# Statistical tools for the *r*-process nucleosynthesis studies

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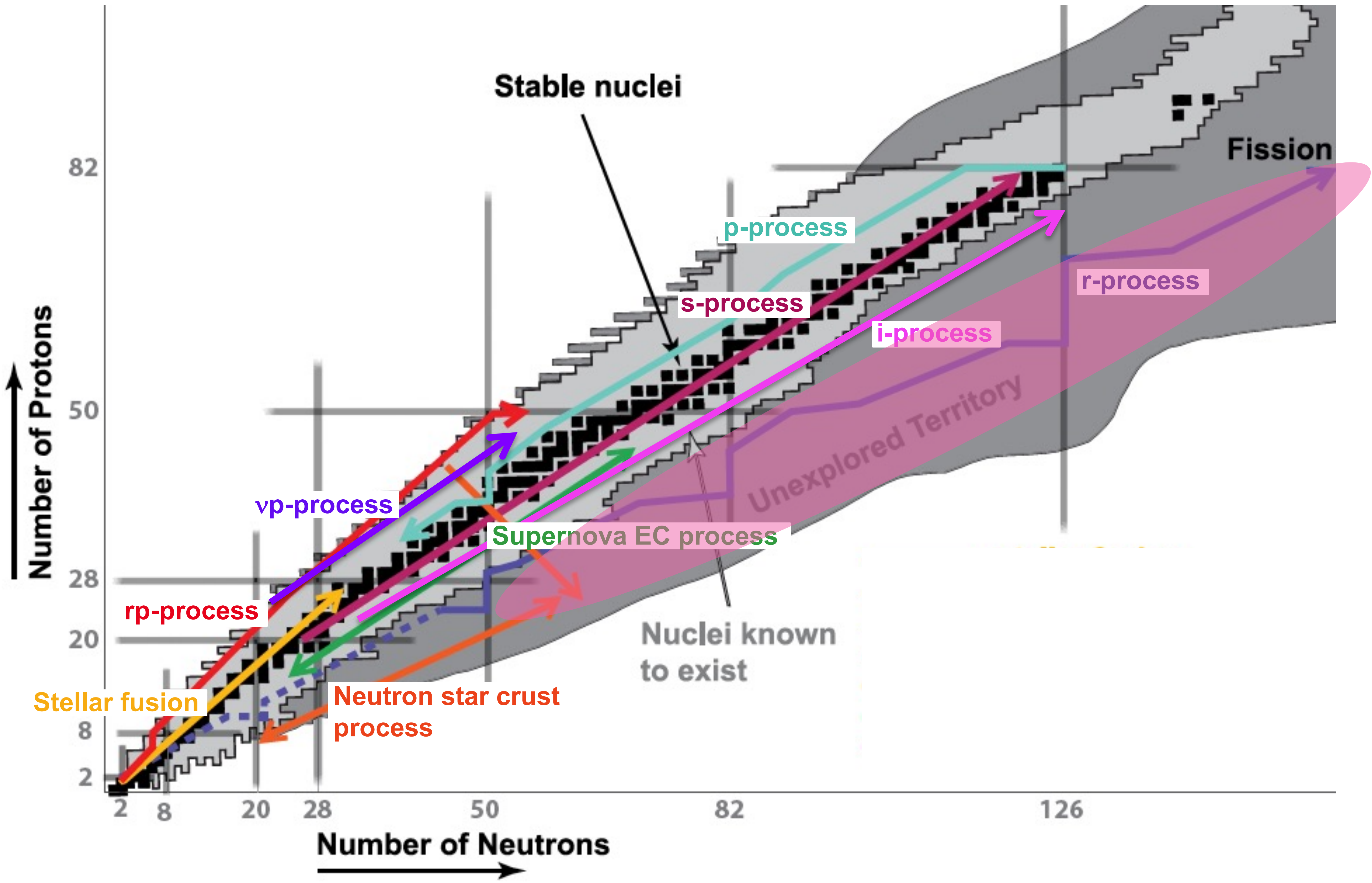
RIKEN TRIP Symposium
2025-03-10

