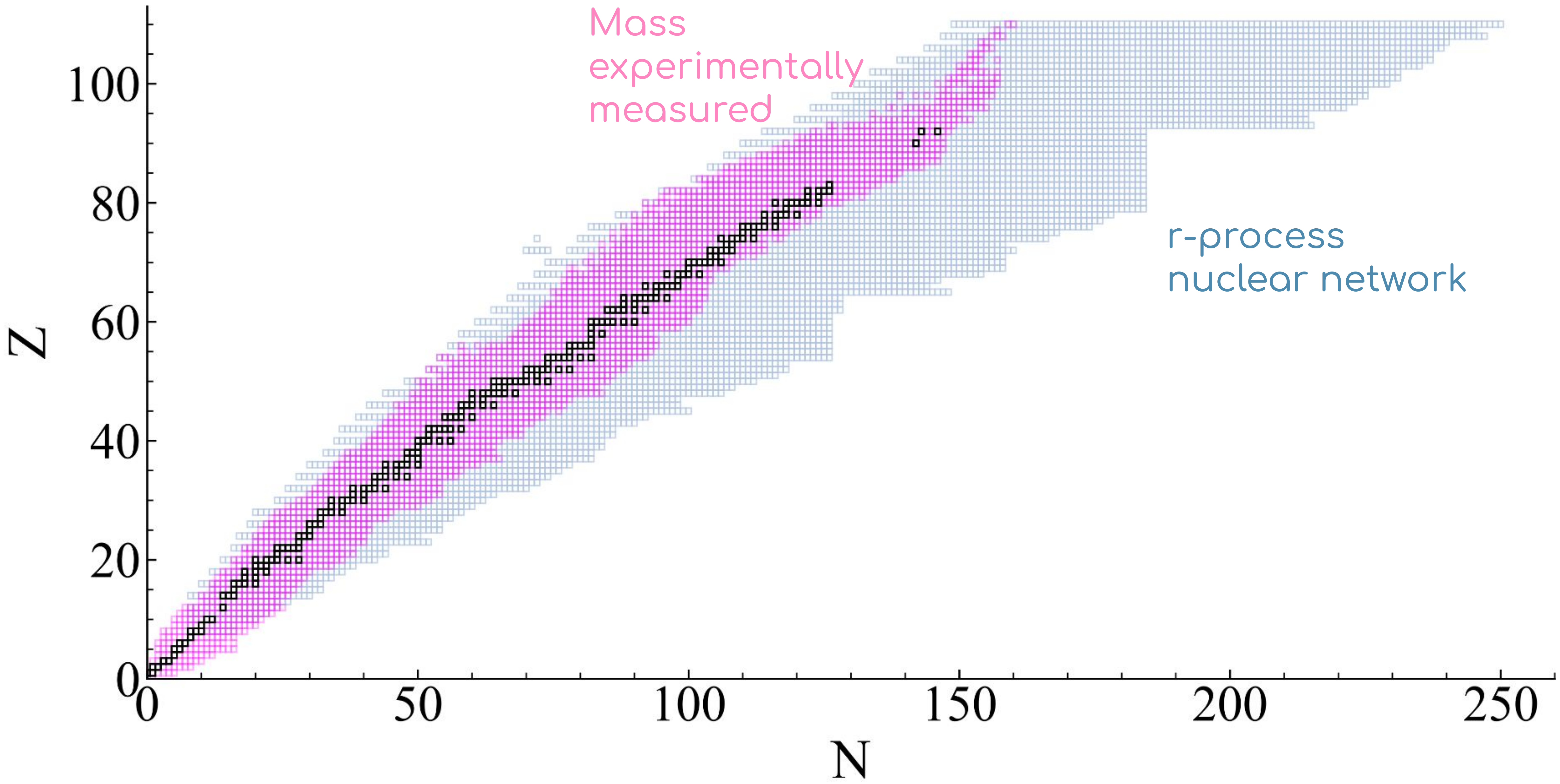

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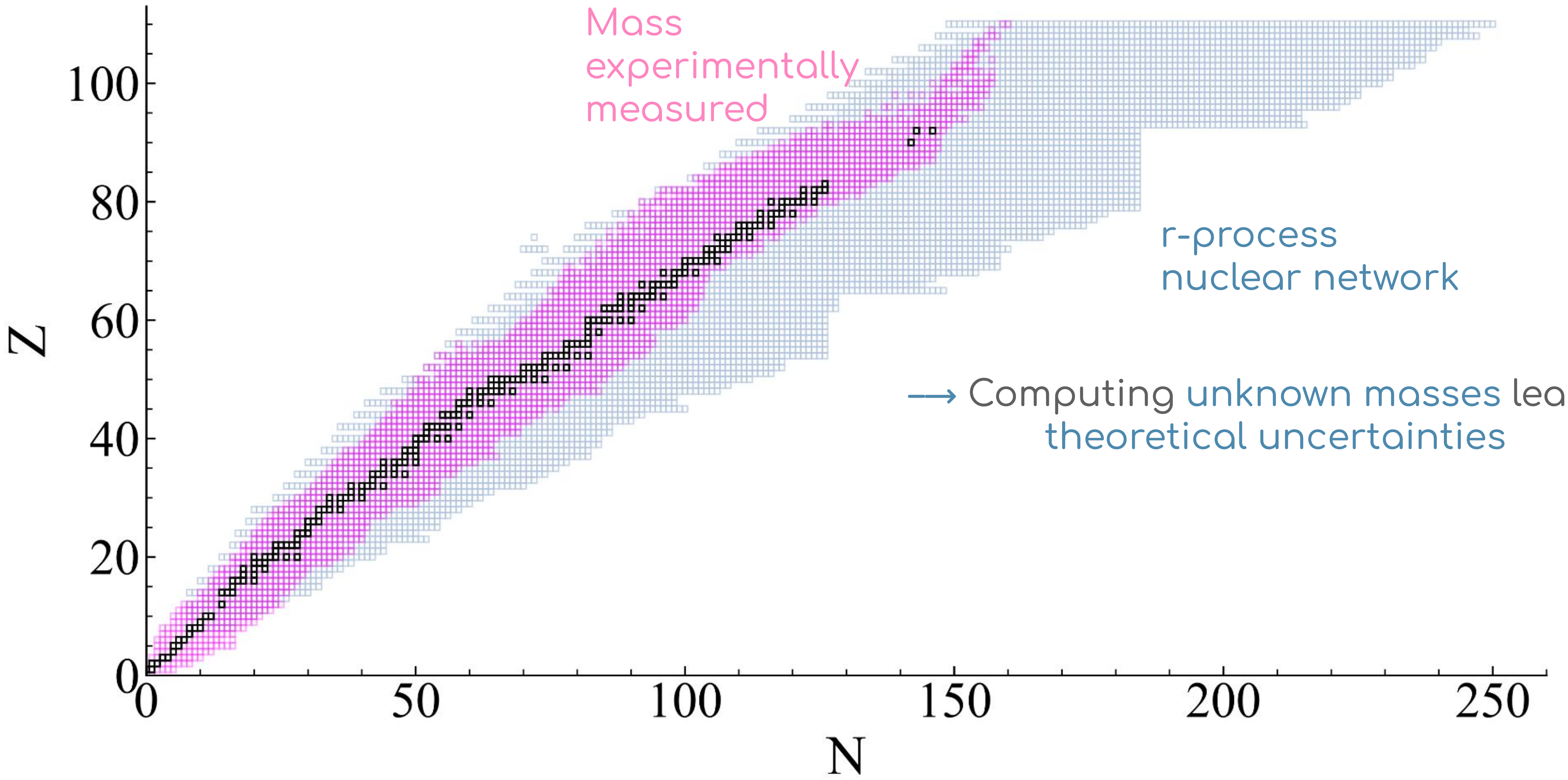
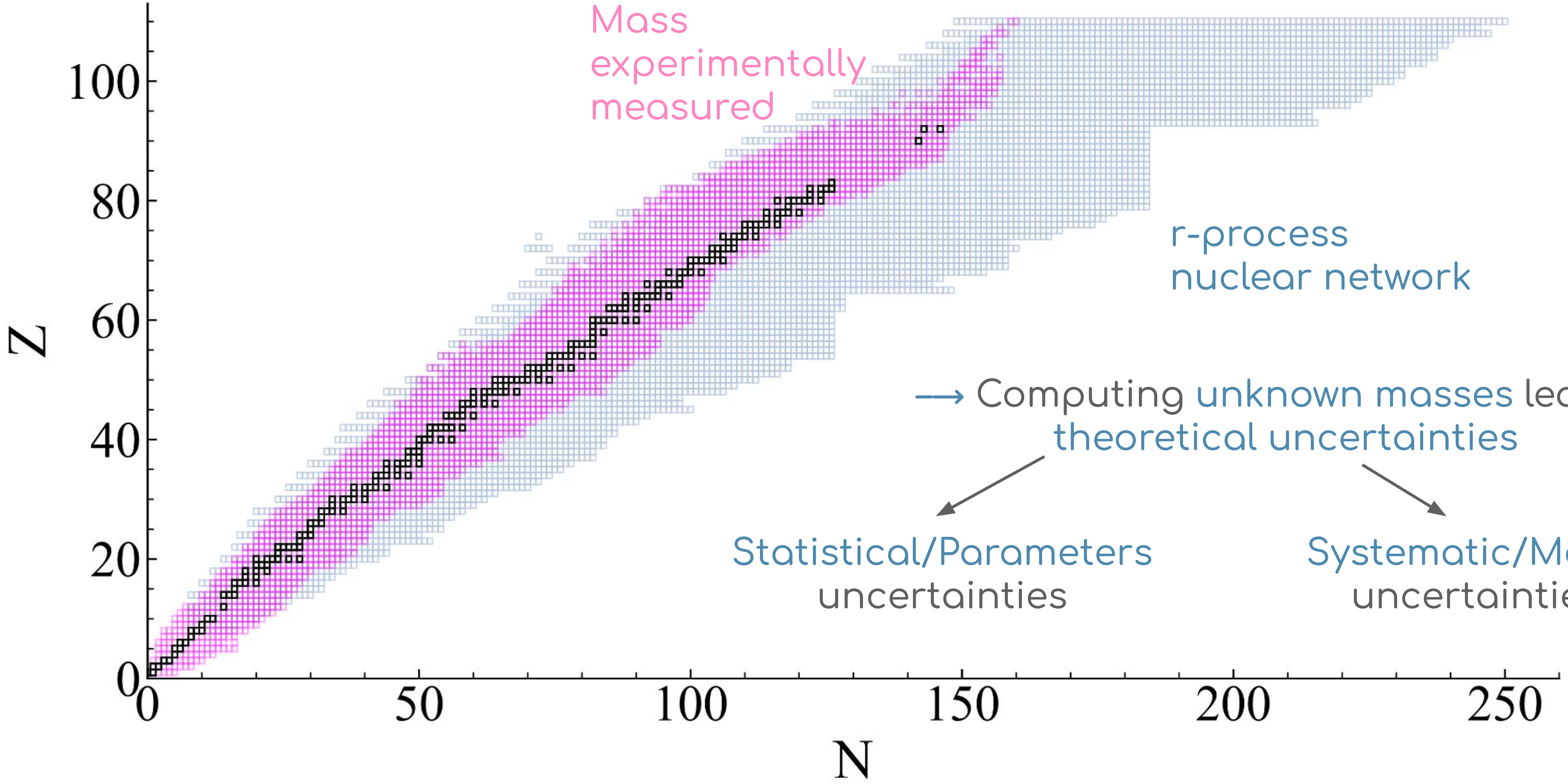


→ Computing unknown masses lead to theoretical uncertainties

Estimating Nuclear Uncertainties

Experimentally known masses vs r-process network needed



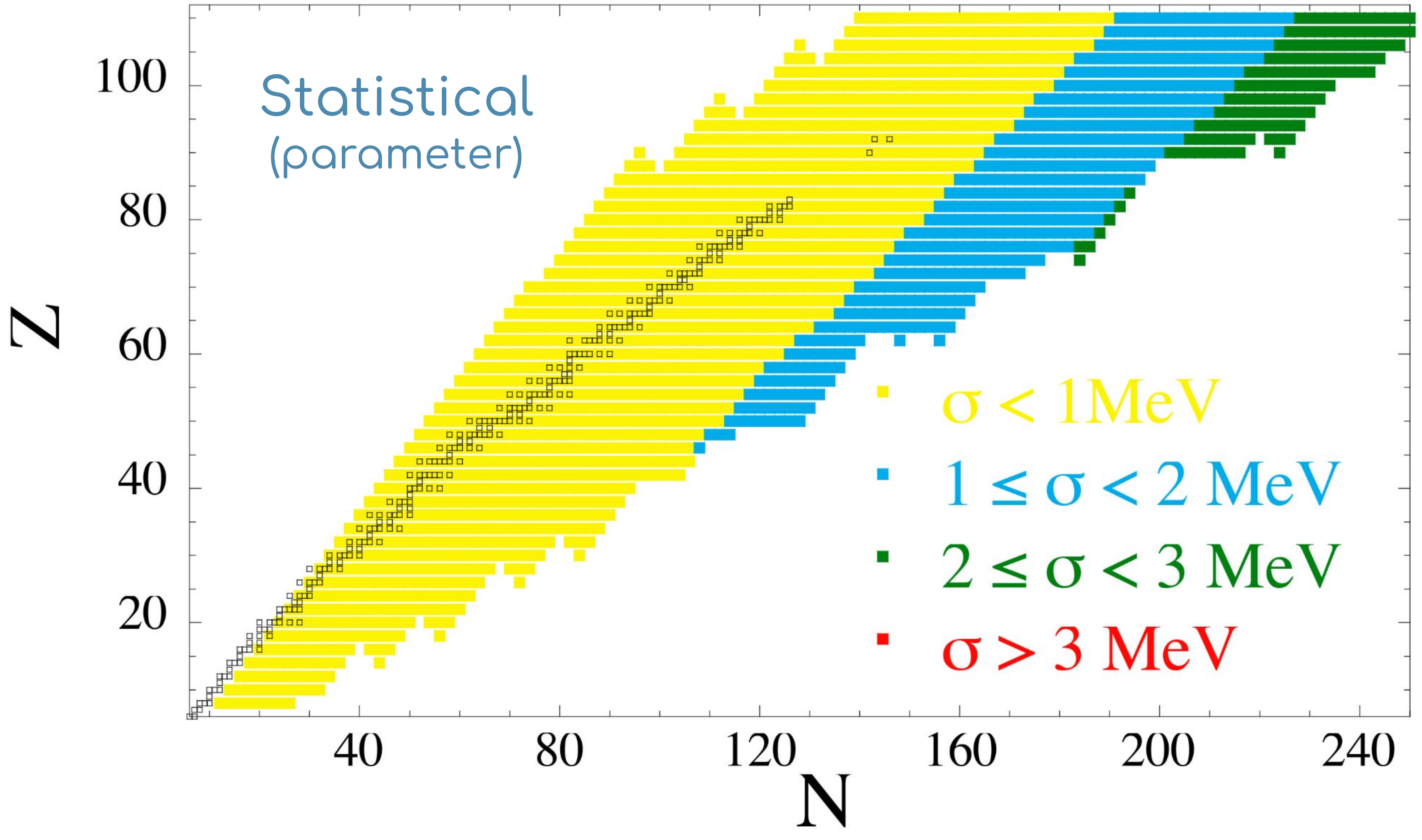
→ Computing unknown masses lead to theoretical uncertainties

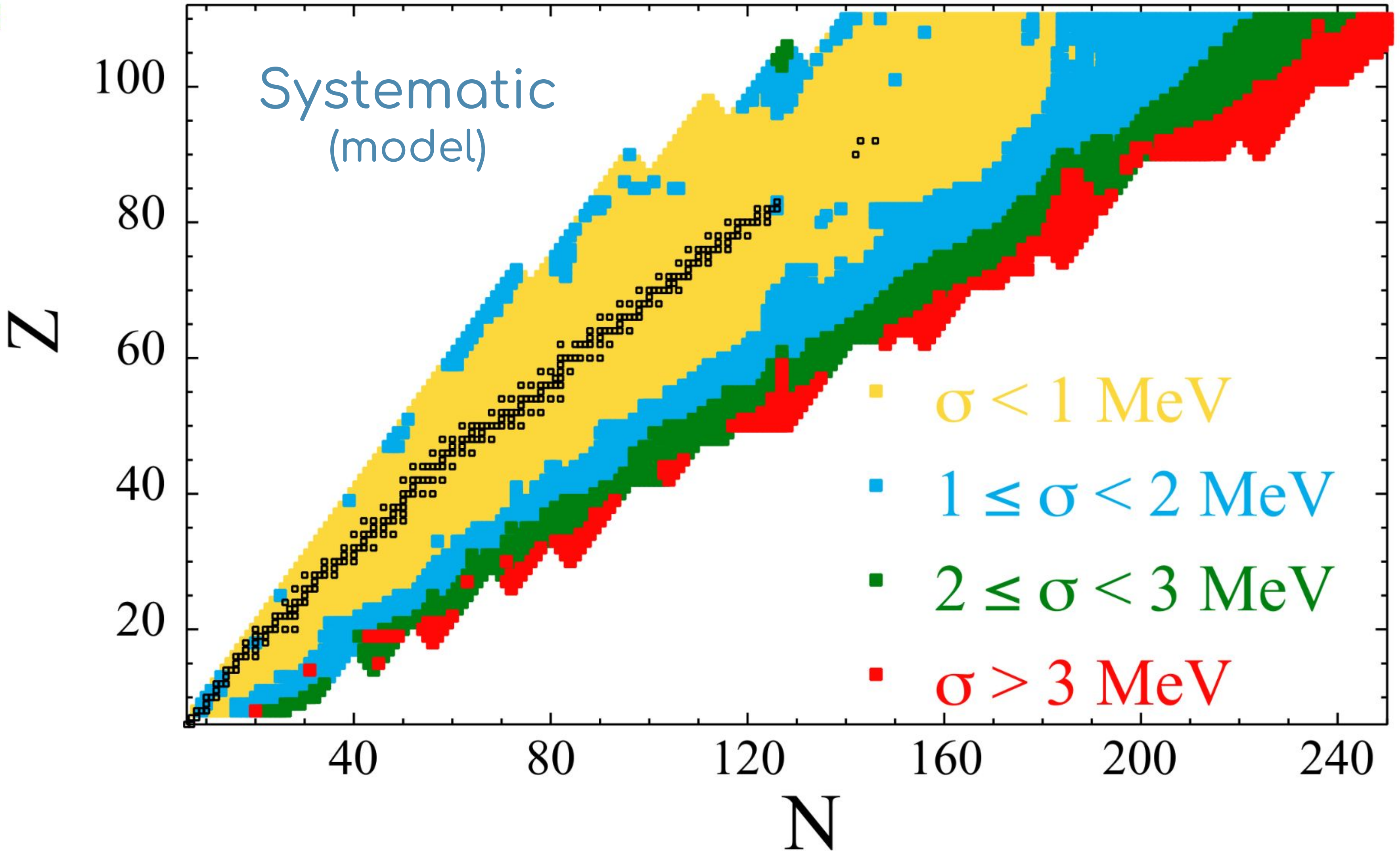
Statistical/Parameters uncertainties

Systematic/Model uncertainties

Estimating Nuclear Uncertainties

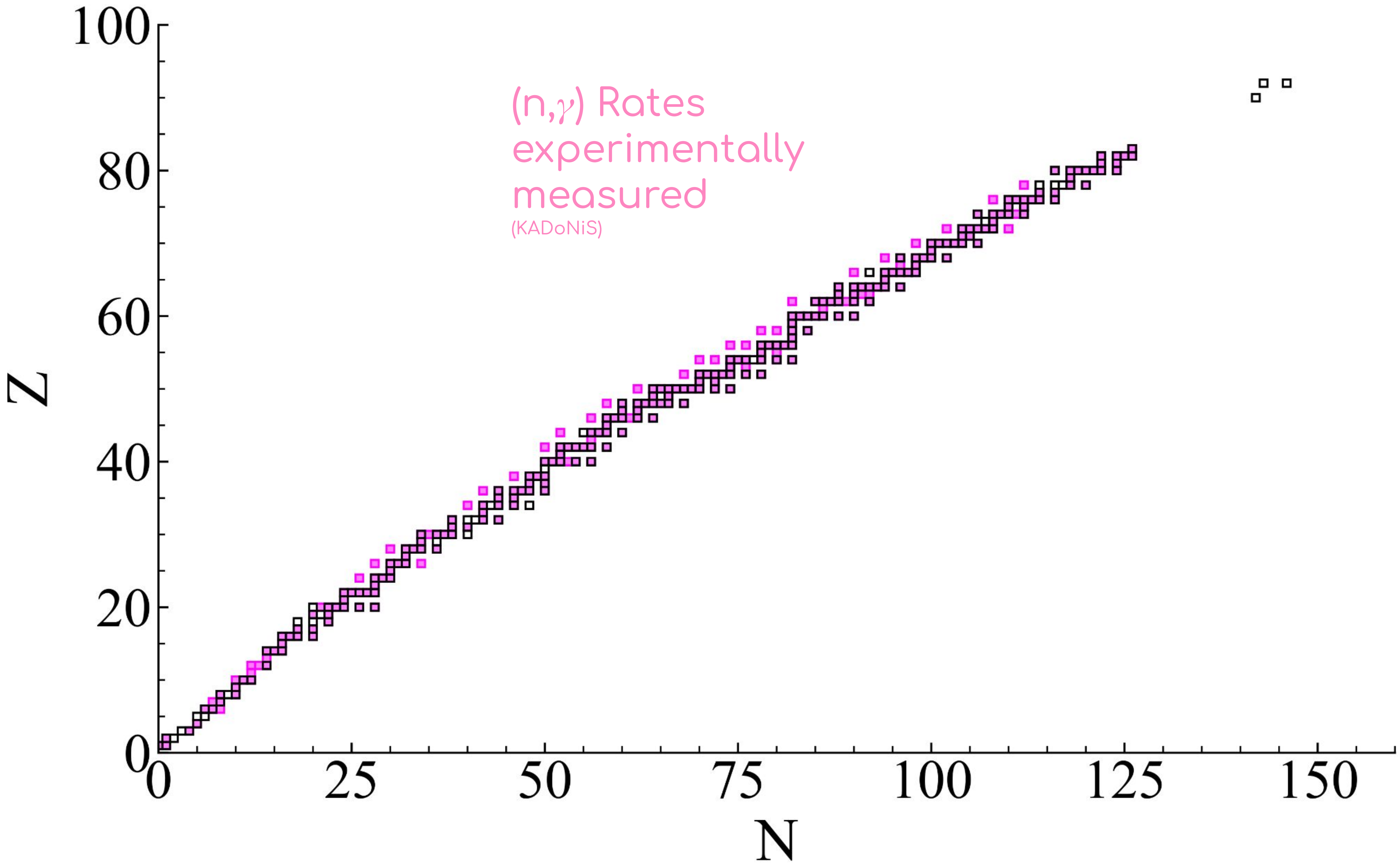
Overestimating uncertainties





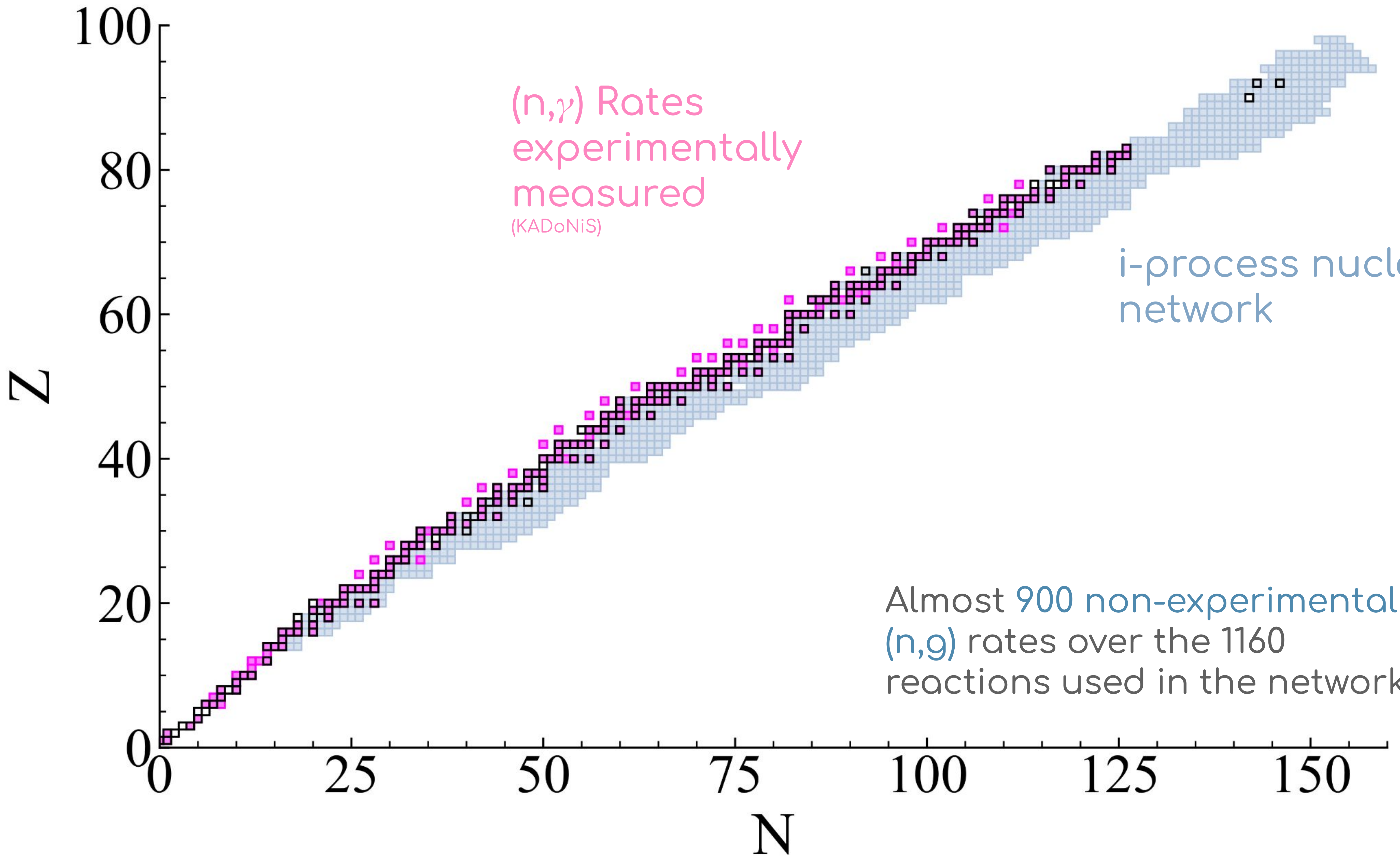
Estimating Nuclear Uncertainties

I-process in early AGB phase



Estimating Nuclear Uncertainties

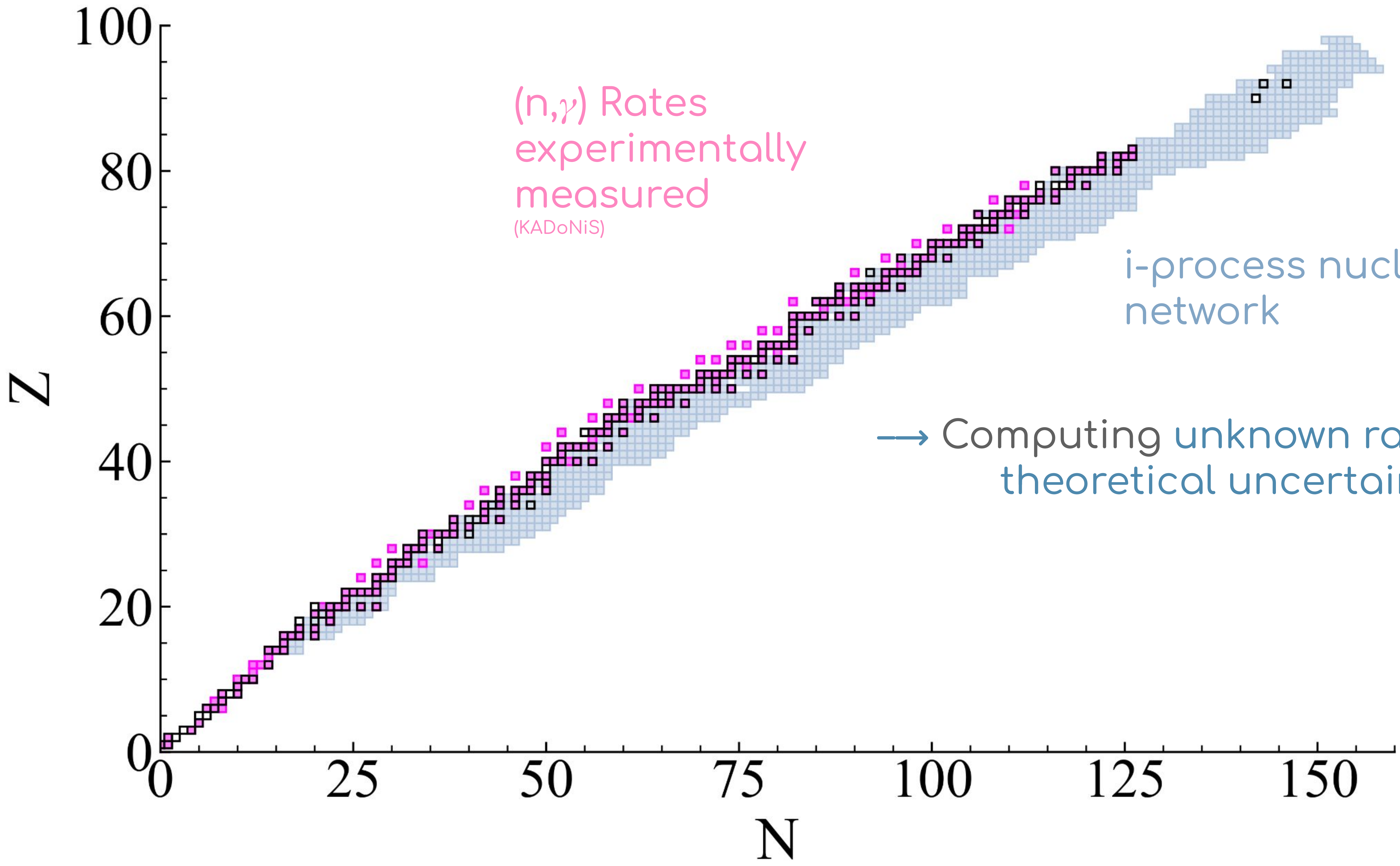
I-process in early AGB phase



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

Estimating Nuclear Uncertainties

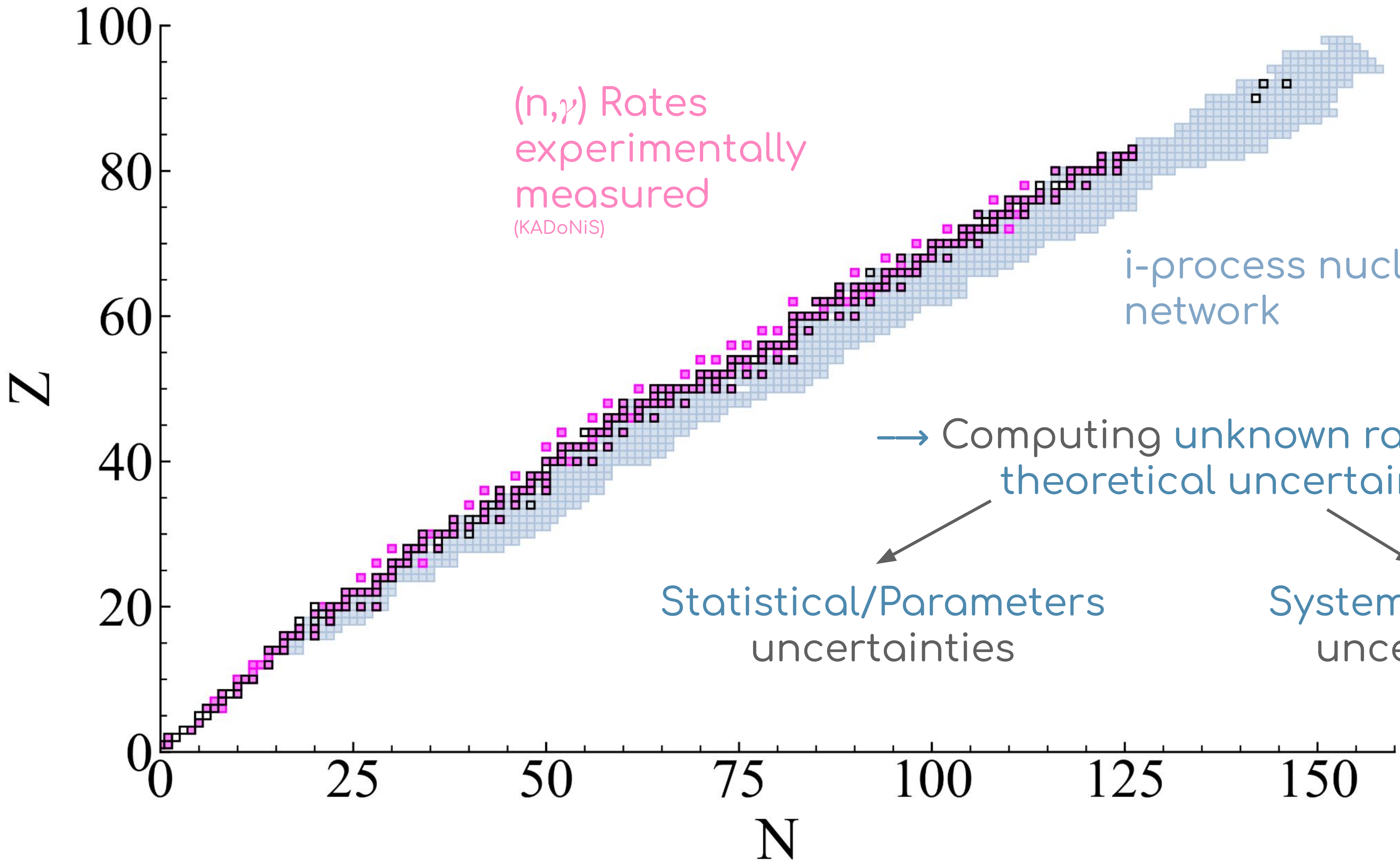
I-process in early AGB phase



⟶ Computing unknown rates lead to theoretical uncertainties

Estimating Nuclear Uncertainties

I-process in early AGB phase



⟶ Computing unknown rates lead to theoretical uncertainties

Statistical/Parameters uncertainties

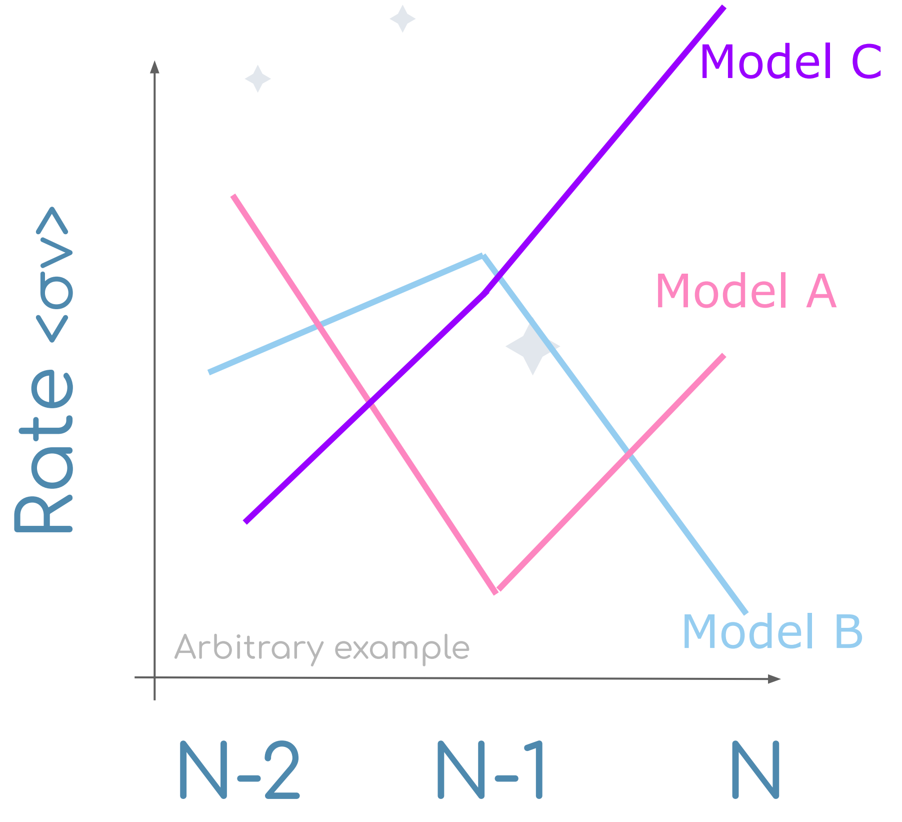
Systematic/Model uncertainties

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

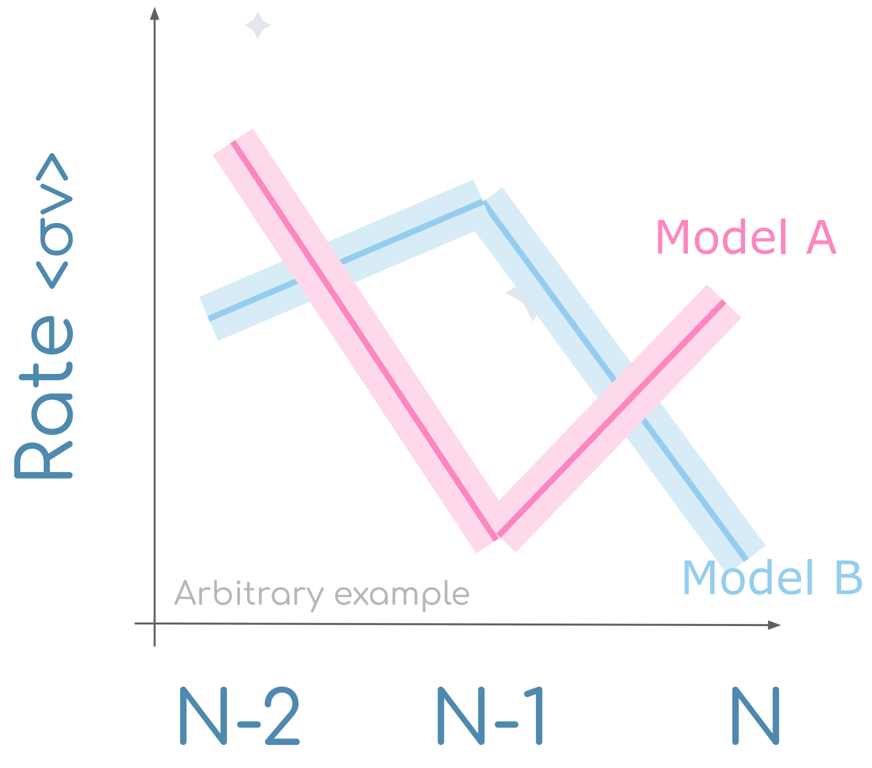
Overestimating uncertainties

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.

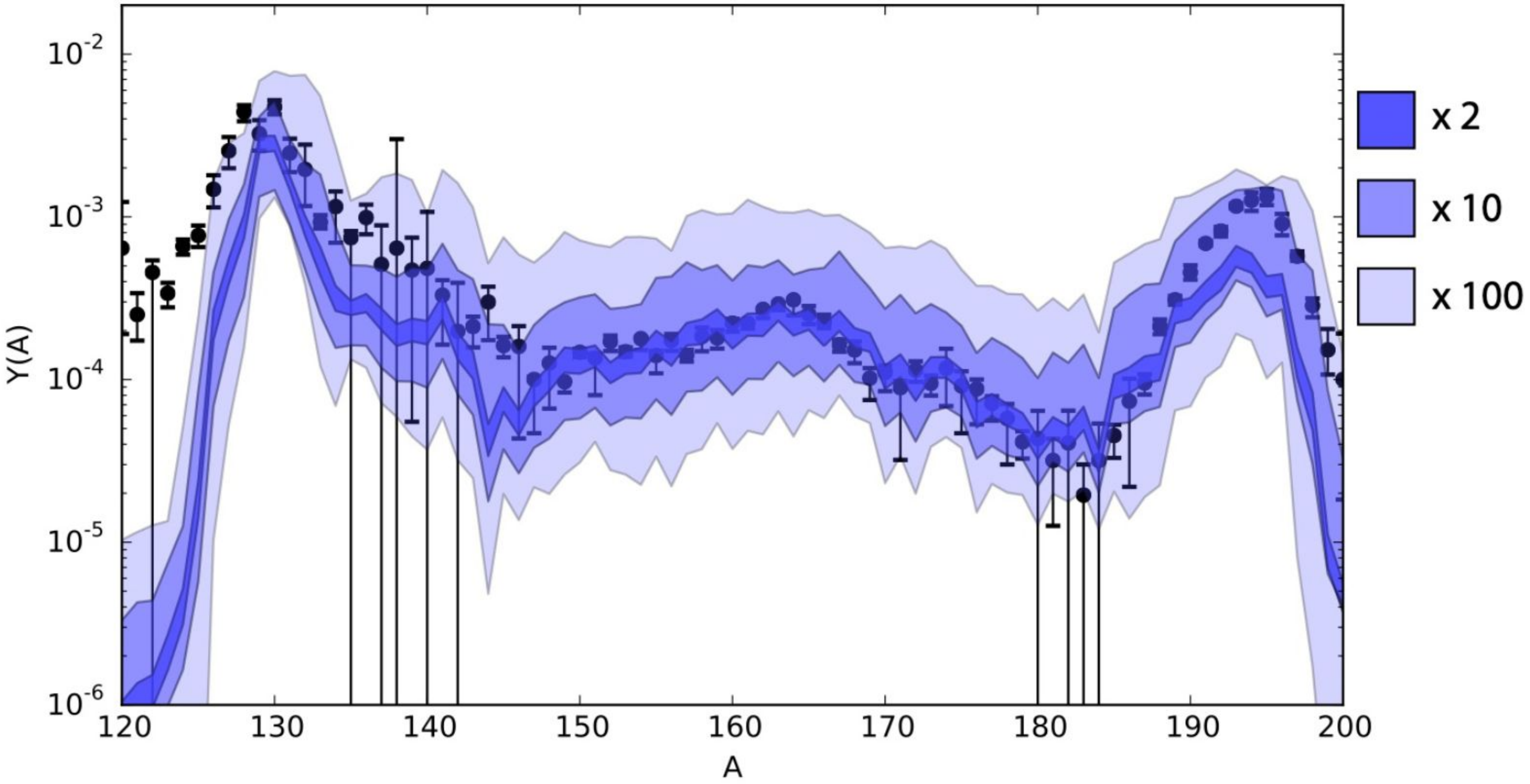
→ Parameter uncertainties are <u>non-correlated</u>

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

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

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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

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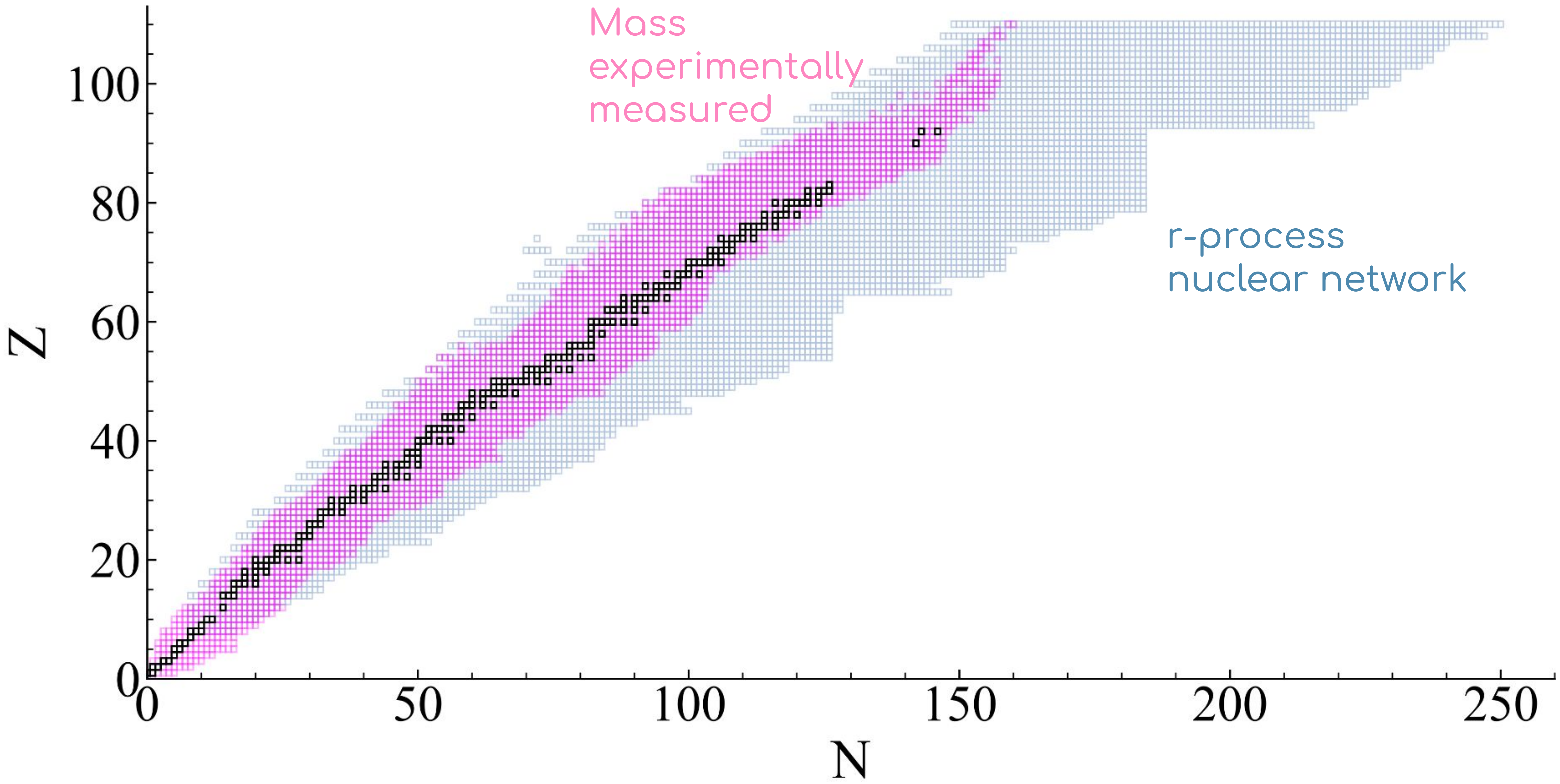
↔

Anchor values to experimental uncertainties

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

Determining coherently parameter uncertainties

Parameters uncertainties obtained from the BFMC method



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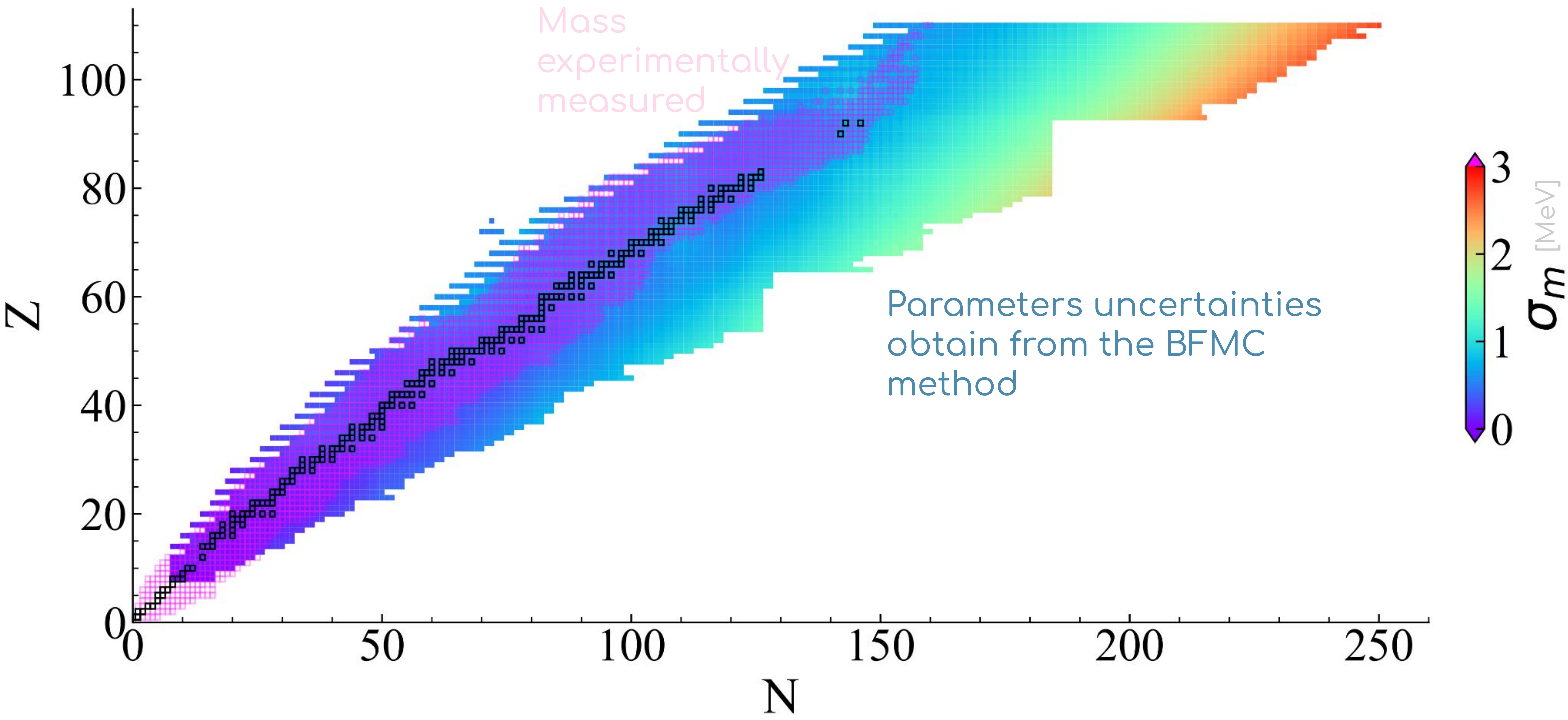

Estimating Nuclear Uncertainties

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

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4 parameters

4 parameters

Statistical/Parameter Uncertainties
(Non-correlated)