# Rapid neutron capture process (*r*-process)

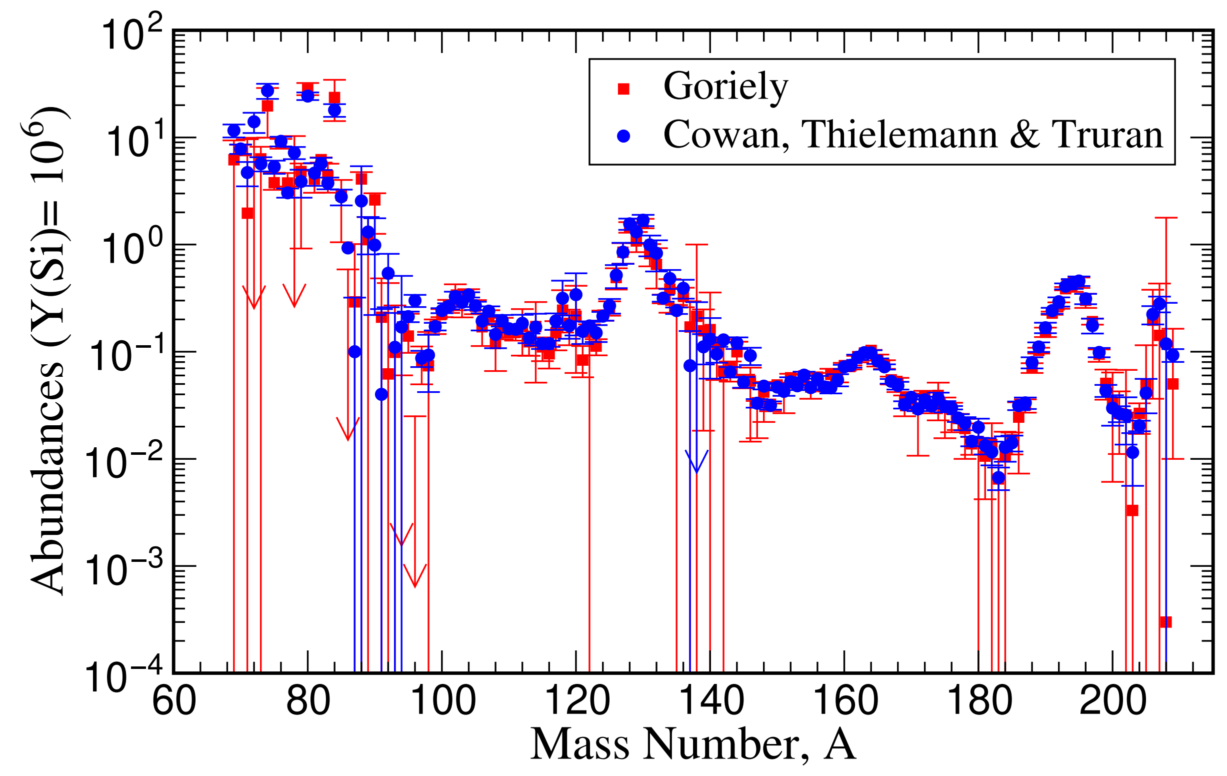


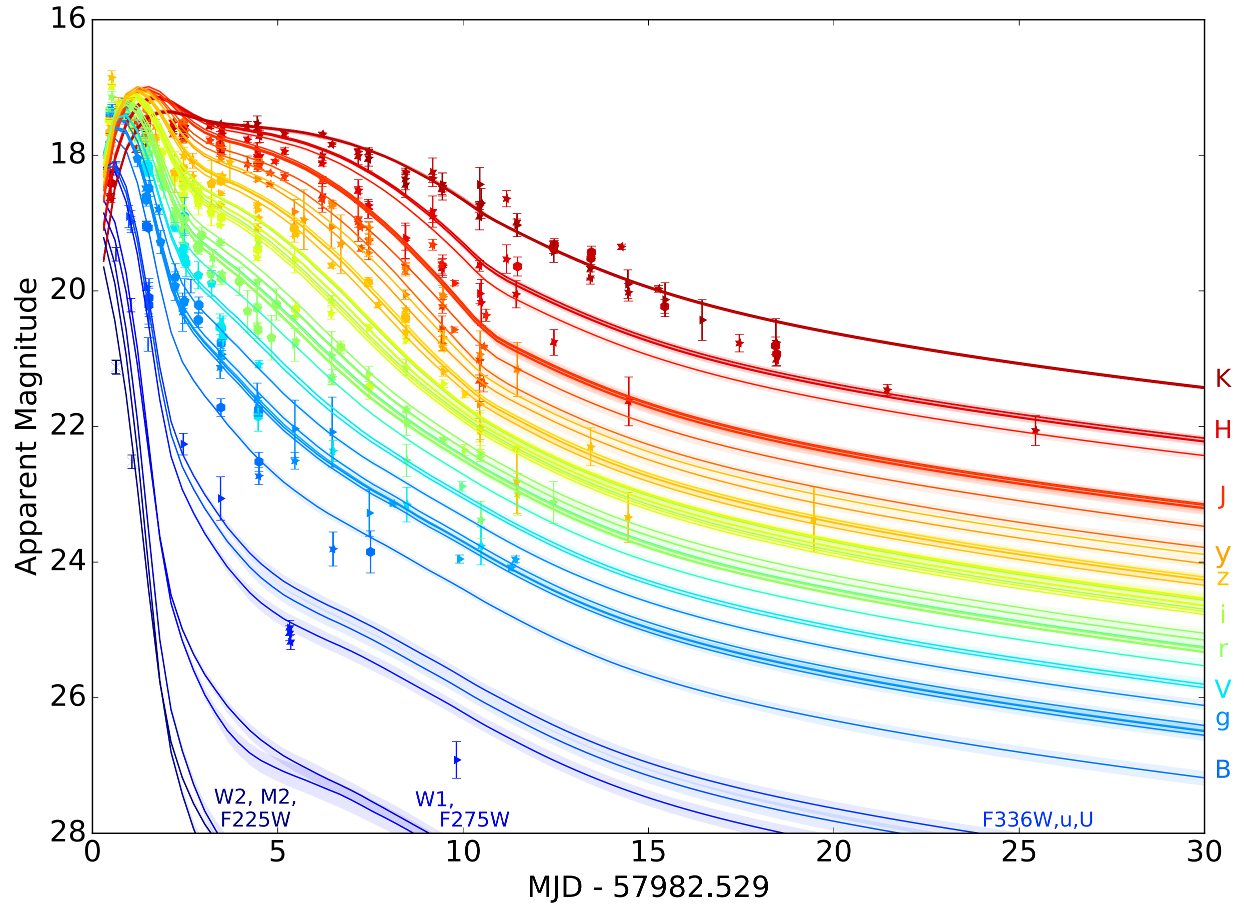

From Schatz et al. (2022), J. Phys. G: Nucl. Part. Phys. 49 110502

- Responsible for ~50% of the abundance of heavy elements
- High neutron density, temperature can reach > 10 GK
  - Compact binary mergers
  - Some types of core-collapse SNe
  - ?
- Required nuclear data
  - Nuclear masses
  - Neutron capture & photodissociation
  - $\beta$-decay & $\beta$-delayed neutron emission
  - Fission
  - …
- **Contains neutron-rich nuclear physics**

# *r*-process post-processing

Understand / reproduce
*r*-process observables




Hydrodynamical simulation of astrophysical events

$T(t), \rho(t)$,
initial conditions
etc.

**Nuclear reaction network calculation**

Nuclear heating

Experimental/theoretical properties of nuclei

Nuclear reaction/
decay rates,
Fission properties, etc.

# Propagation of nuclear physics uncertainty in nuclear reaction network calculations



**Nuclear mass model**

Uncertainty in
phenomenological/microscopic
description of ground state

→

**Reaction/decay rates**

Mass uncertainty propagated to
- Neutron capture