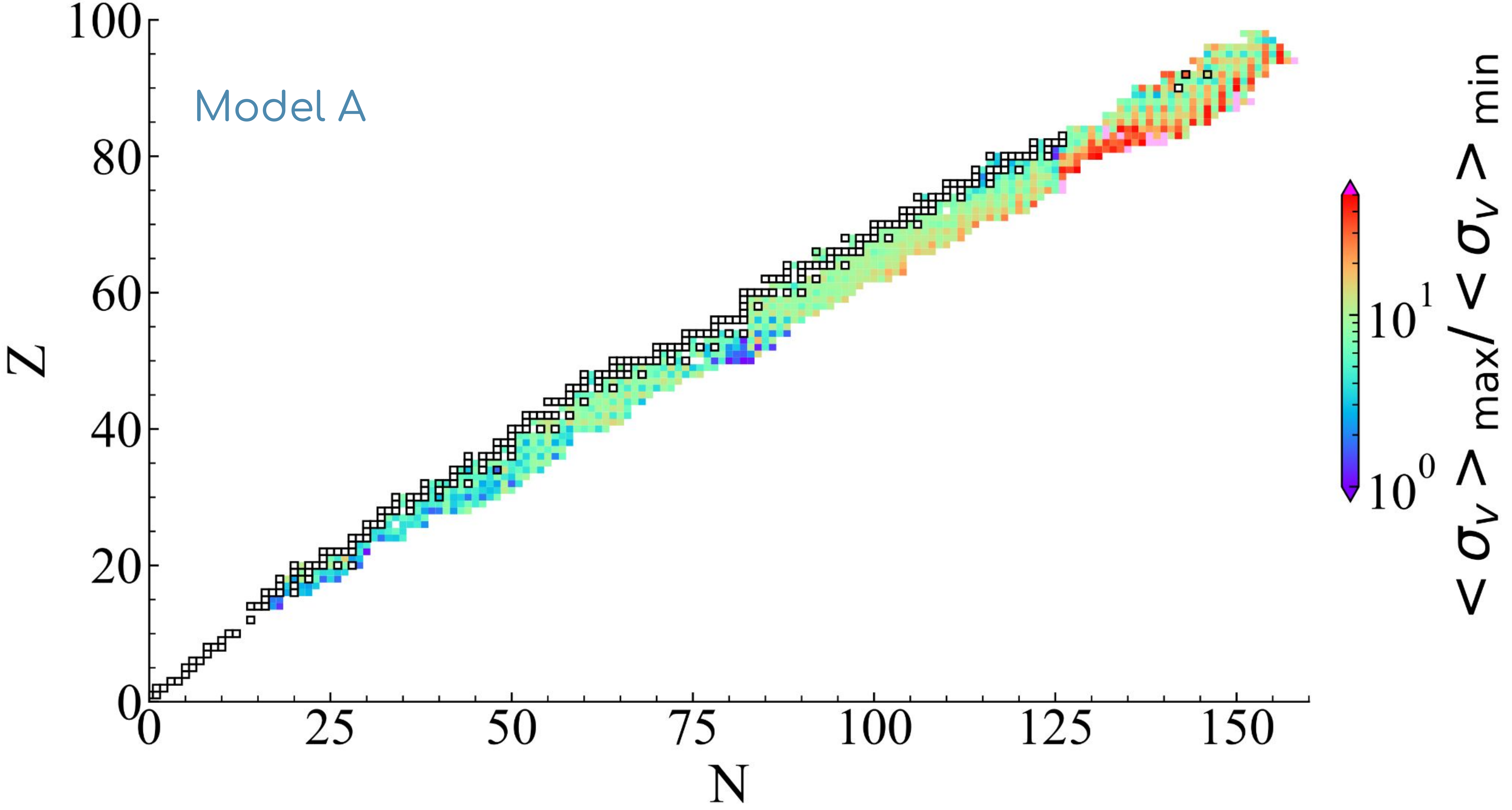
2 parameters affecting nuclear level densities

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



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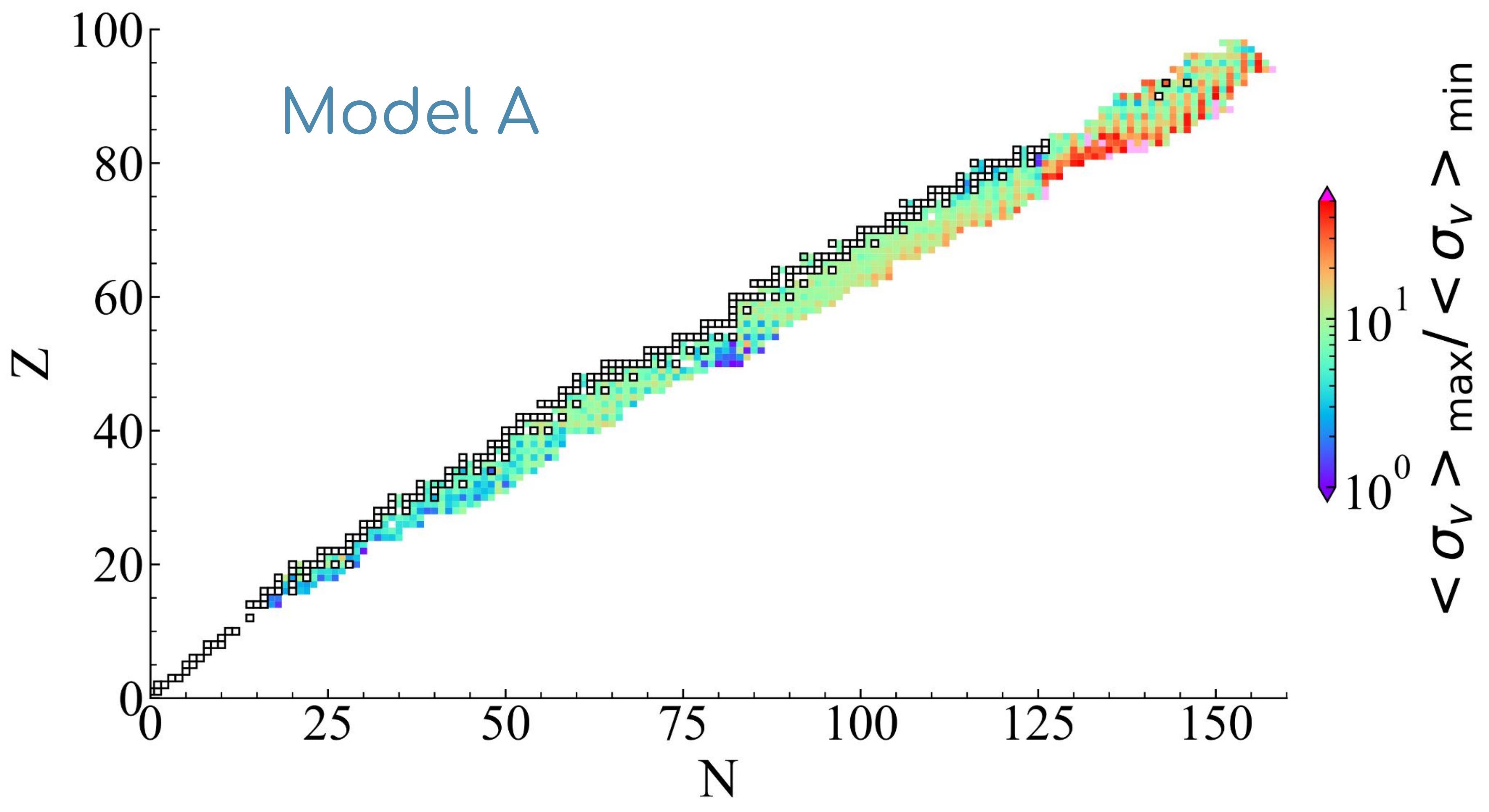
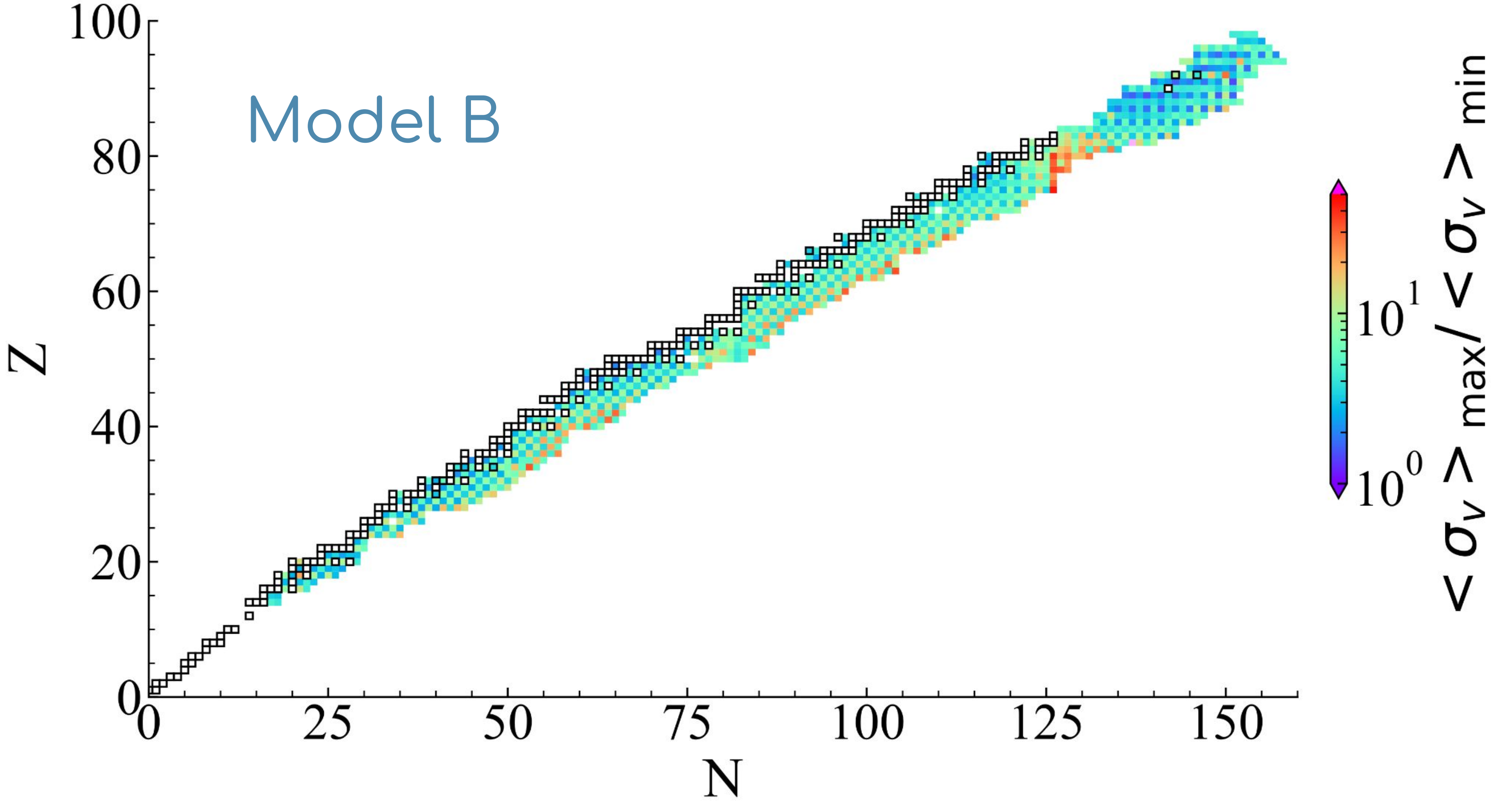




Impact of Nuclear Uncertainties on the i-process in AGB Stars

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

STAREVOL code (Siess et al. 2006)

→ i-process nucleosynthesis

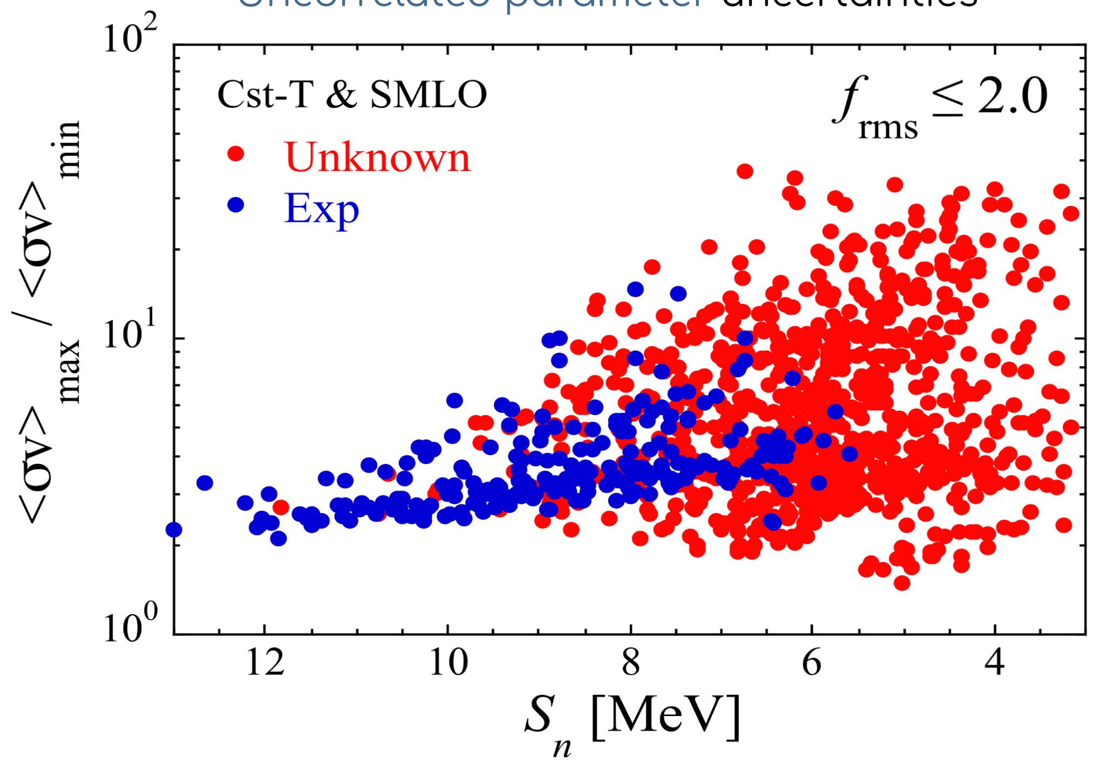
1 Msol at [Fe/H]=-2.5

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) Si31(n,g)	2) P32(n,g)	3) Si32(n,g)	....	862) 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

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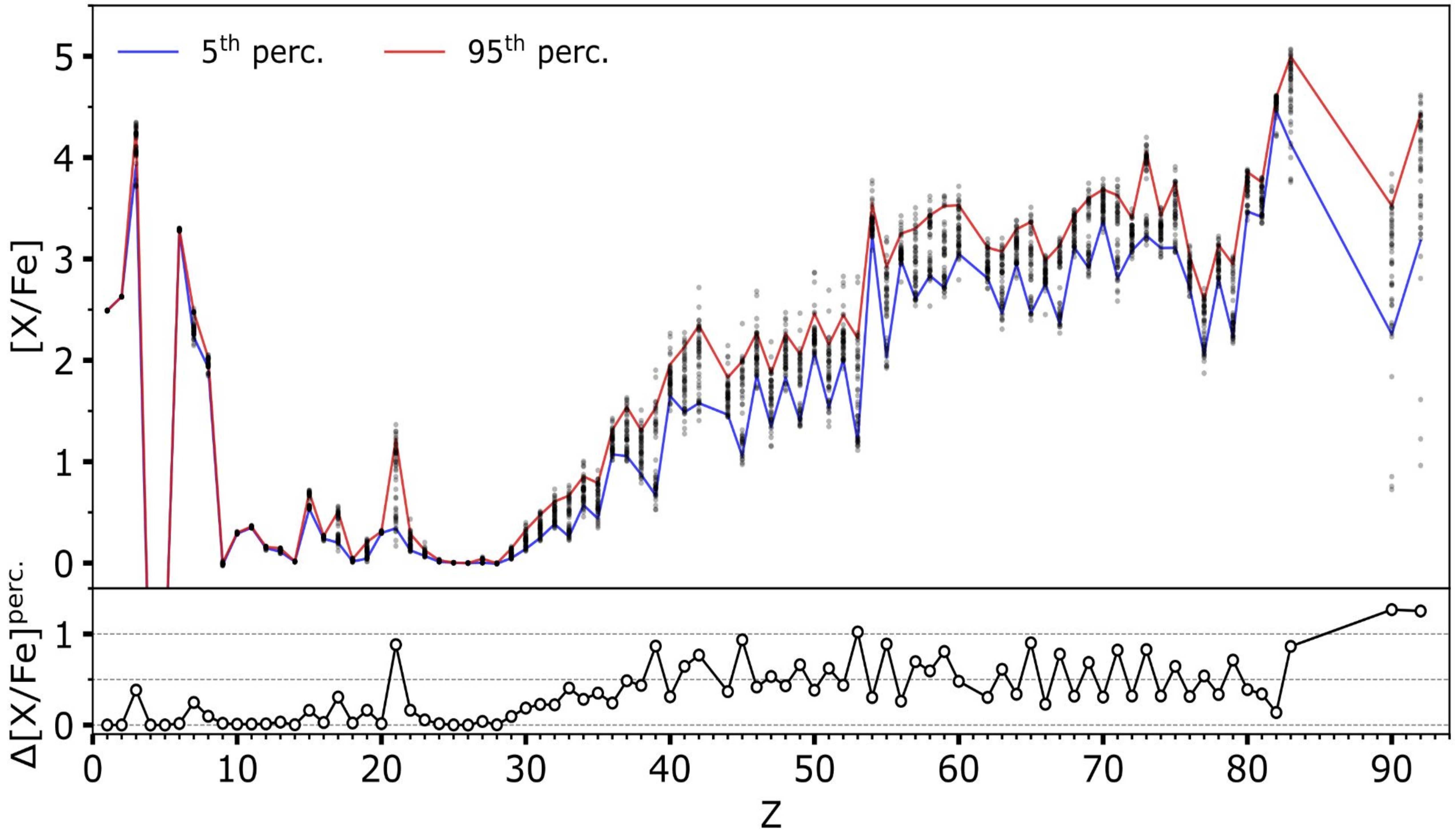
Non-correlated parameter uncertainties



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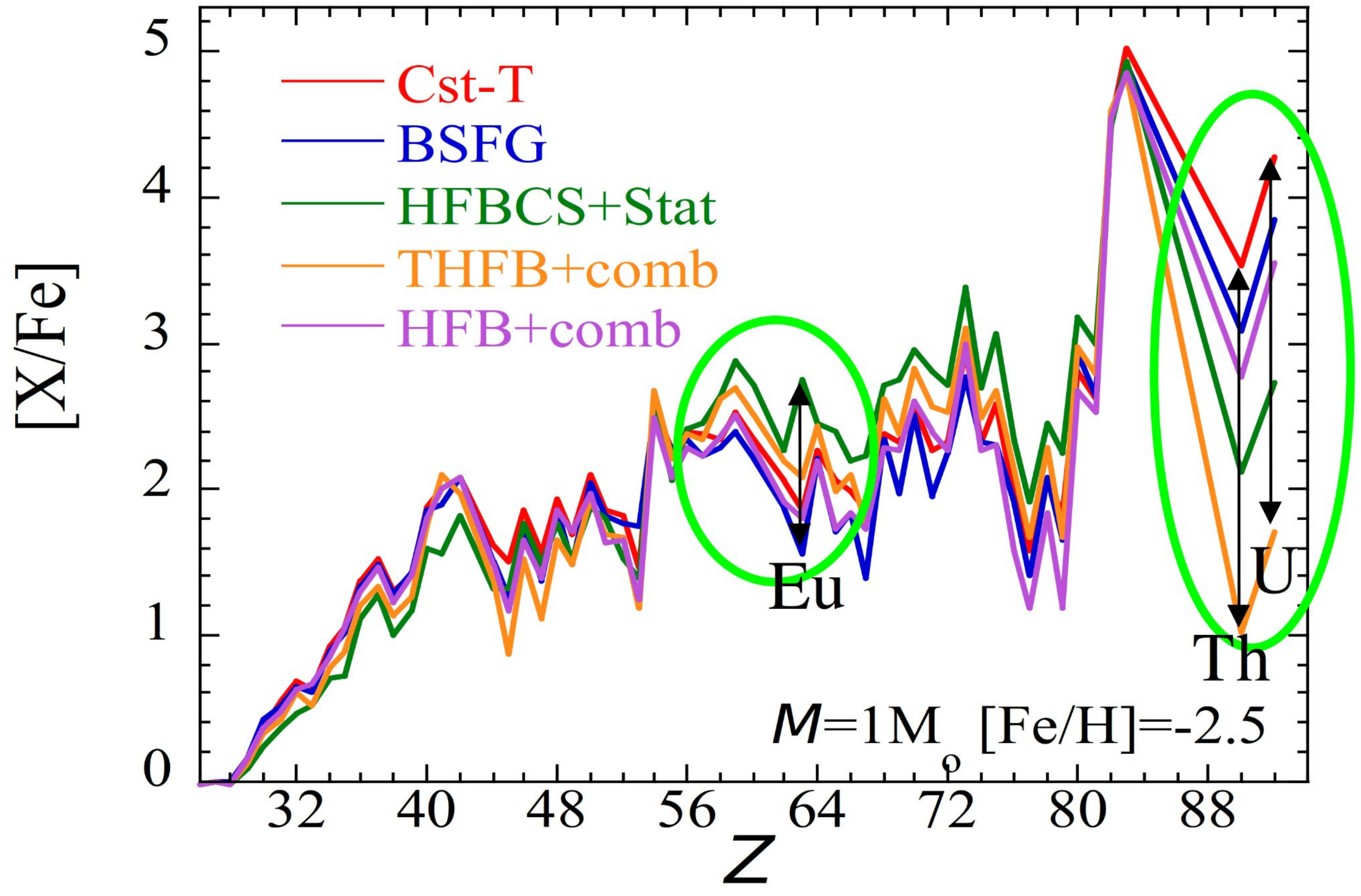
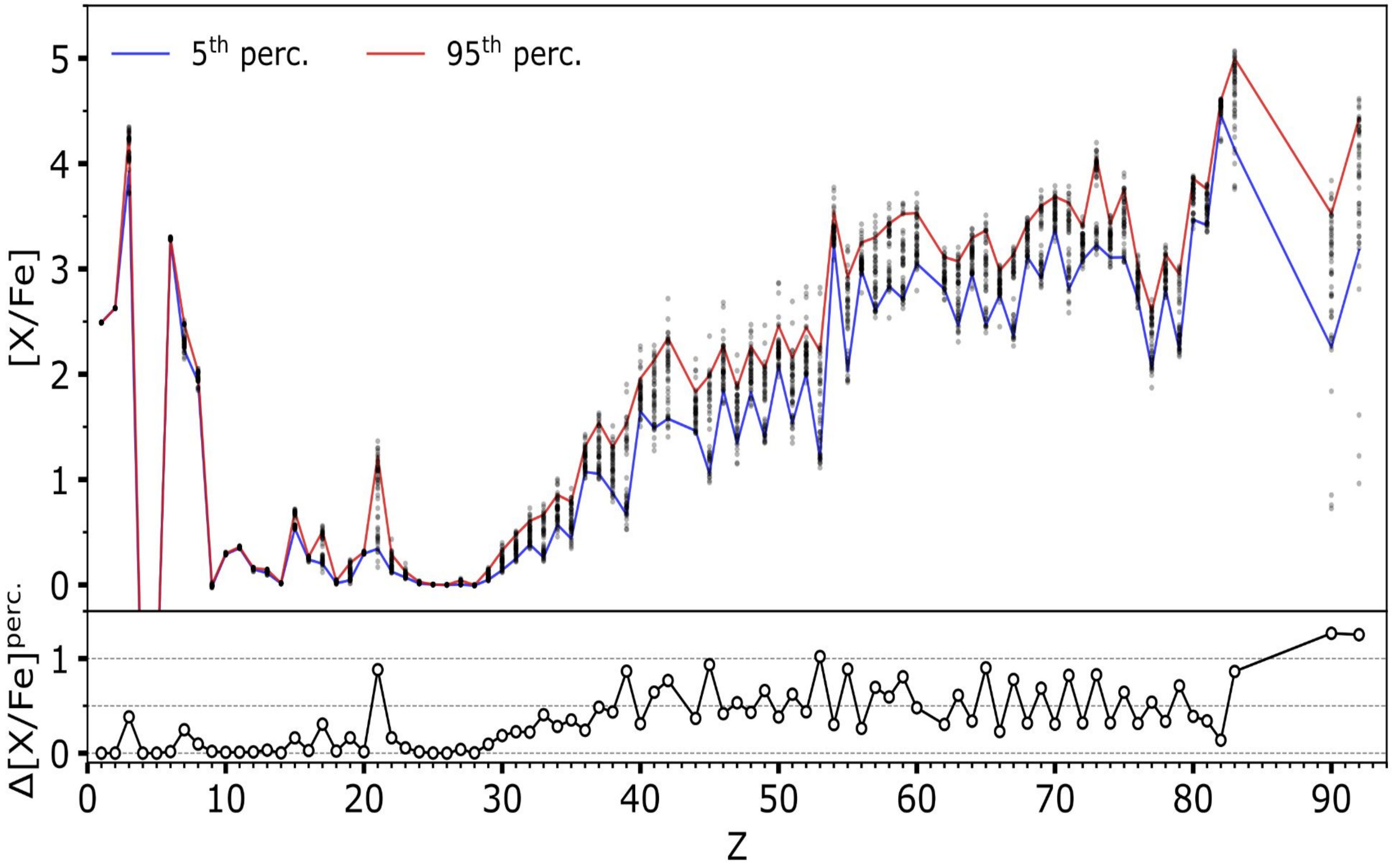
Correlated model uncertainties



Non-correlated parameter uncertainties



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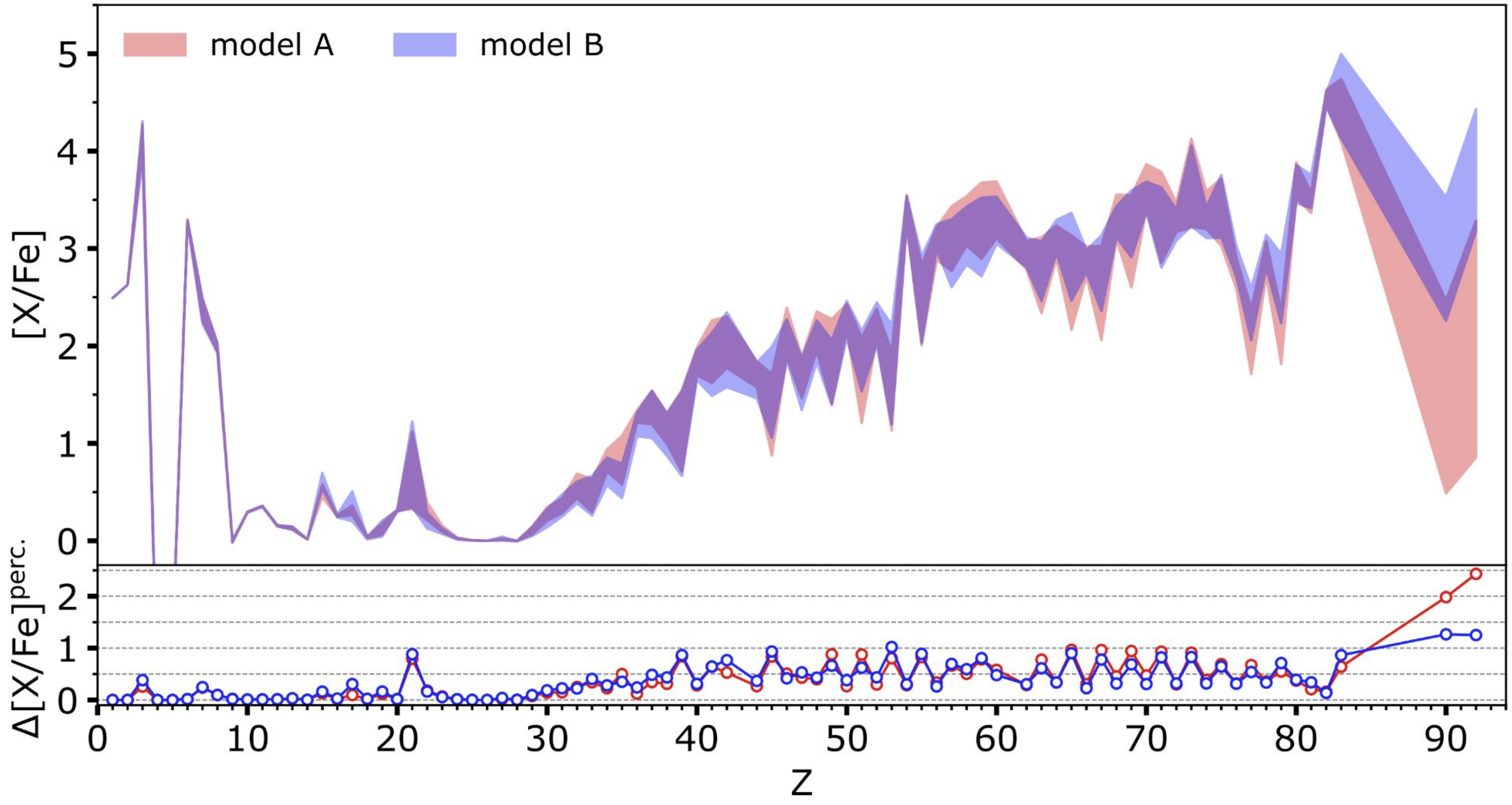
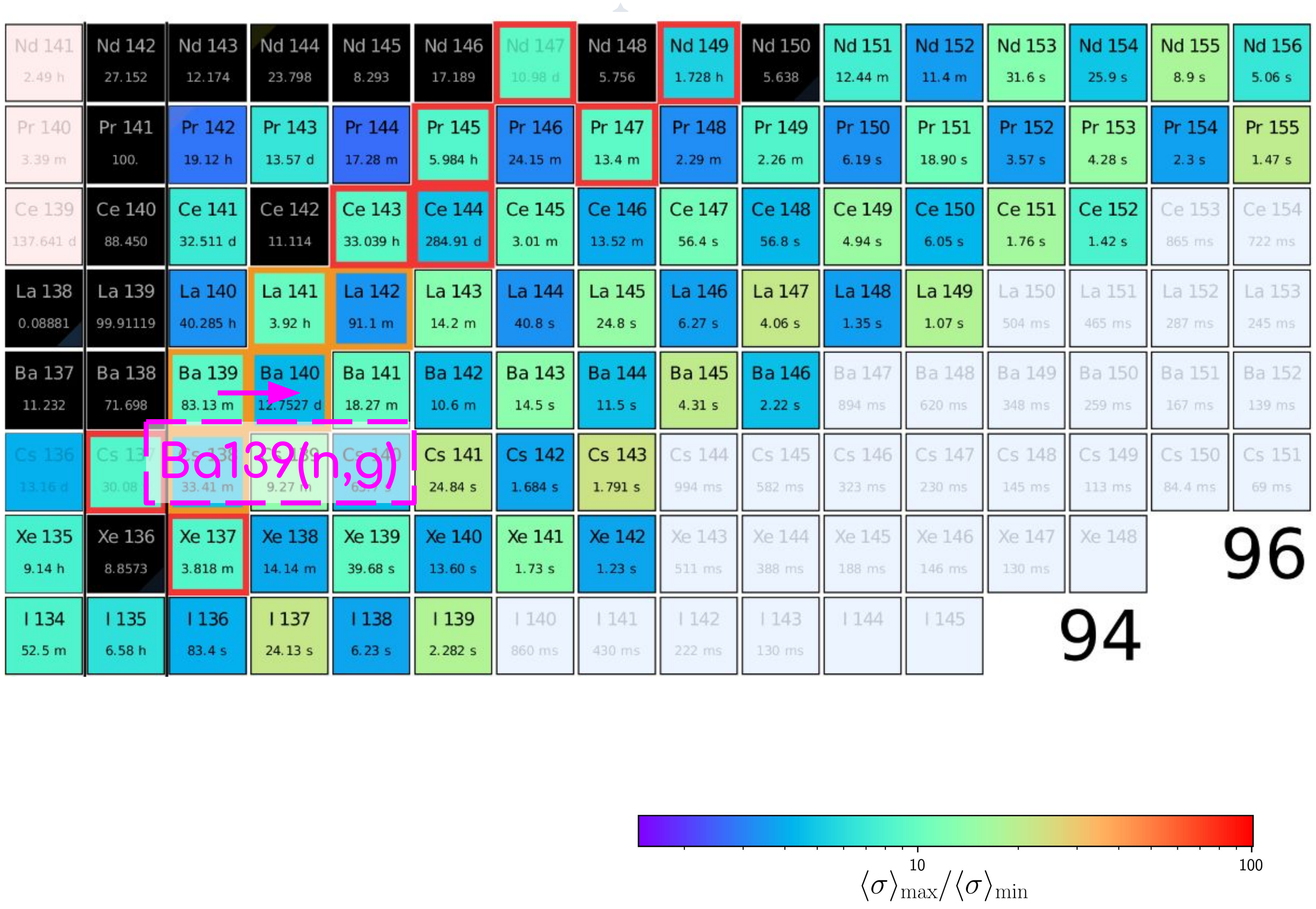


Impact of Nuclear Uncertainties on the i-process in AGB Stars

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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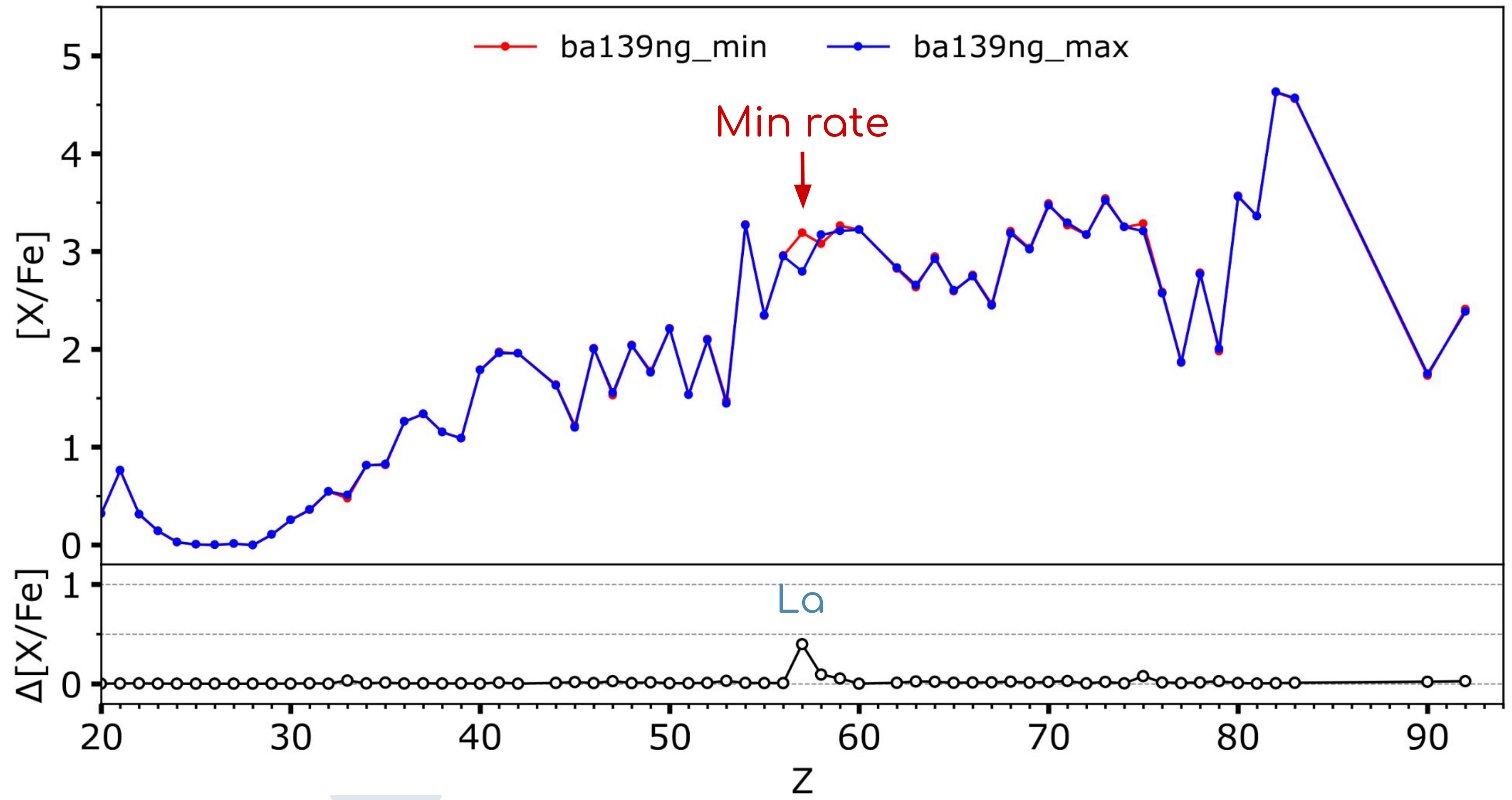

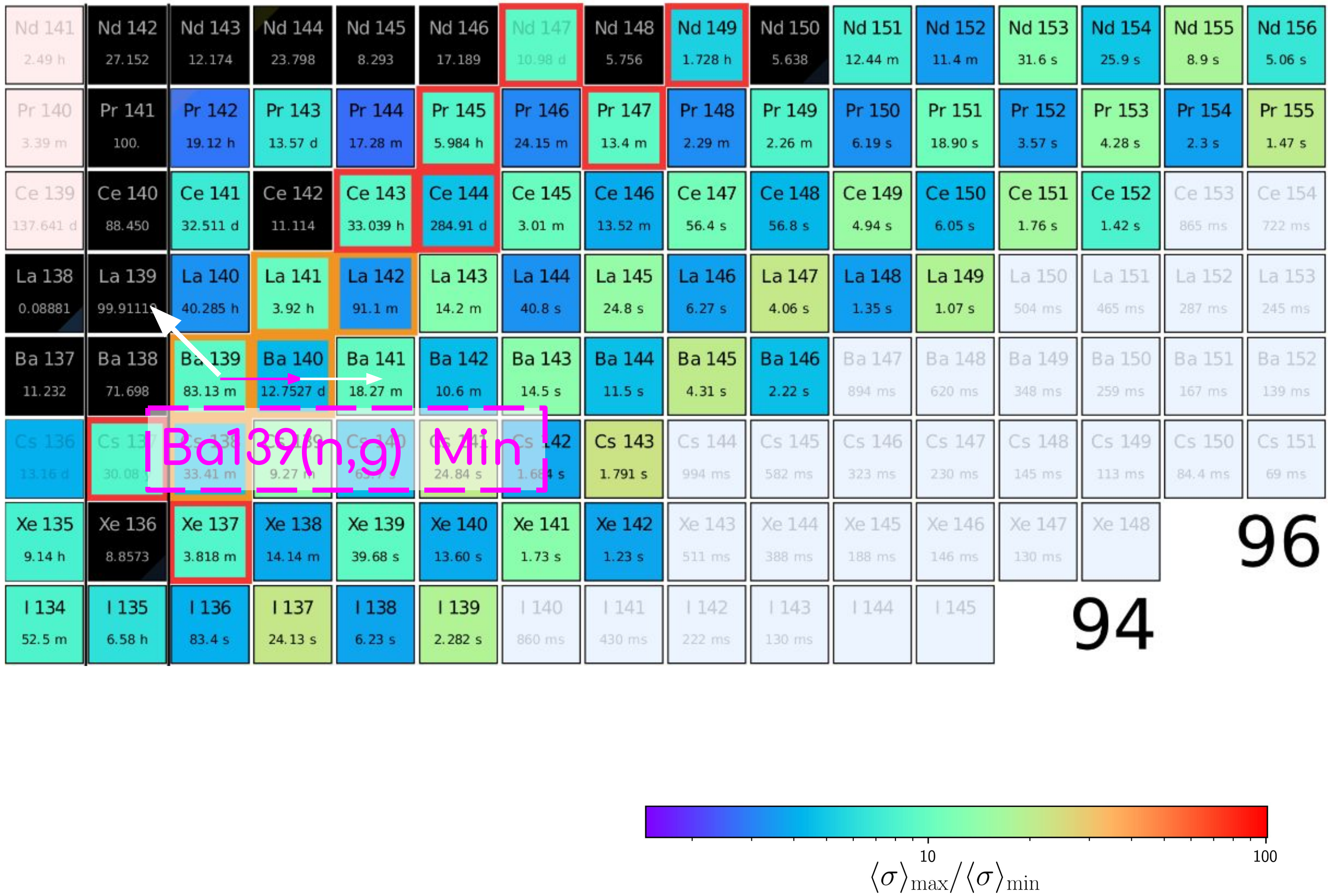

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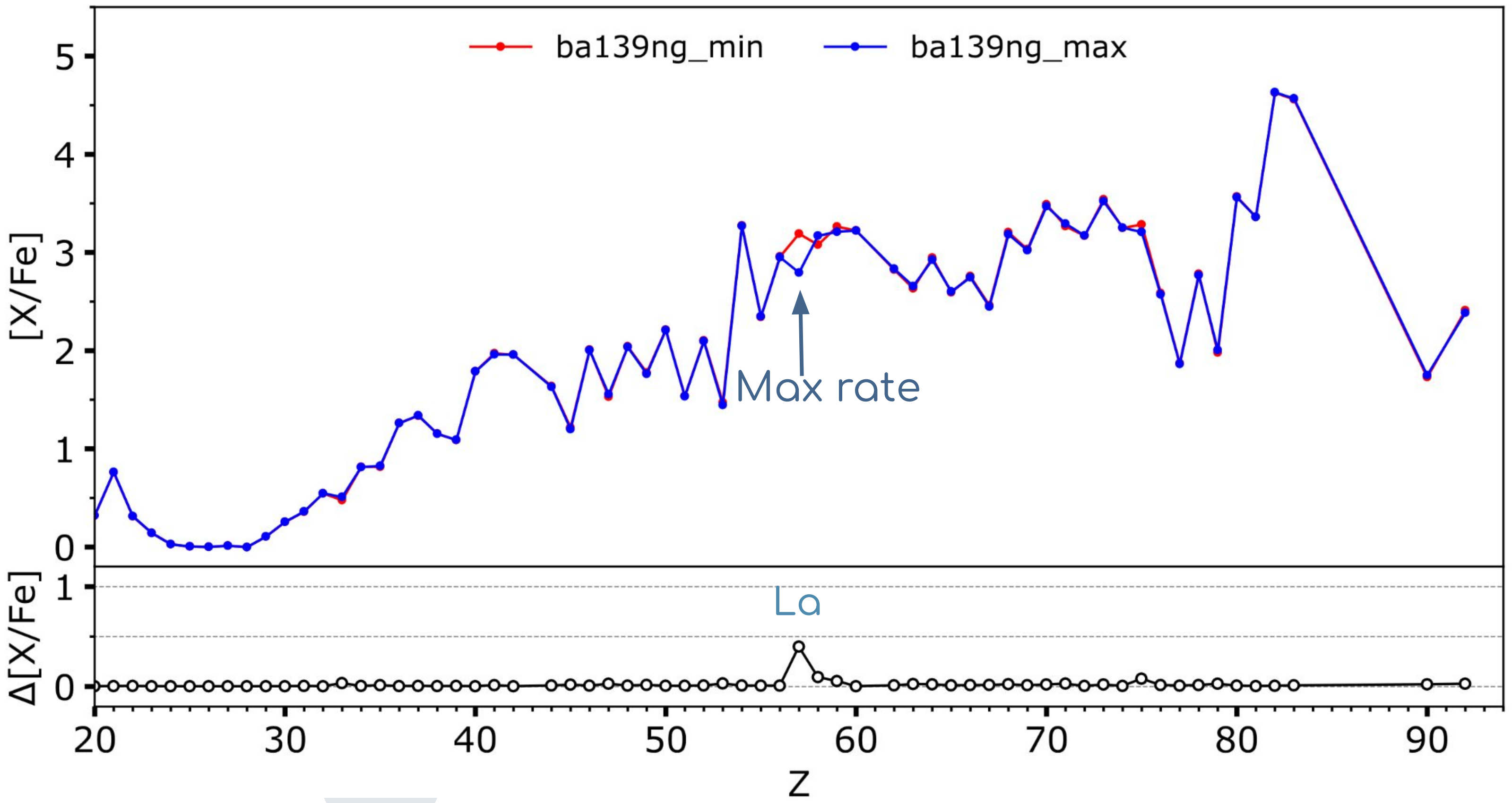

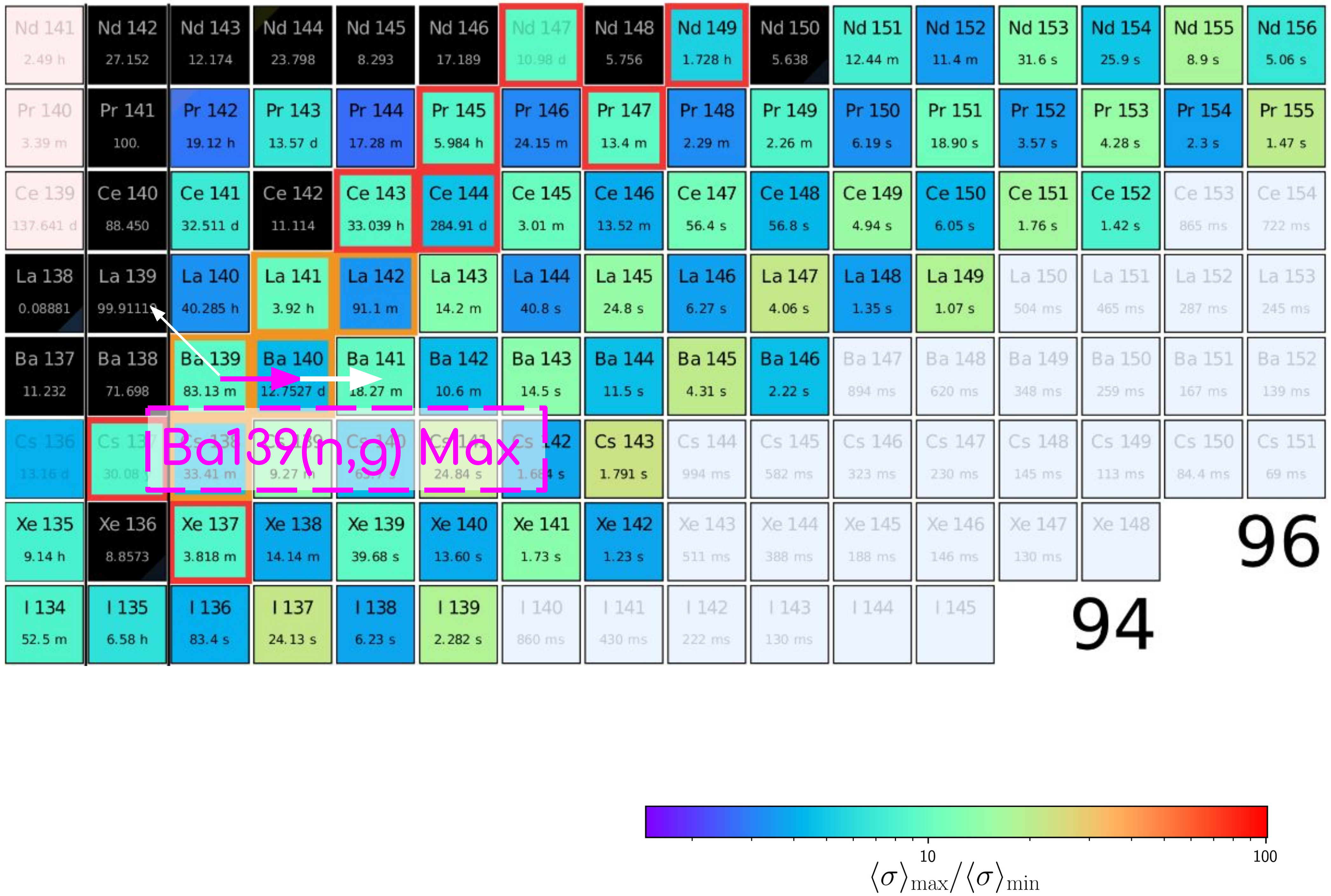

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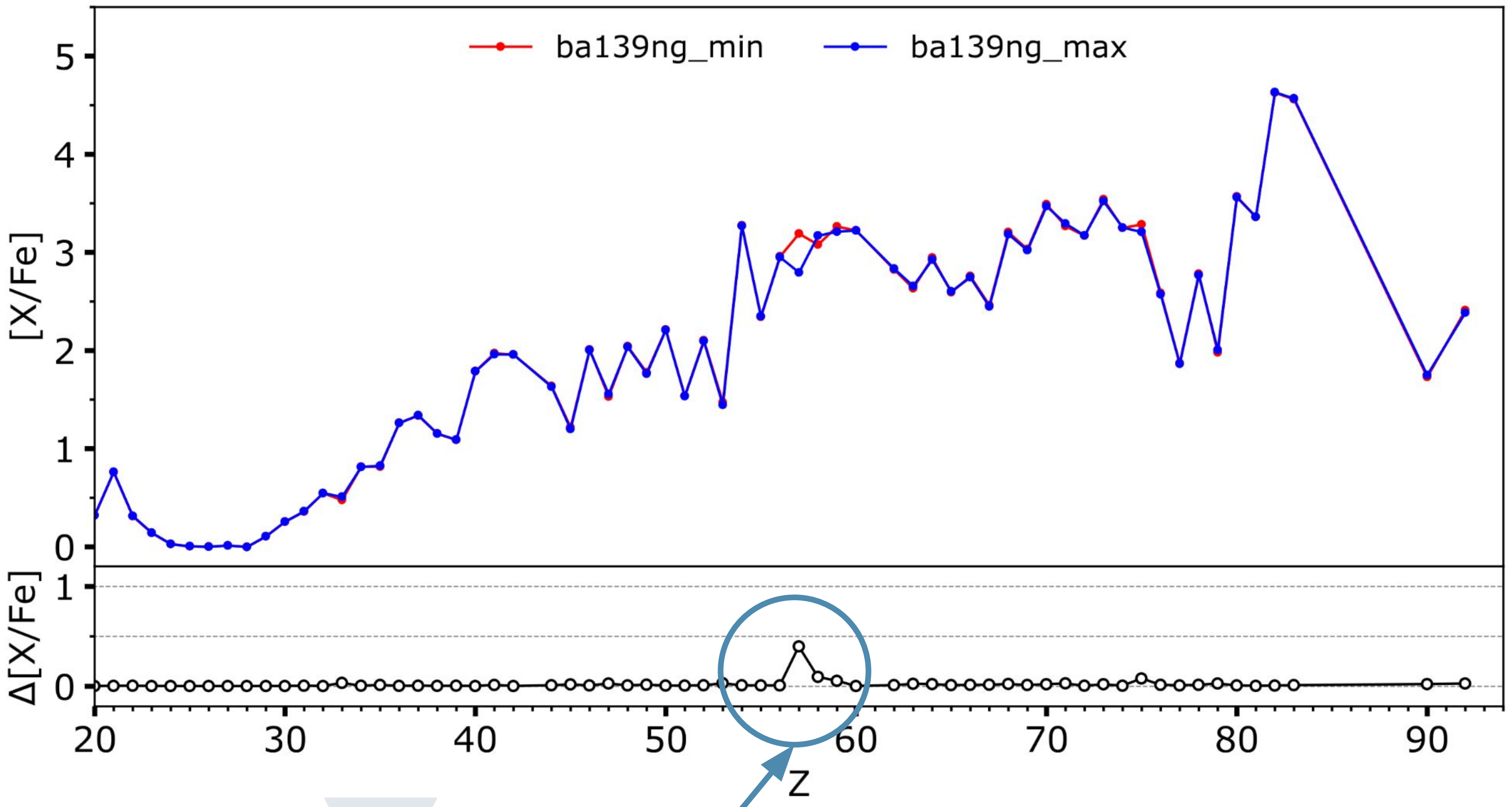