- Photodissociation
- $\beta$-decay
- $\beta$-delayed neutron emission
- Fission rates & products

Systematic uncertainty in
the descriptions of reaction/decay

→

**Nuclear reaction network calc.**

Uncertainty in
- Treatment of heating
- Assumptions in astrophysical trajectory
- Unaccounted for reactions (e.g. neutrinos)

**Underlying nuclear physics models / assumptions are not necessarily consistent.**

# Common mass models in *r*-process nucleosynthesis studies



## Macroscopic-microscopic models

Bulk properties + microscopic (shell, pairing, etc.) corrections

e.g. FRDM (finite-range droplet model), DZ (Duflo-Zucker)
WS (Weizsäcker-Skyrme)

## Microscopic model + phenomenological corrections

e.g. HFB-i (i = 1,…,32) models based on Skyrme-HFB framework

## Microscopic model

Skyrme-HFB mass models (parameter sets e.g. SkM*, UNEDF0/1, …),

Covariant DFT

| Mass model | $\sigma_{\mathrm{rms}}^{\mathrm{AME2020}}$ [MeV] |
|---|---|
| FRDM12 | 0.57 |
| DZ29 | 0.41 |
| WS4 | 0.28 |
| HFB31 | 0.55 |
| SkM* | 7.07 |
| UNEDF1 | 1.71 |

- How can we take into account the uncertainty of having multiple mass models, while considering the performance at the same time?