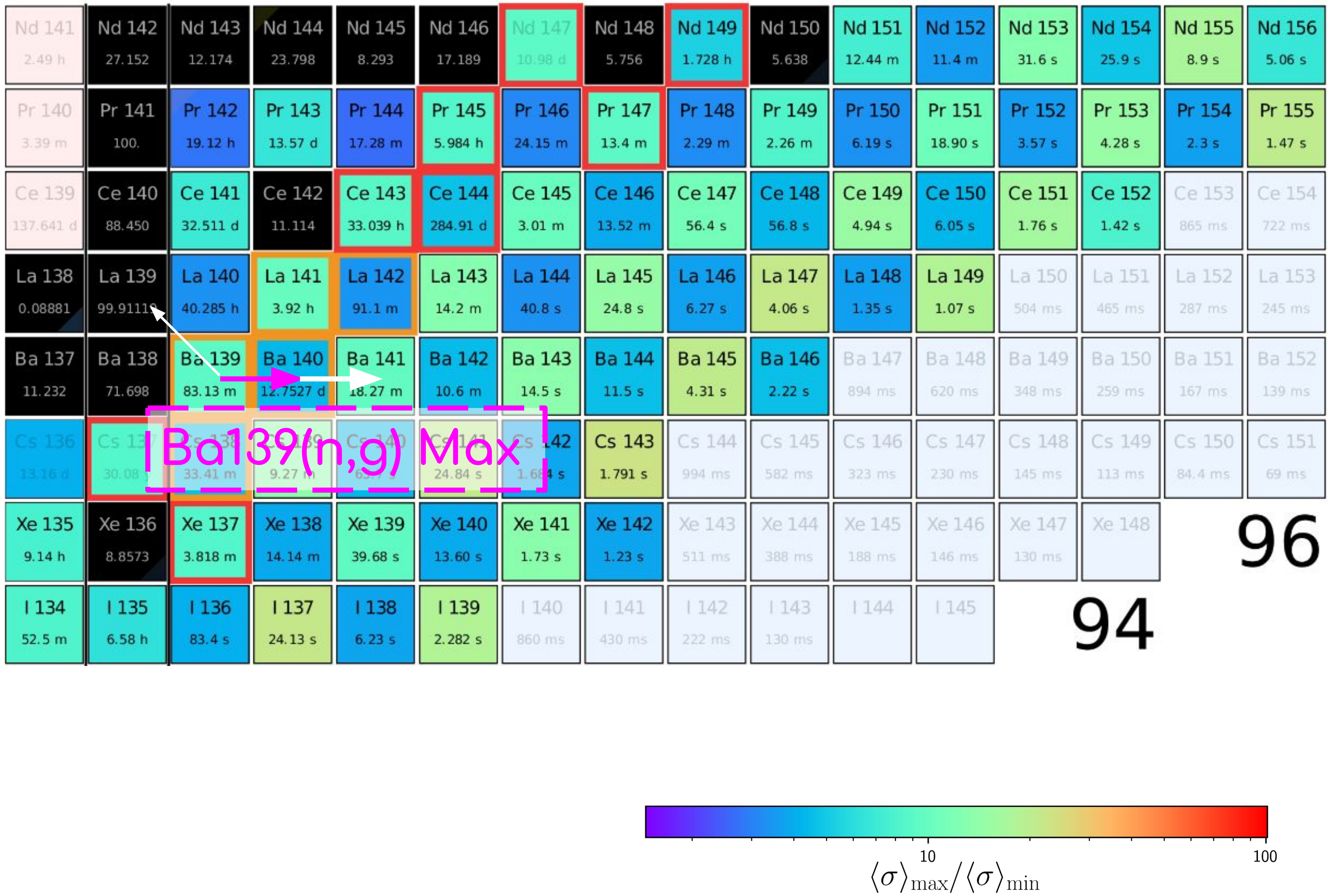

La139 abundance uncertainty: 0.44 dex

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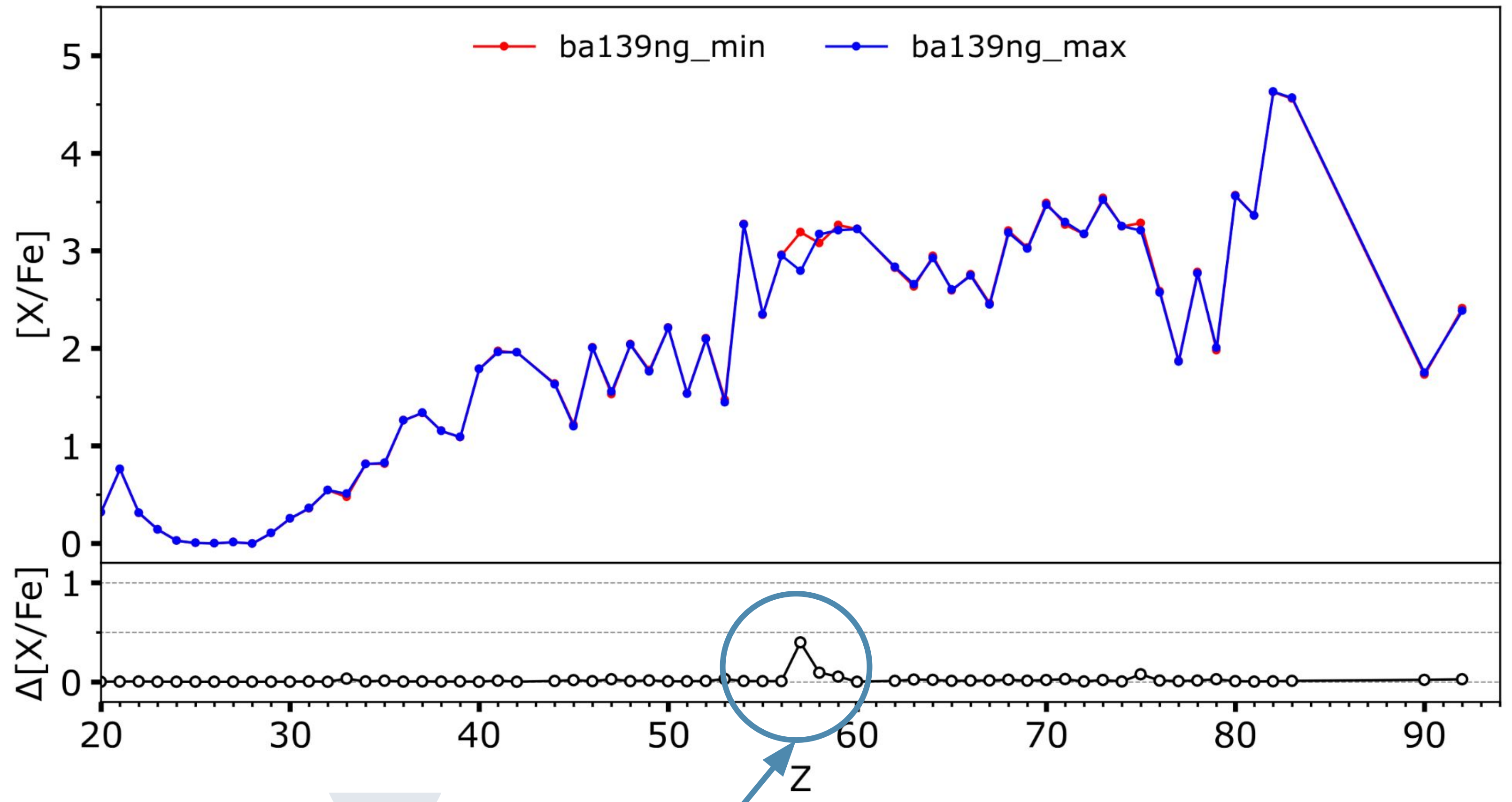

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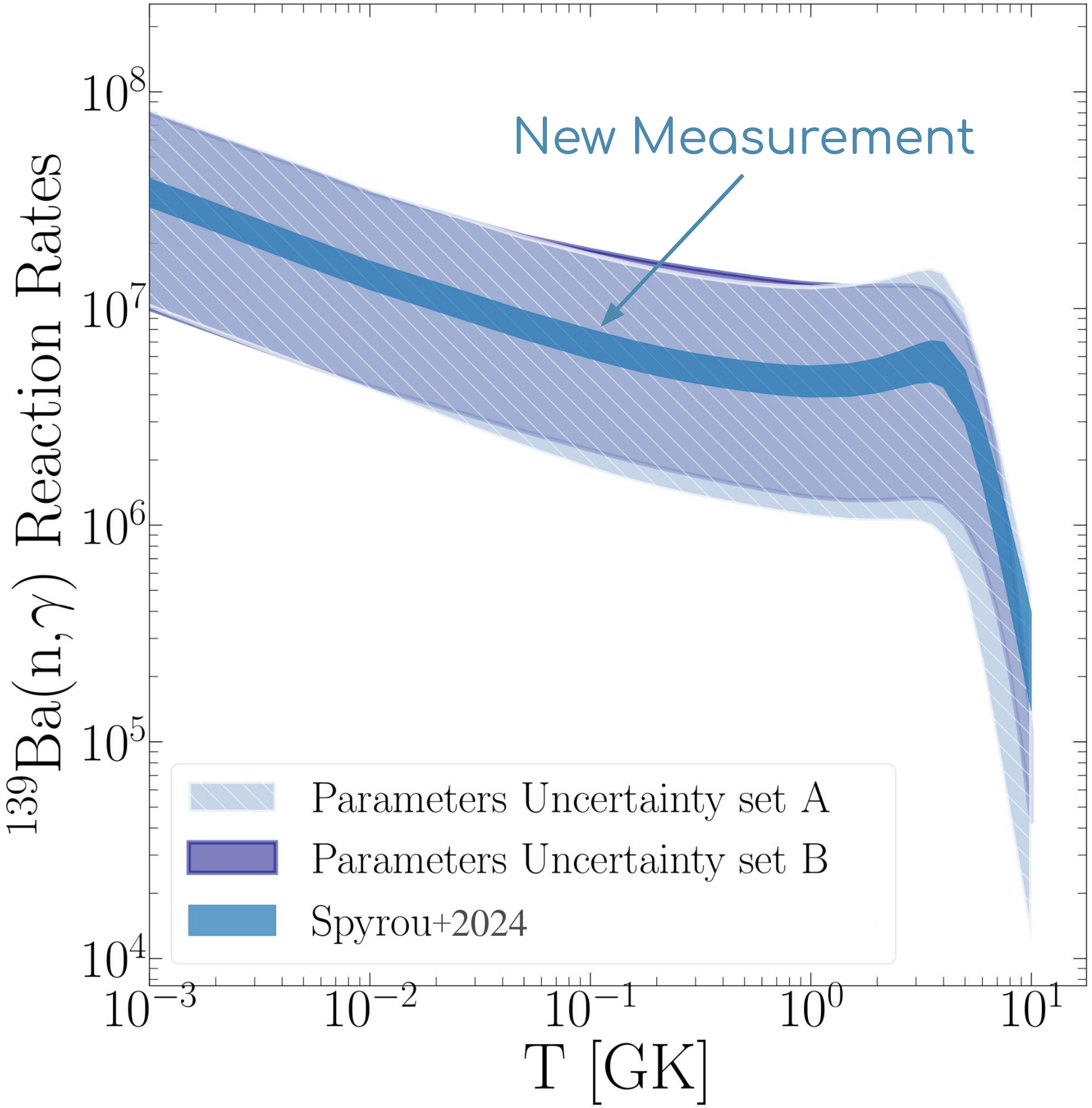

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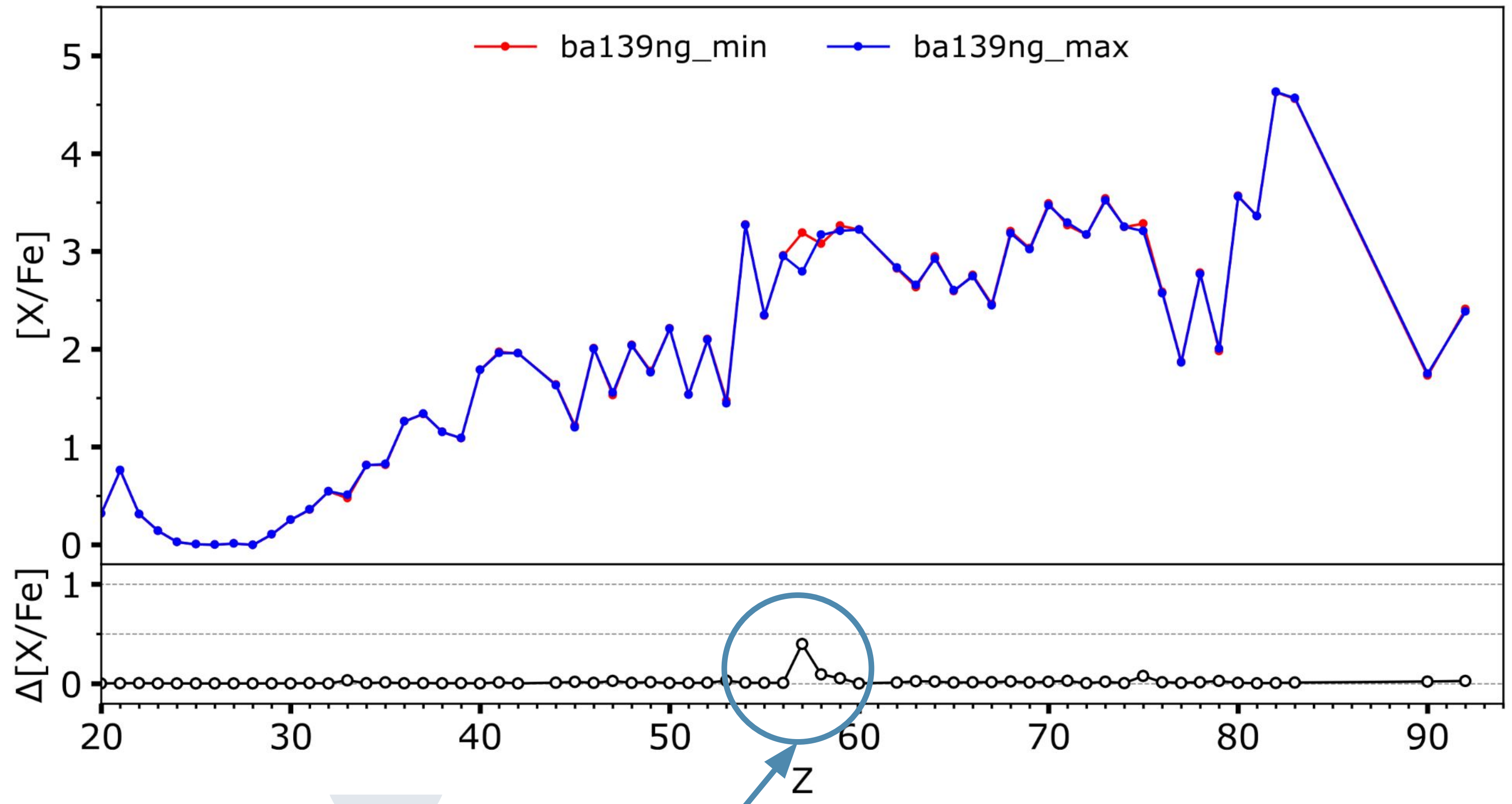
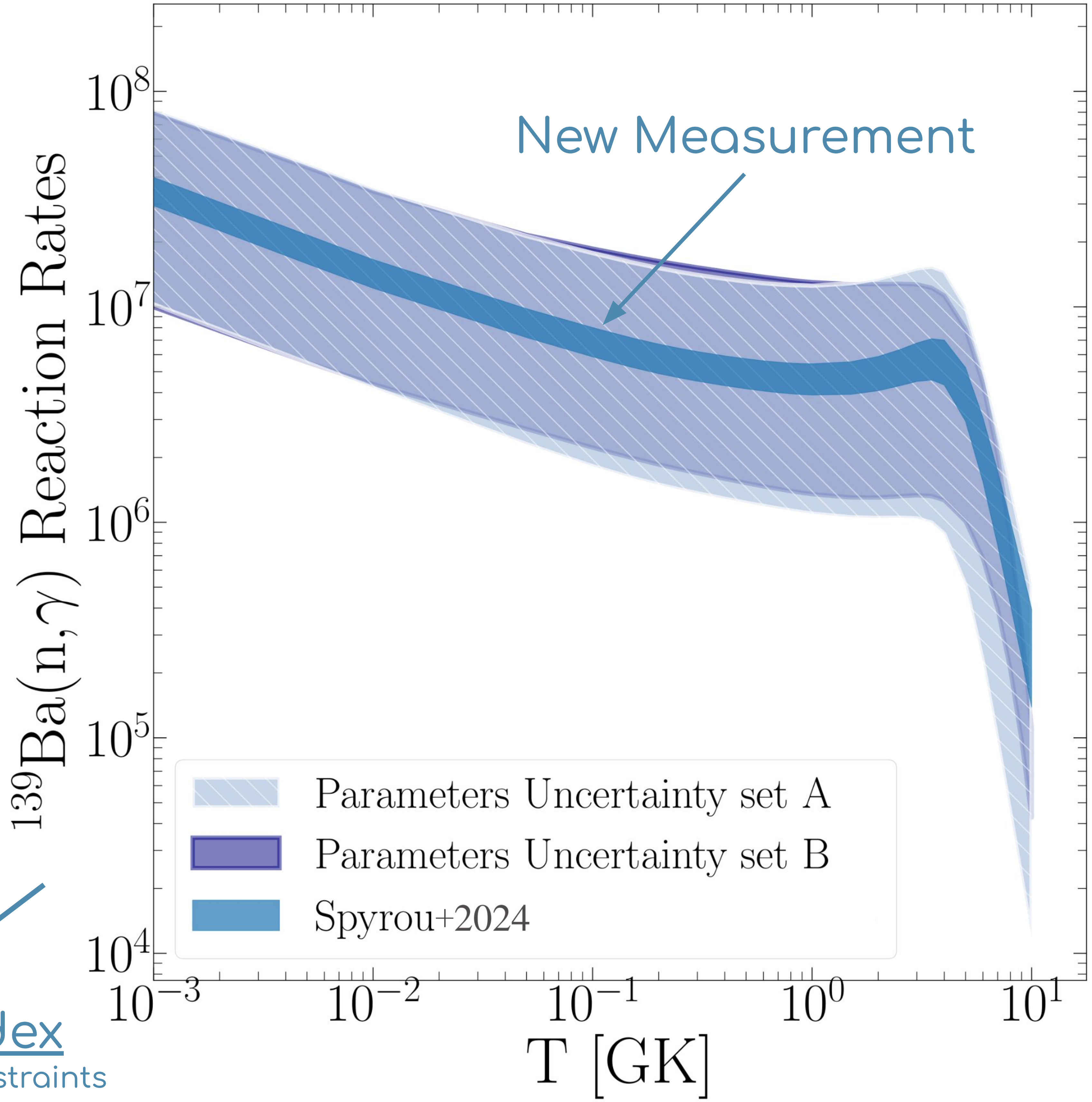


La139 abundance uncertainty: 0.44 dex

Reduced to 0.06 dex
thanks to experimental constraints



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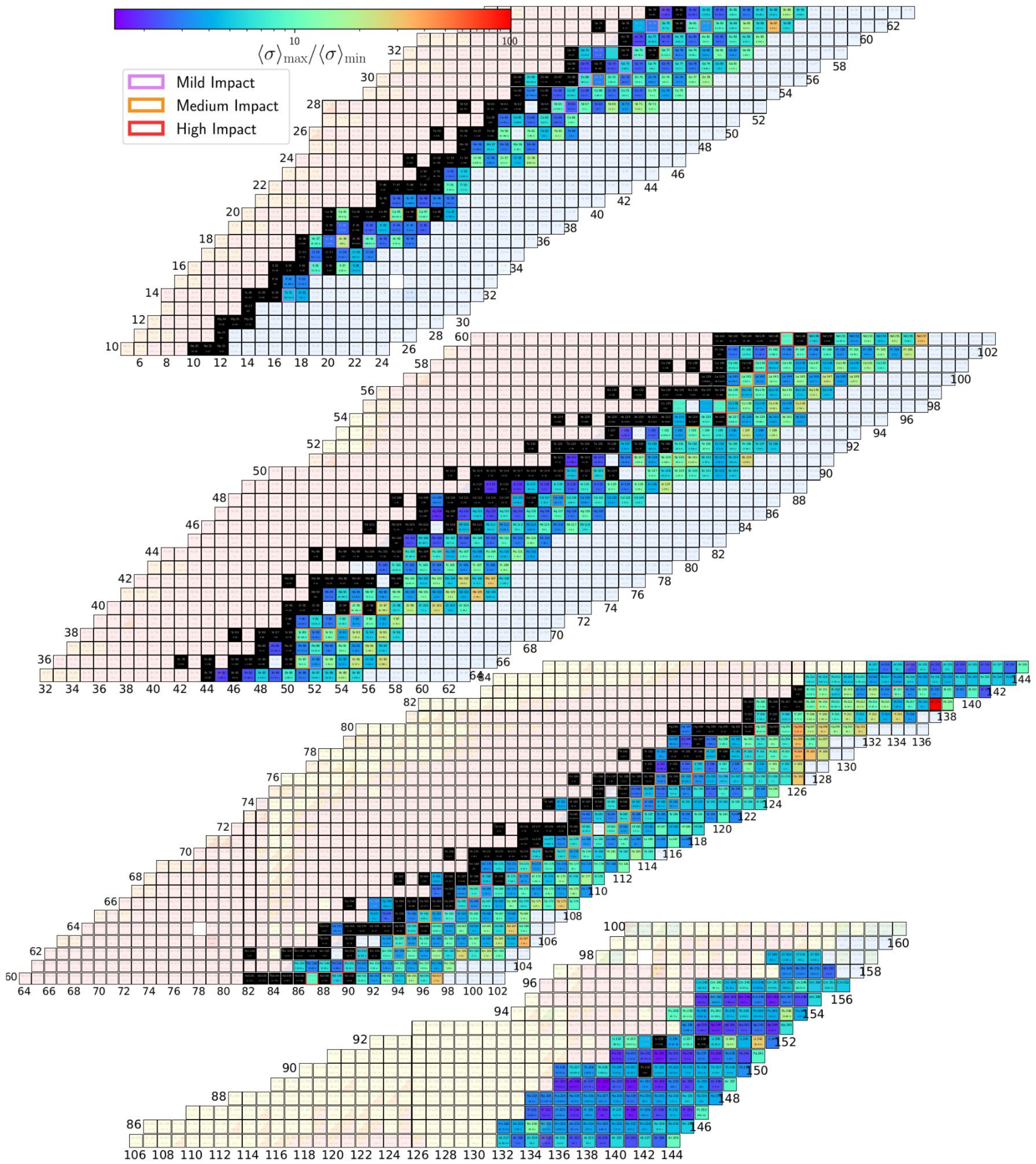
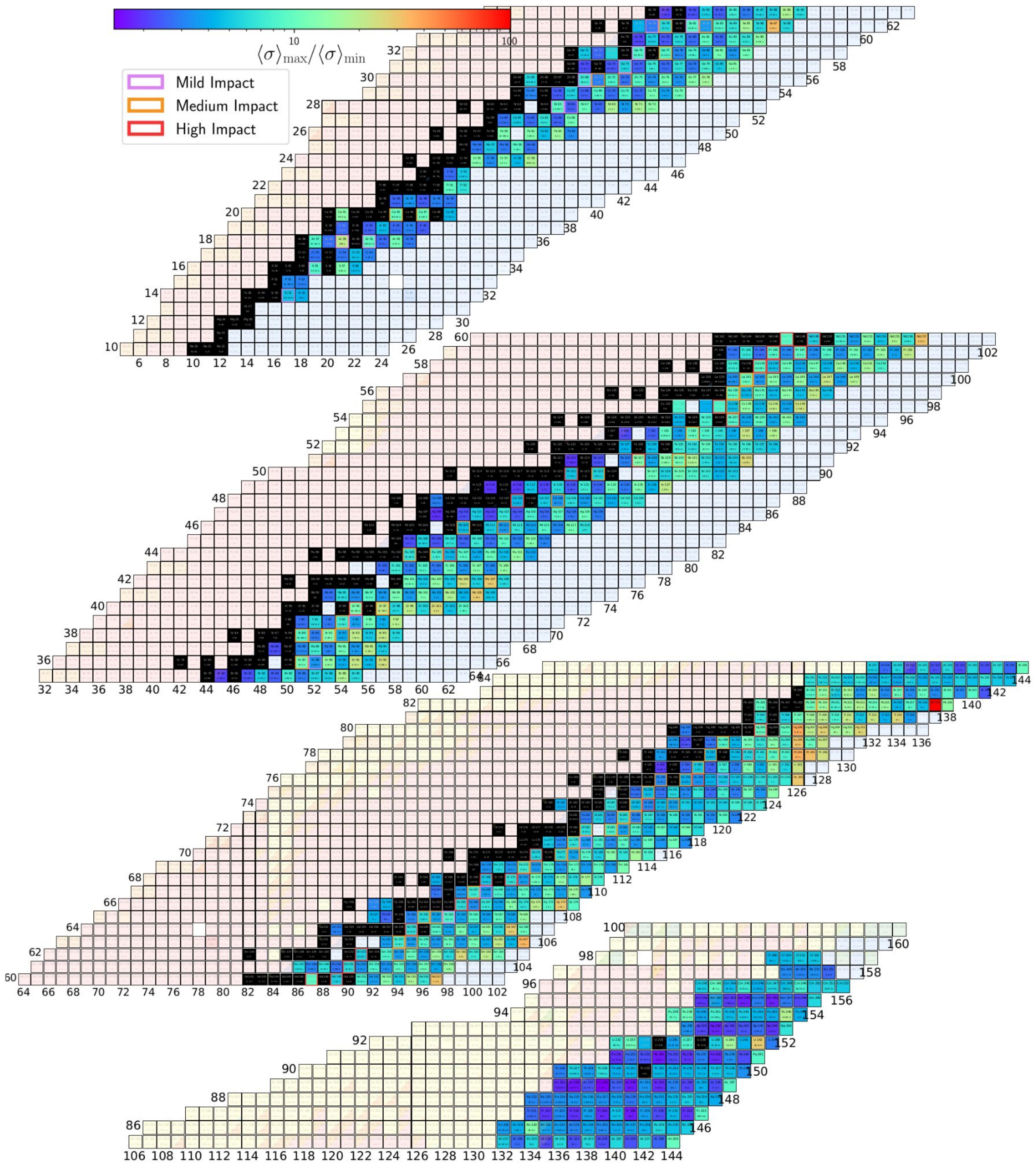


Element	Z	A	Iso. Frac.	Surf. abund. uncertainty (in log) set A	set B	Reaction	$\langle\sigma\rangle_{max}$ / $\langle\sigma\rangle_{min}$ set A	set B
U	92	235	8-51%	2.90	1.37	^{217}Bi(n,γ)	57.2	10.0
U	92	238	49-92%	2.87	1.80	^{217}Bi(n,γ)	57.2	10.0
Th	90	232	100%	2.75	1.36	^{217}Bi(n,γ)	57.2	10.0
Dy	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

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
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Sm	62	150	0-4%	1.31	1.08	^{149}Nd(n,γ)	7.3	5.4
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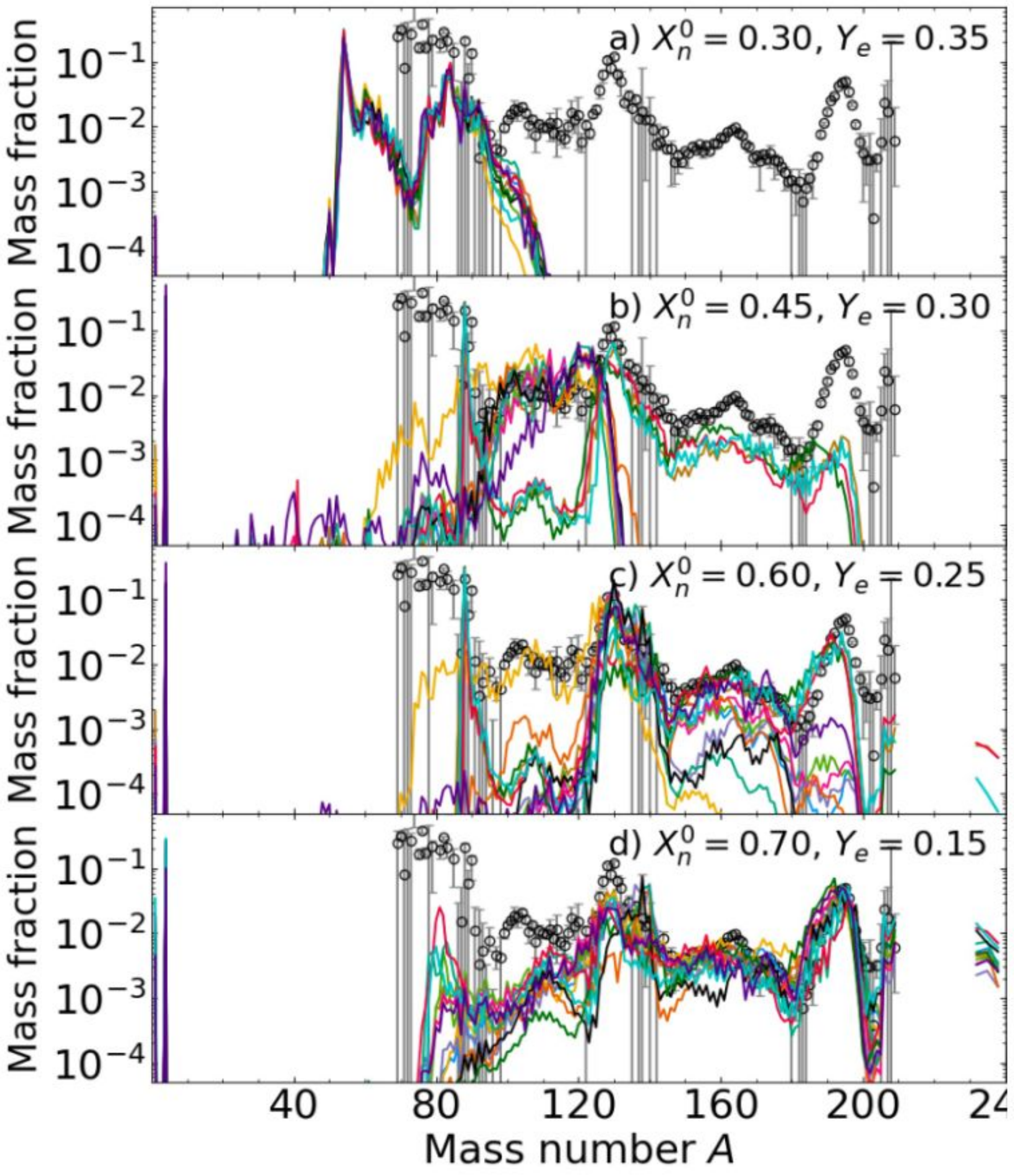
Martinet+2024

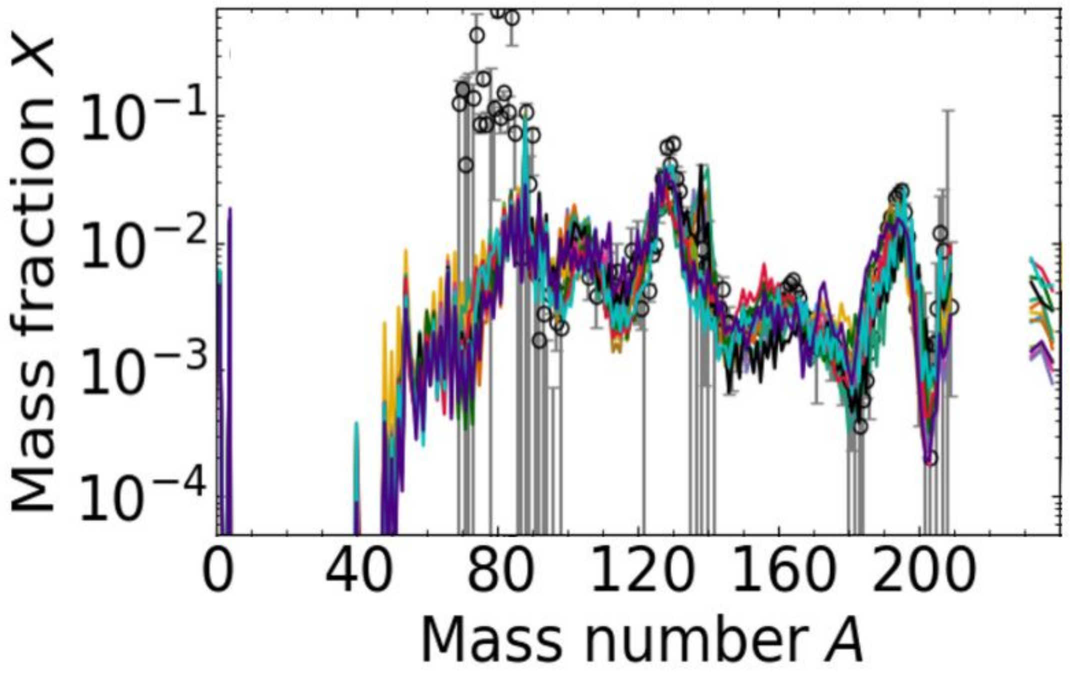
Propagating nuclear uncertainties to r-process simulations

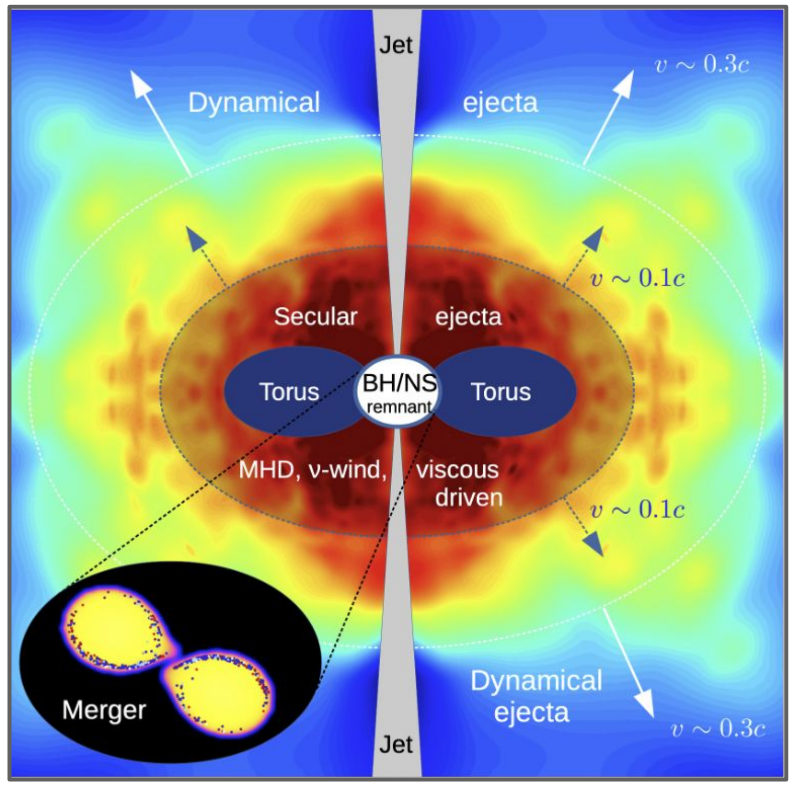
Importance of using multiple trajectories representing the whole NSM event

Prompt dynamical ejecta



Multiple trajectories

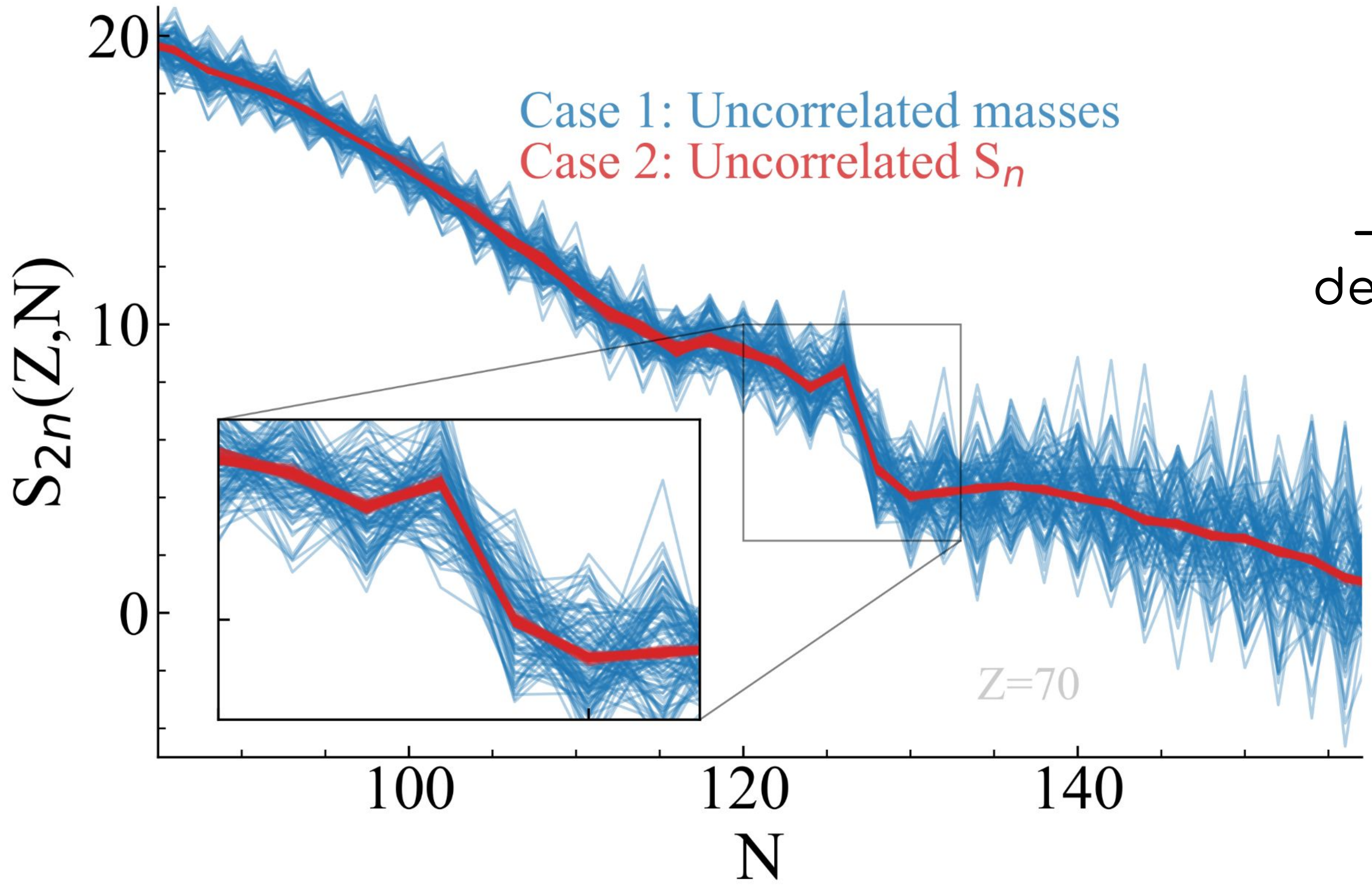




358 trajectories representing the total ~2500 trajectories

Propagating nuclear uncertainties to r-process simulations

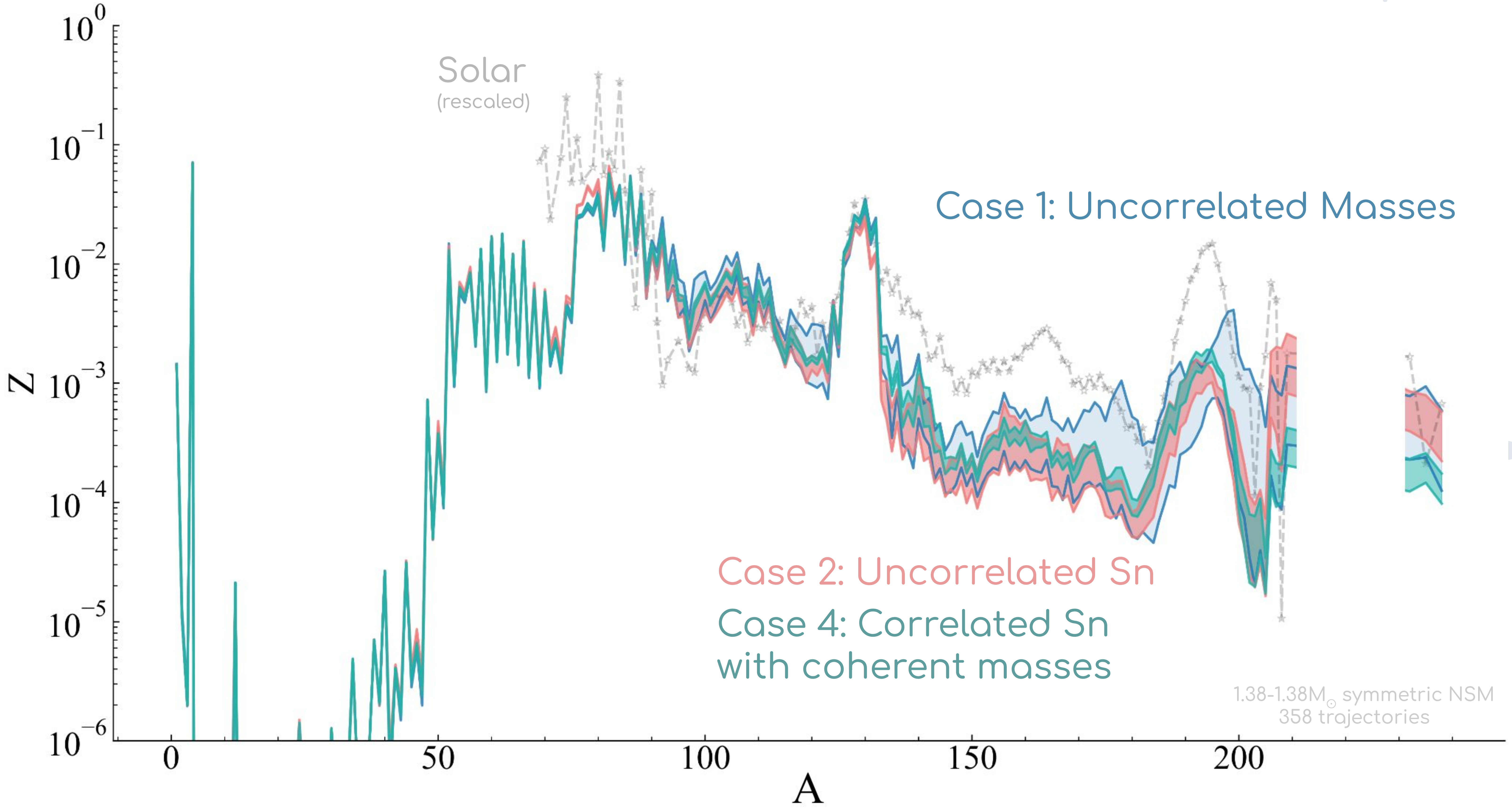
Importance of using multiple trajectories representing the whole NSM event



→ However, photodissociation reaction rates depend exponentially on the separation energy Sn

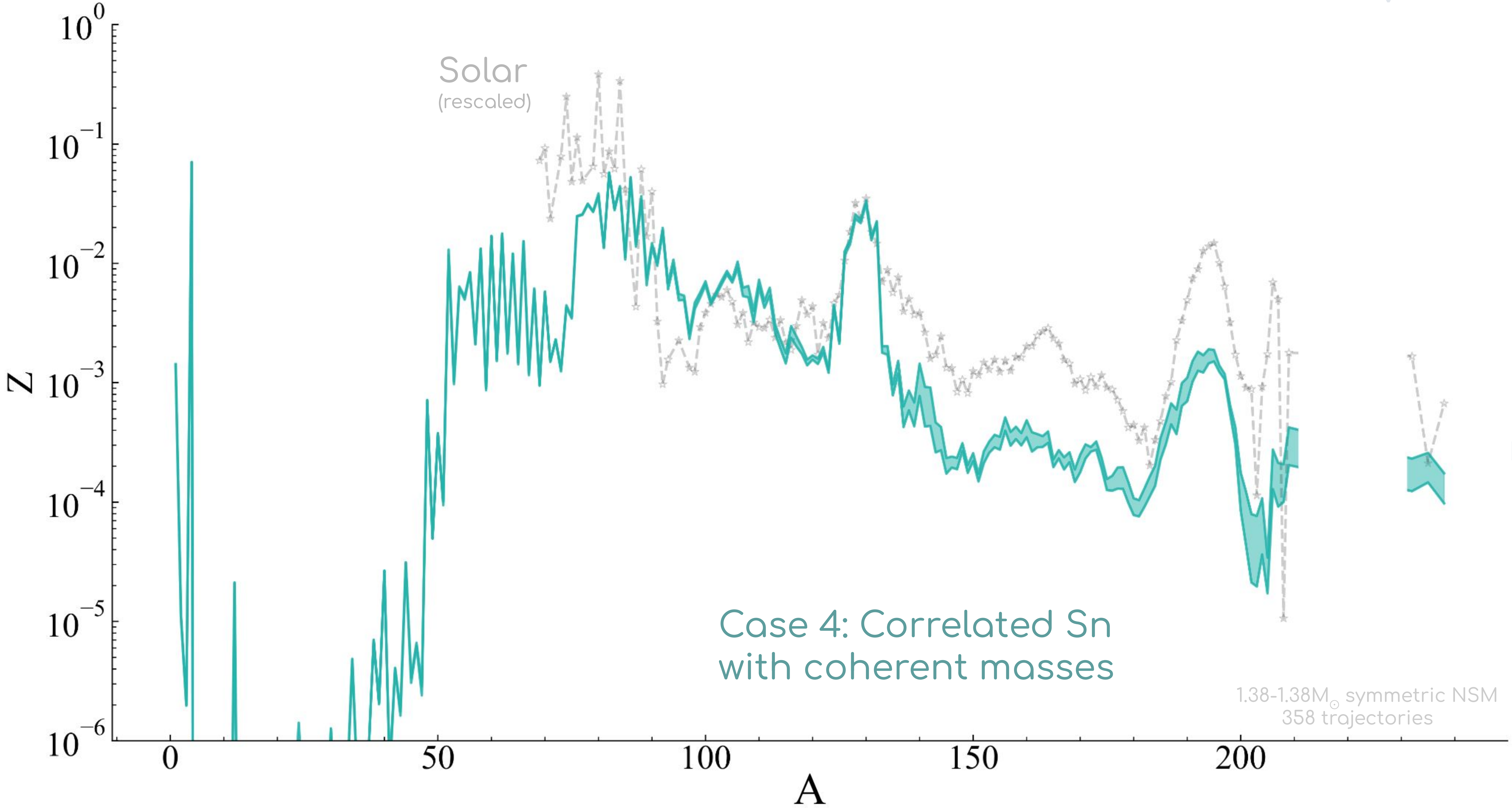
Propagating nuclear uncertainties to r-process simulations

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



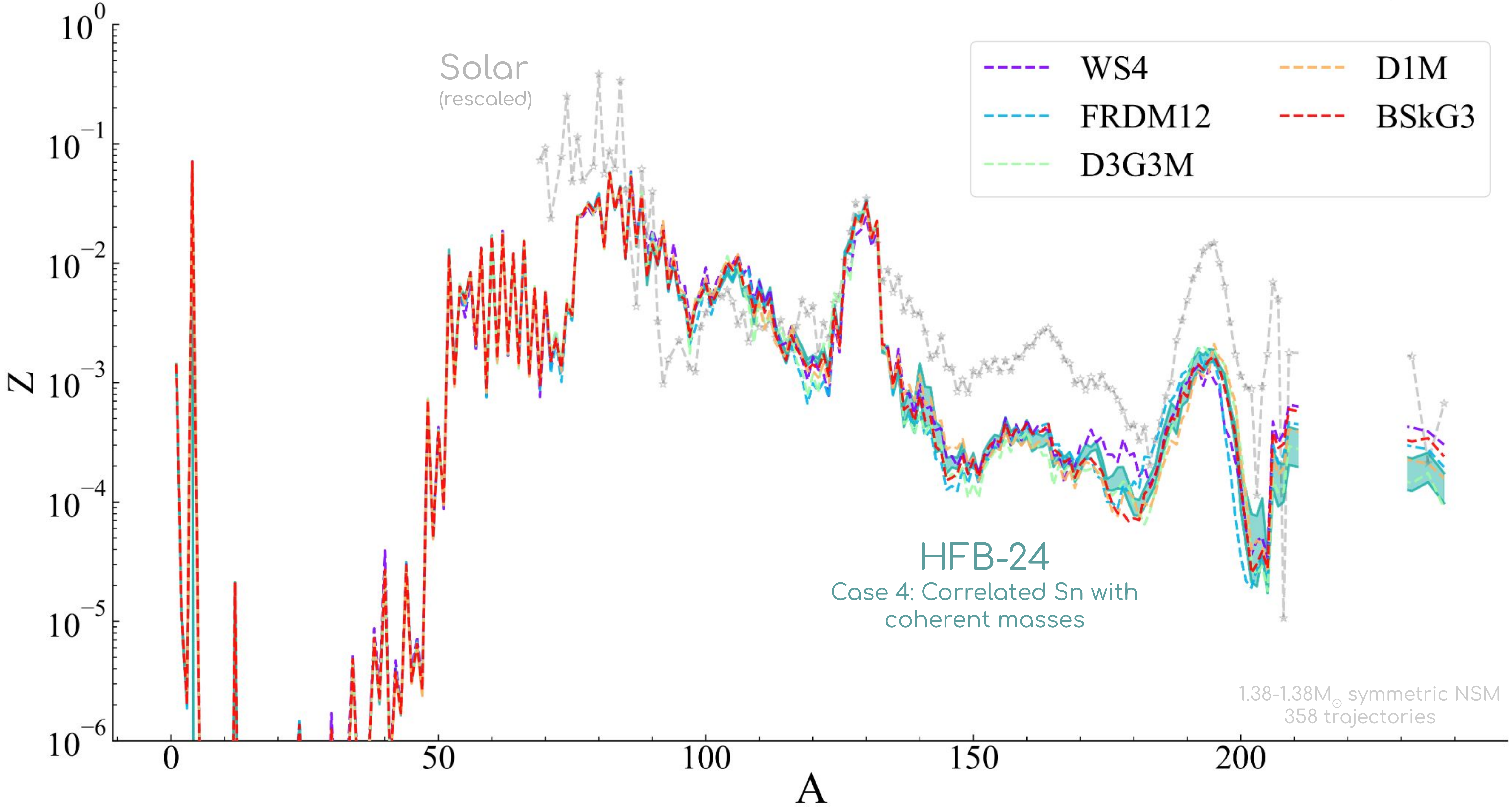
Propagating nuclear uncertainties to r-process simulations

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



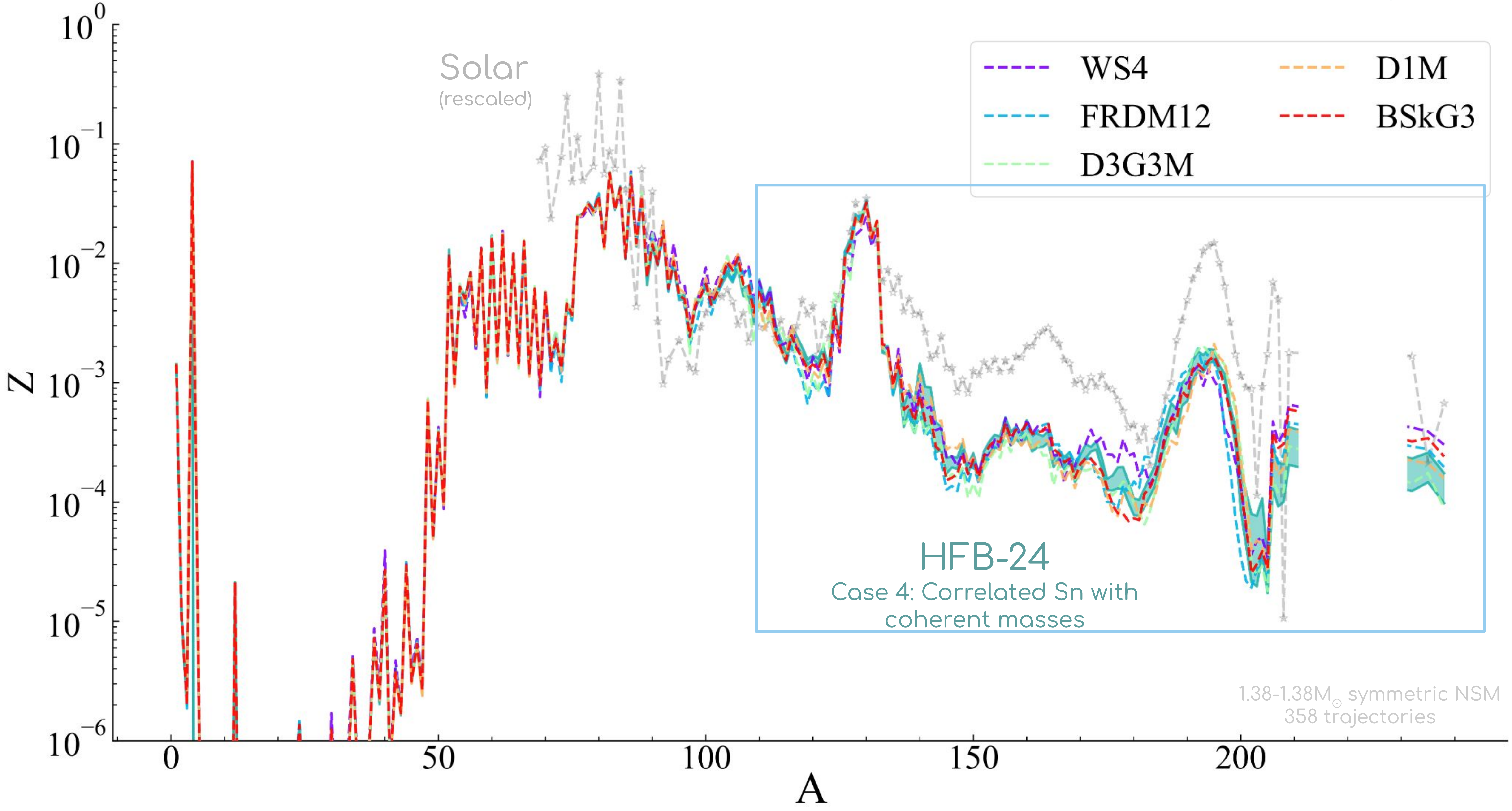
Propagating nuclear uncertainties to r-process simulations

Model uncertainties vs Parameter uncertainties (Martinet & Goriely subm..)



Propagating nuclear uncertainties to r-process simulations

Model uncertainties vs Parameter uncertainties (Martinet & Goriely subm..)



Propagating nuclear uncertainties to r-process simulations

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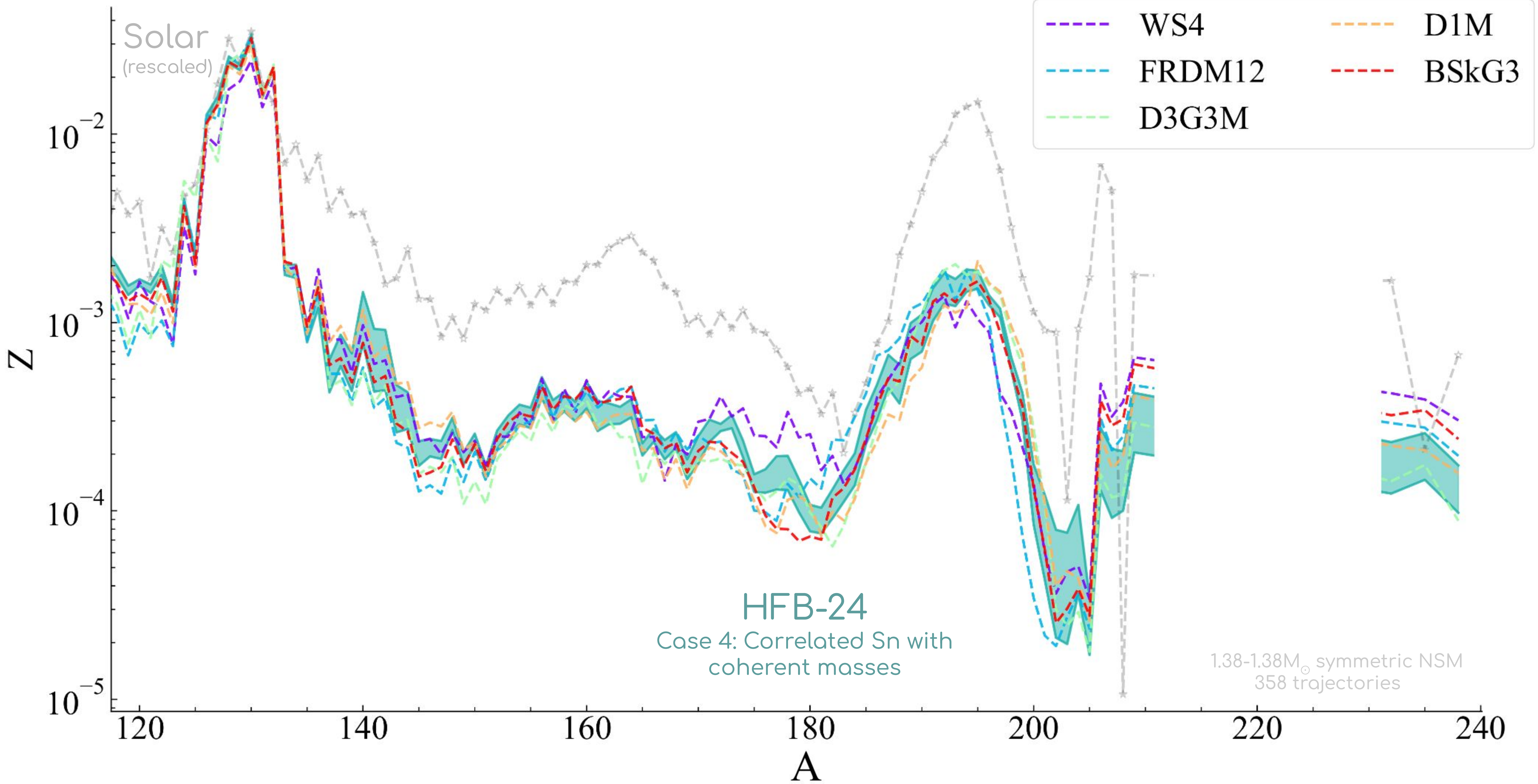

Conclusions

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

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Systematic and Statistical nuclear uncertainties

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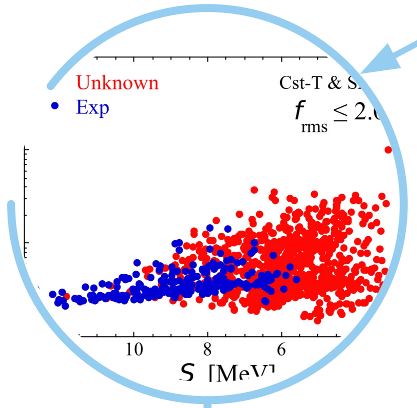
The impact of Systematic and Statistical nuclear uncertainties on the i-process nucleosynthesis

Systematic and Statistical nuclear uncertainties



Correlated model vs Non-correlated parameter Uncertainties

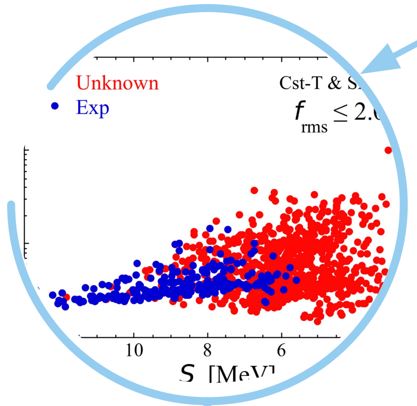
Correlated model uncertainties of the same order than non-correlated parameters uncertainties

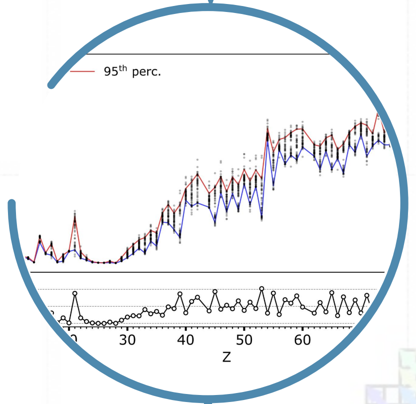
Important to use correctly model/parameters uncertainty

Conclusions

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

Systematic and Statistical nuclear uncertainties





Correlated model vs Non-correlated parameter Uncertainties

Correlated model uncertainties of the same order than non-correlated parameters uncertainties

Important to use correctly model/parameters uncertainty

Impact on i-process nucleosynthesis

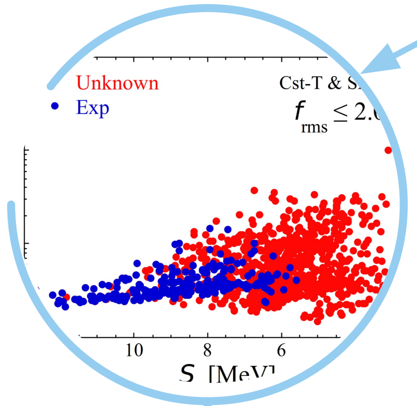
Important impact on the production of observable tracers (surface abundance uncertainties by 1 dex for La, 3 dex for Th/U, 1.2 dex Eu, ...)

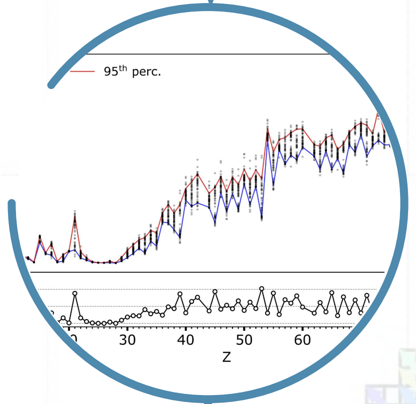
Results consistent for model A and B

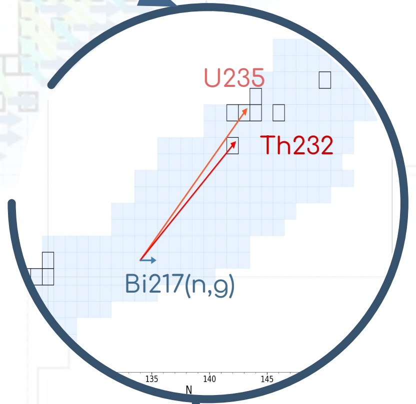
Conclusions

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

Systematic and Statistical nuclear uncertainties







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Impact on i-process nucleosynthesis

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 model A and B

Identifying important reactions

Interesting reactions such as Bi217(n,g) for Th/U.
Possibility to quantify the impact of these reactions, especially for the ones that impact observable tracers.
Results consistent for model A and B.

Conclusions

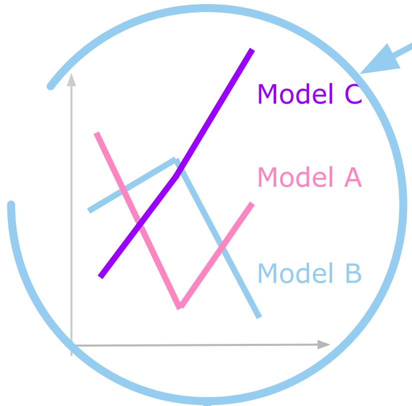
The impact of Systematic and Statistical nuclear uncertainties on the r-process nucleosynthesis

Systematic and Statistical nuclear uncertainties

Conclusions

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

Systematic and Statistical nuclear uncertainties



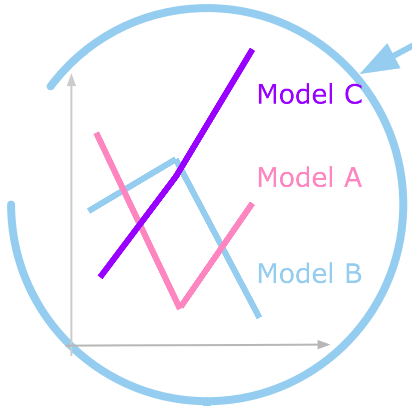
Correlated model vs Non-correlated parameter Uncertainties

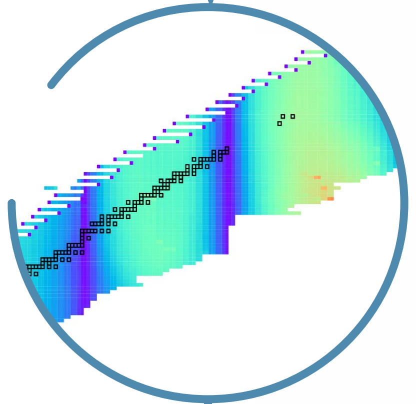
Extra care needed with the misuse of Correlated model uncertainties and the use of non-correlated parameters uncertainties

Conclusions

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

Systematic and Statistical nuclear uncertainties





Correlated model vs Non-correlated parameter Uncertainties

Extra care needed with the misuse of Correlated model uncertainties and the use of non-correlated parameters uncertainties

Determining coherently parameter uncertainties

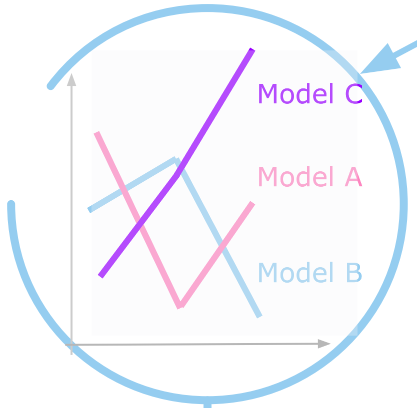
Using the BFMC we can determine coherently the parameter uncertainties.

Different cases to be considered between uncertainties from Mass and from Sn

Conclusions

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

Systematic and Statistical nuclear uncertainties



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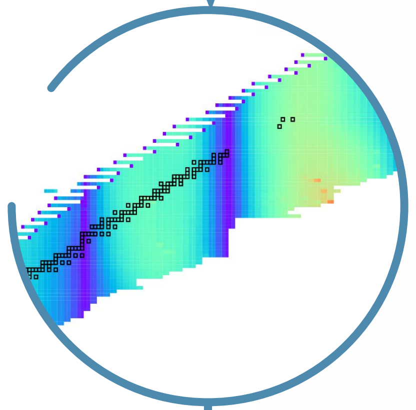


Determining coherently parameter uncertainties

Using the BFMC we can determine coherently the parameter uncertainties.

Different cases to be considered between uncertainties from Mass and from Sn

Impact on r-process nucleosynthesis in Neutron Star Mergers

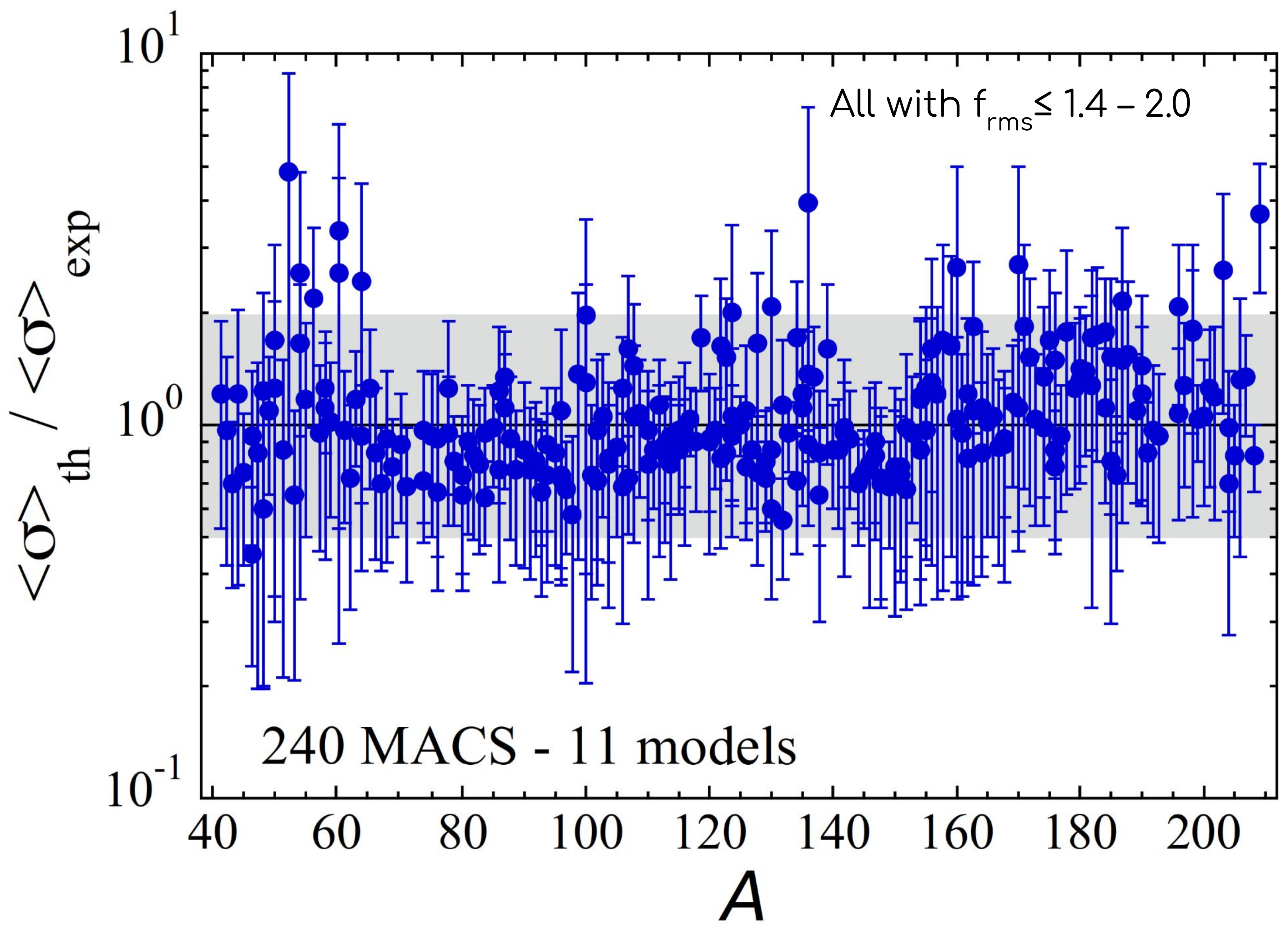
Multiple trajectories needed to represent the real impact of nuclear uncertainties.

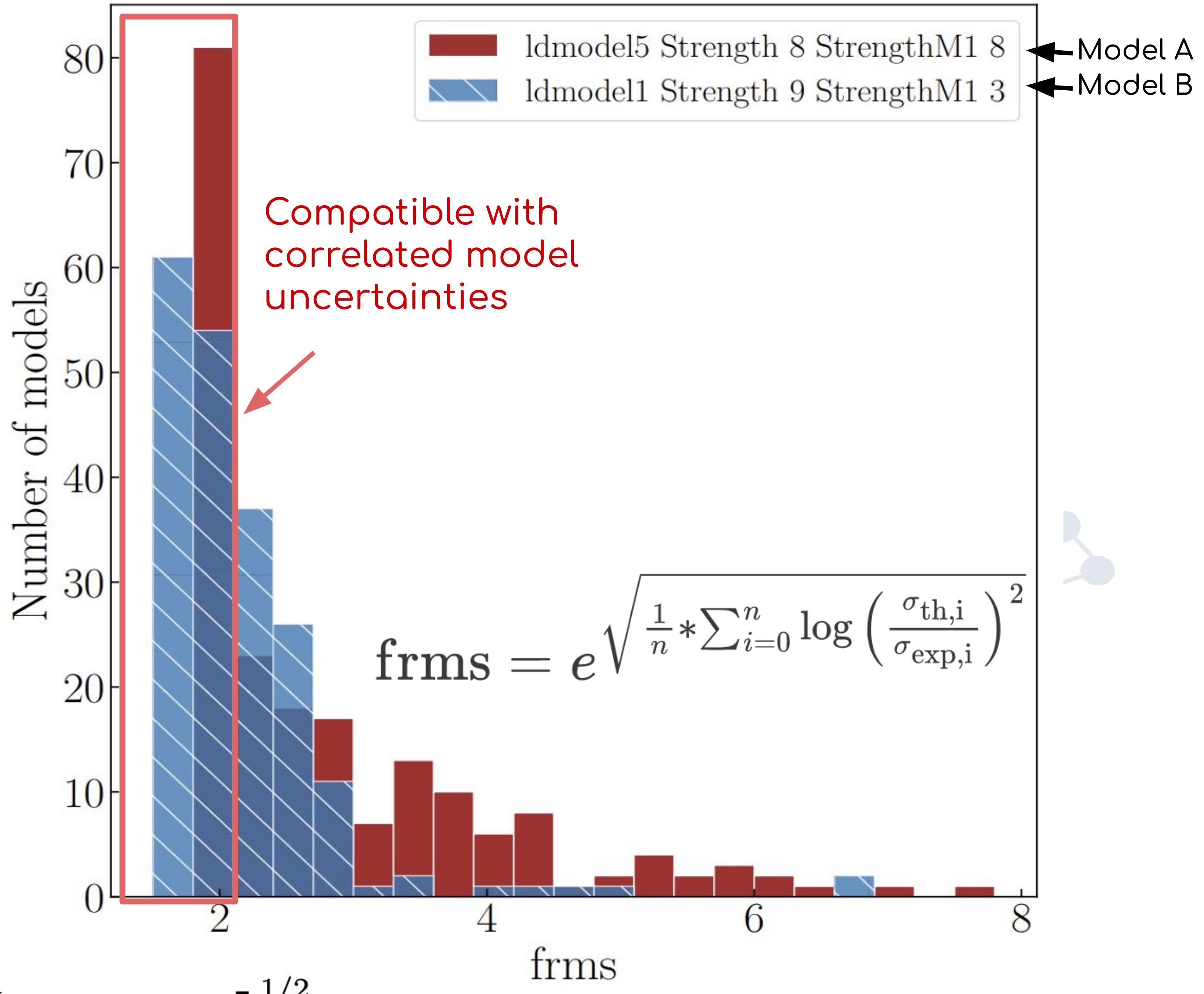
Mostly affects abondances of nuclei with A > 135. Model uncertainties leads to larger uncertainties on abondances than parameter ones

Estimating Nuclear Uncertainties

Radiative Neutron Capture Rates - Parameters uncertainty range constrain by experimental uncertainties

Correlated model uncertainties





$$f_{rms} = \exp\left[\frac{1}{N_e}\sum_{i=1}^{N_e}\ln^2\frac{\langle\sigma\rangle_{th,i}}{\langle\sigma\rangle_{exp,i}}\right]^{1/2}$$

Estimating Nuclear Uncertainties

Compatibility with experiment uncertainties

→ Random combinations of these 4 parameters to probe statistical uncertainties of (n,g) reaction

Model A

Model B

Compatible with correlated model uncertainties

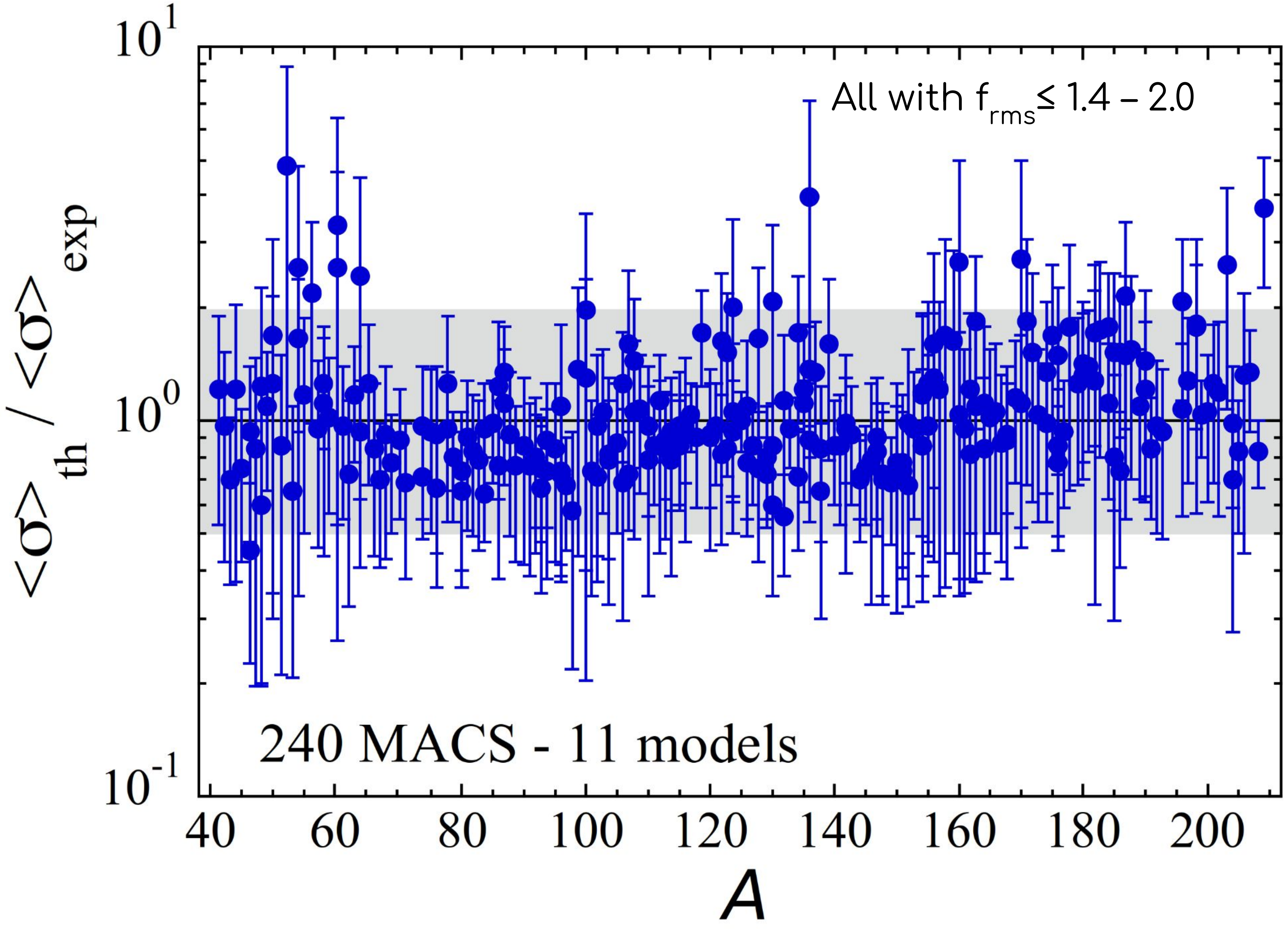
Estimating Nuclear Uncertainties

Compatibility with experiment uncertainties

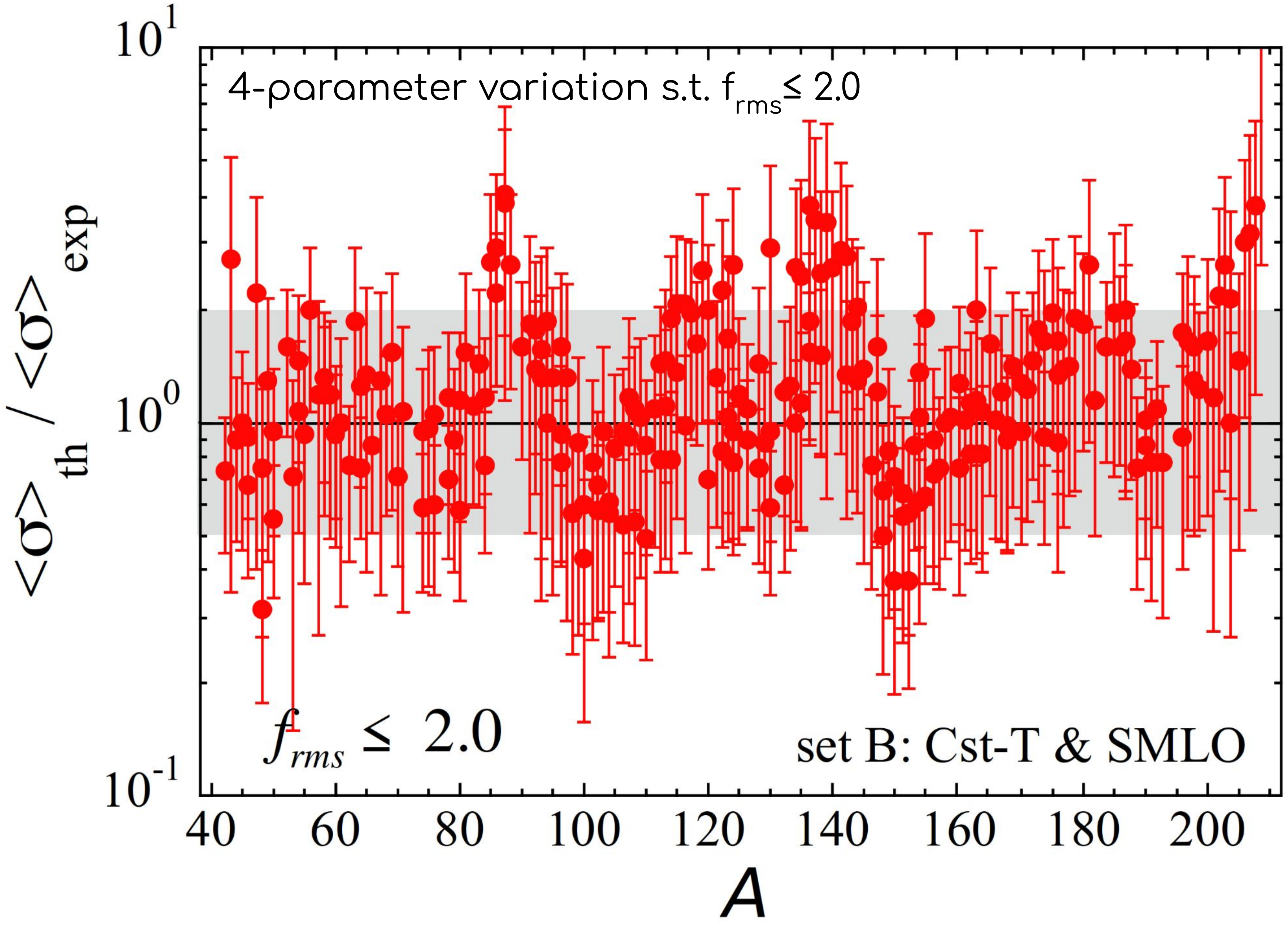
Estimating Nuclear Uncertainties

Radiative Neutron Capture Rates - Parameters uncertainty range constrain by model uncertainties

Correlated model uncertainties



Non-correlated parameter uncertainties

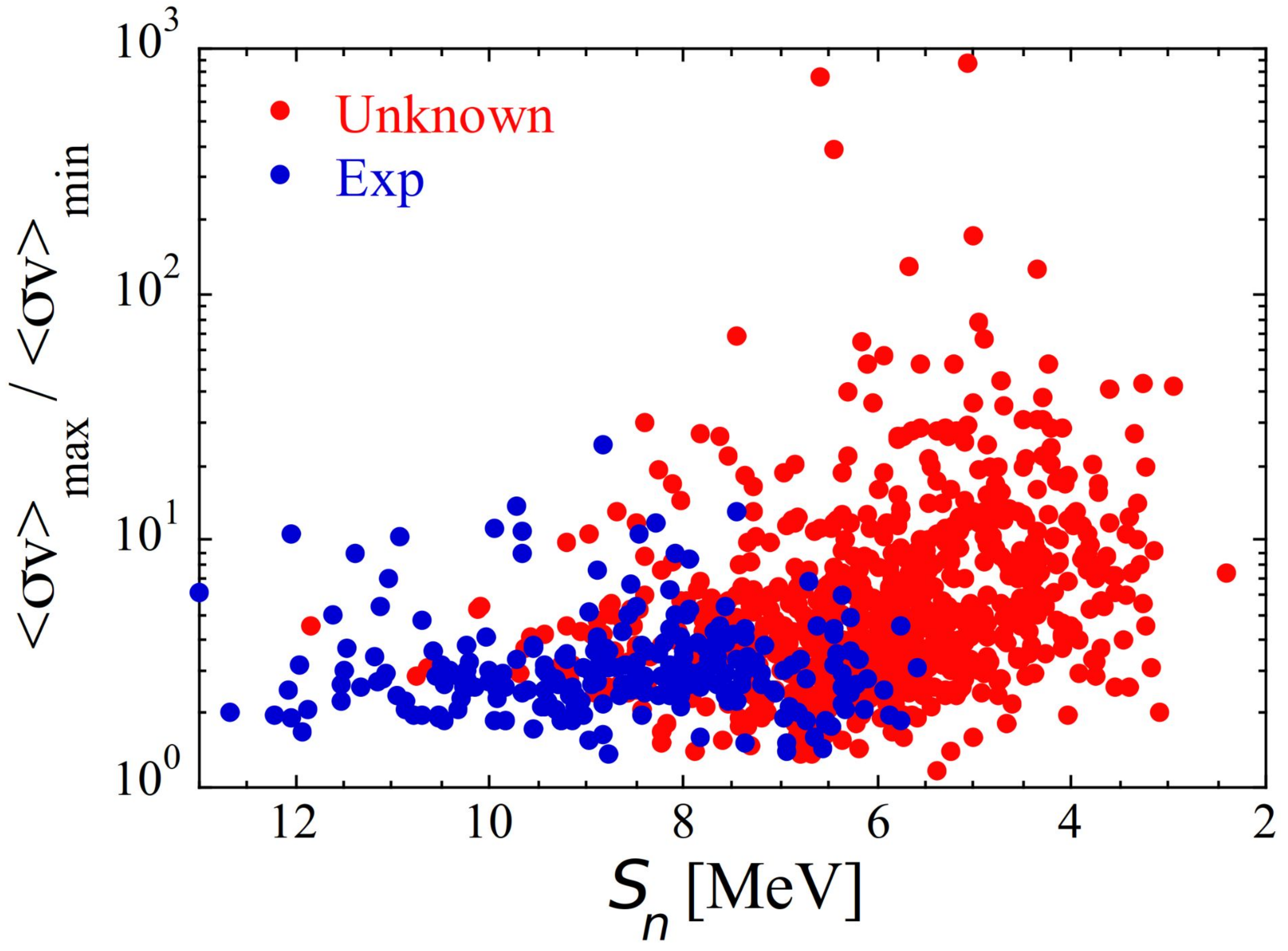


$$f_{rms} = \exp\left[\frac{1}{N_e}\sum_{i=1}^{N_e}\ln^2\frac{\langle\sigma\rangle_{th,i}}{\langle\sigma\rangle_{exp,i}}\right]^{1/2}$$

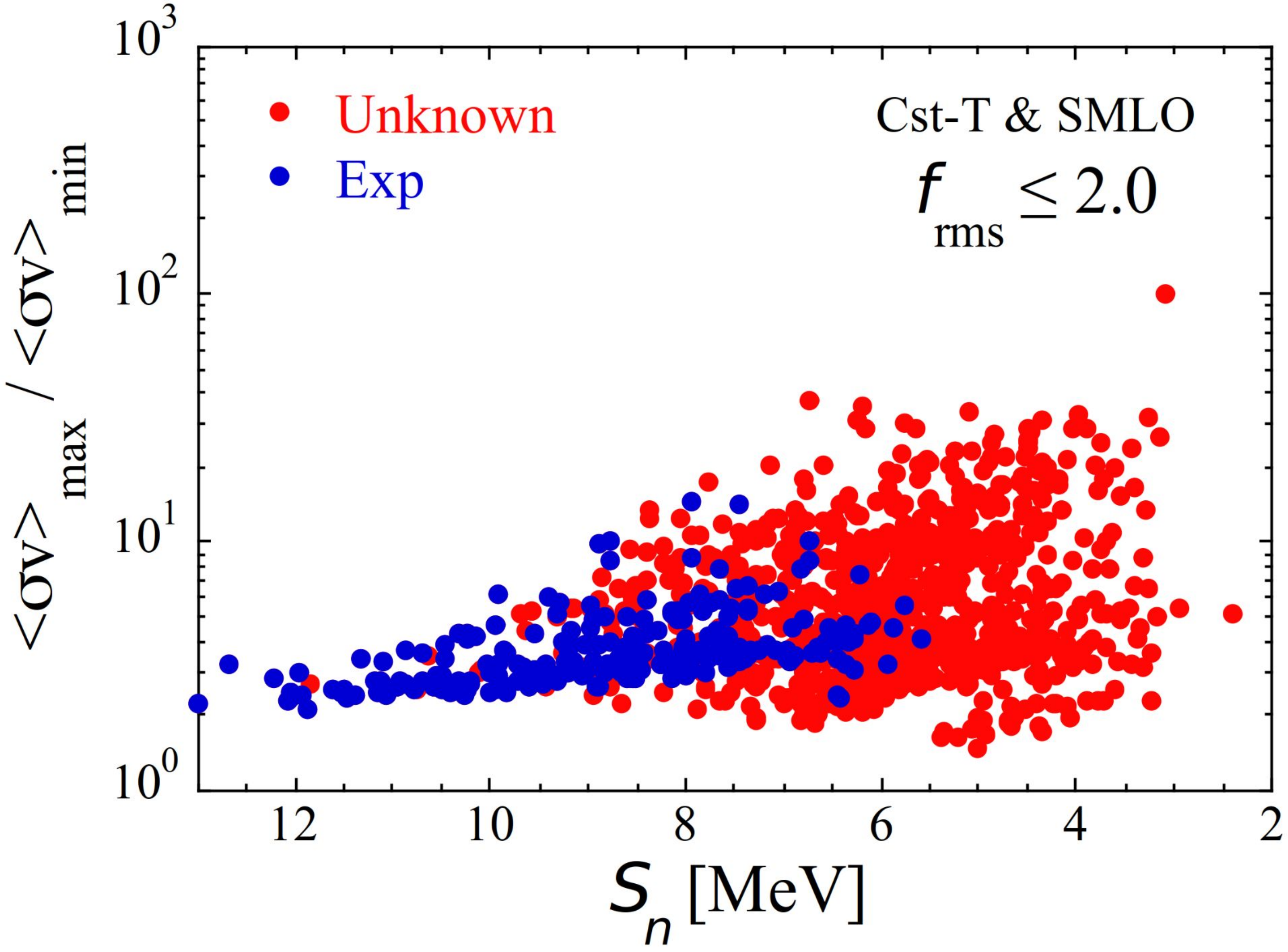
Estimating Nuclear Uncertainties

Radiative Neutron Capture Rates - Extension to non-experimental (n,g) reactions

Correlated model uncertainties



Non-correlated parameter uncertainties



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

Effect of statistical uncertainties on the surface enrichment of early AGB stars

STAREVOL code (Siess et al. 2006)

→ i-process nucleosynthesis

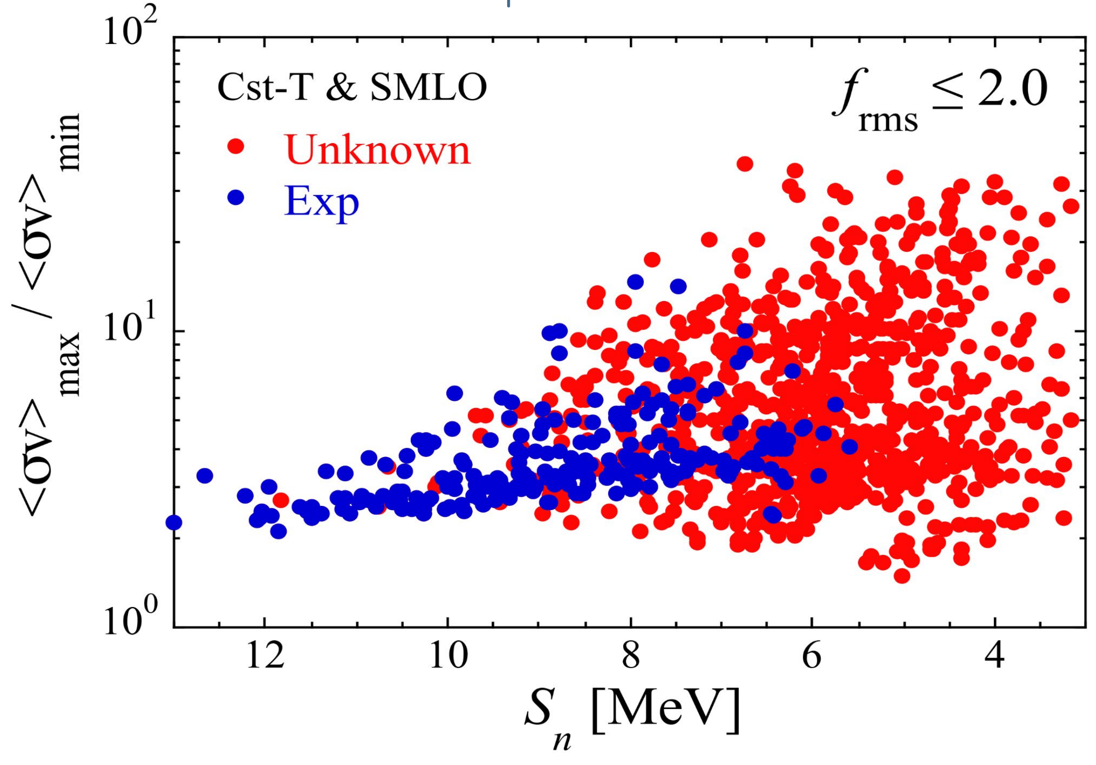
1 Msol at [Fe/H]=-2.5

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) Si31(n,g)	2) P32(n,g)	3) Si32(n,g)	....	862) 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

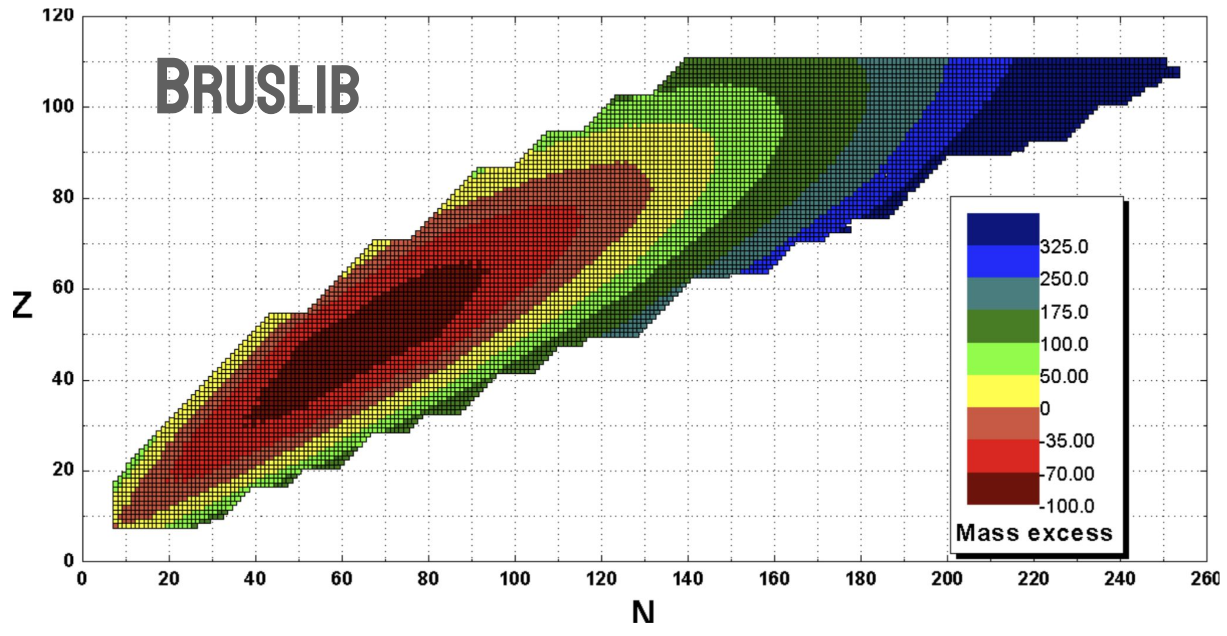
Update to Bruslib and NetGen

Updates of mass model for Brusslib

→ New reactions updated (e.g. $^{12}C+^{12}C$)

→ Plan for regular updates integrating ChaNUREPS entries

http://www.astro.ulb.ac.be/Netgen/



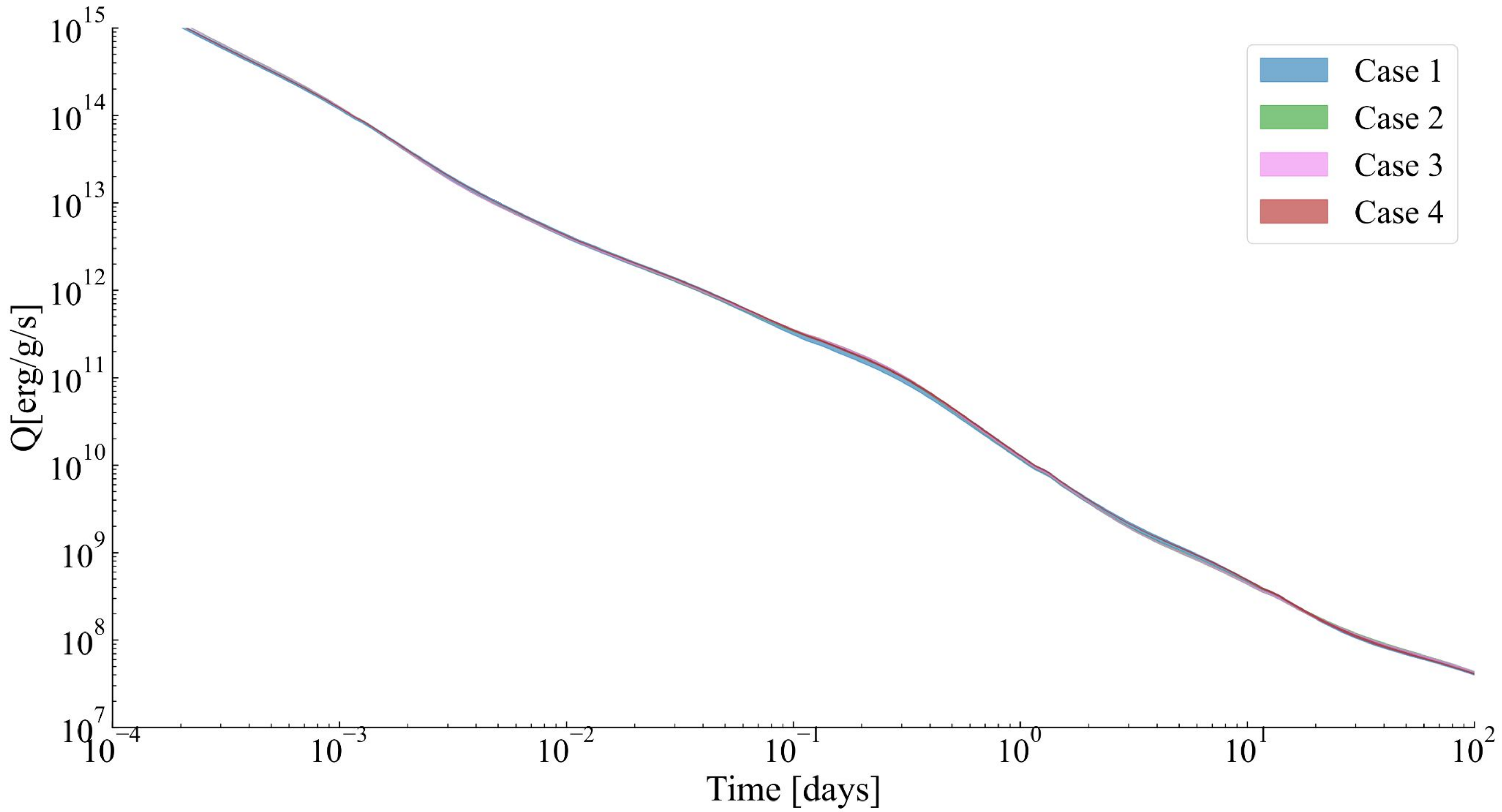
Masses updated with new mass model BSkg3 (Grams+2023), density, potentials, … will be updated too

- Triaxiality, time-reversal symmetry breaking & octupole GS deformation
- Microscopic pairing from "realistic" calculations
- Stiff EoS
- Accurate masses: s(2457M)=0.63MeV
- Accurate fission barriers s(45B f)=0.33MeV including triaxial & octupole deformations simultaneously

http://www.astro.ulb.ac.be/bruslib/

Nuclear uncertainties on NSM simulations

Q for various Cases

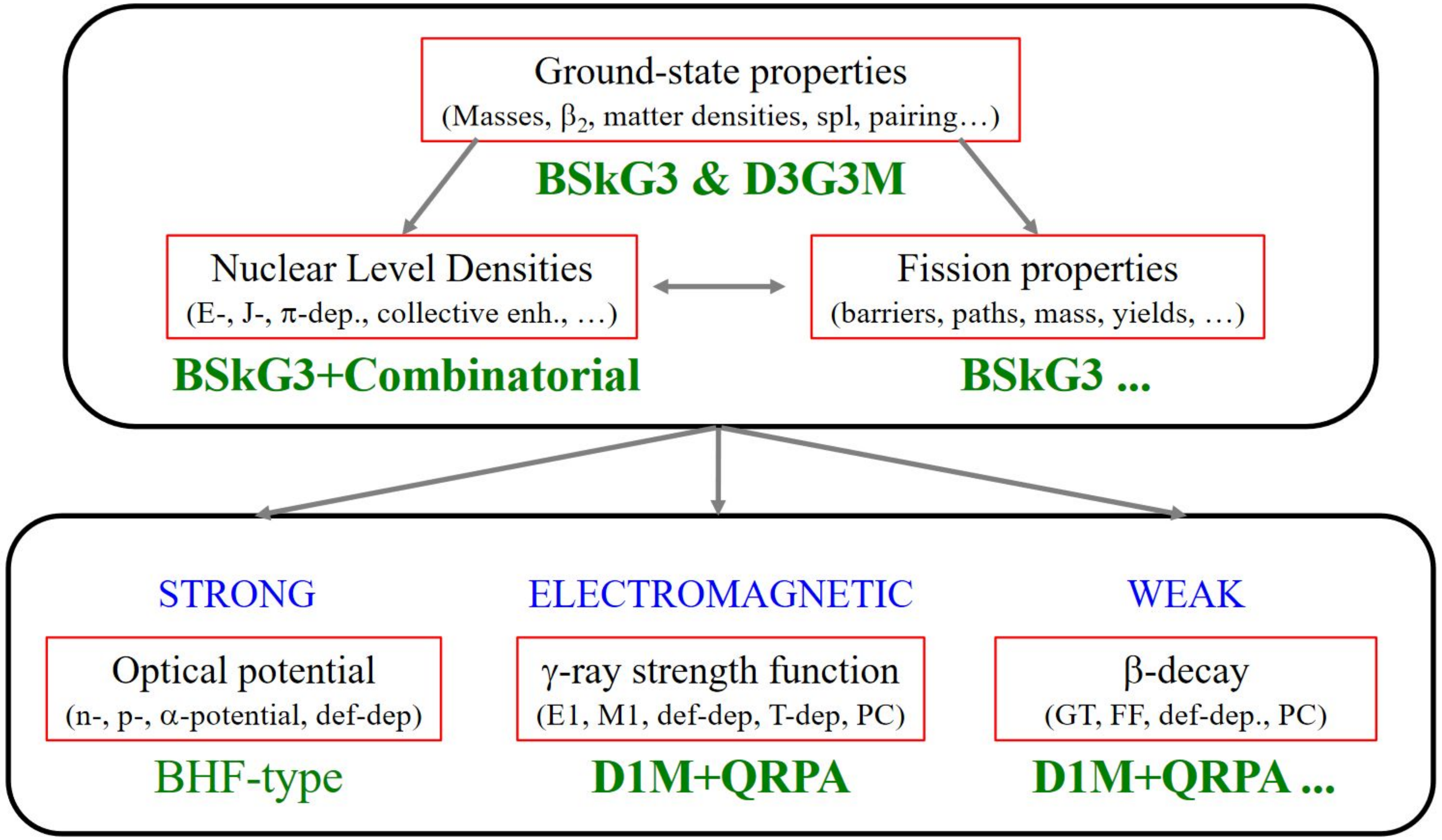


Nuclear models

Nuclear inputs

Some new efforts to improve the nuclear predictions for r-process applications

Nuclear inputs to nuclear reaction & decay calculations



"Microscopic" approach is a necessary but not a sufficient condition !
"(Semi-)Microscopic" models must be competitive in reproducing exp. data !

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)