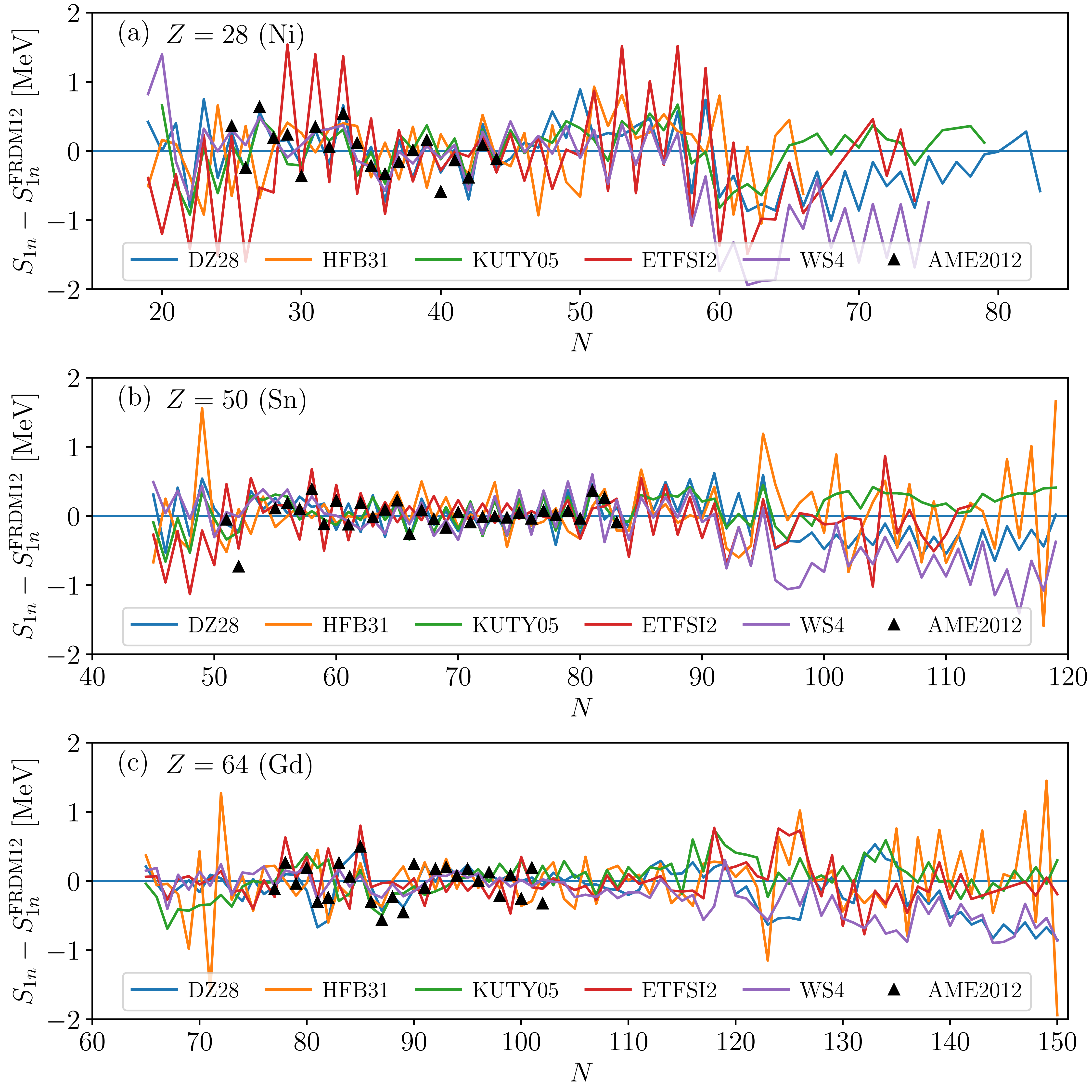
# Modelling the uncertainty of mass models

## Uncertainty to be modelled

- Discrepancies from experiments
- Discrepancies between mass models
- "Choice" of mass models
  - Quantitative measure of which model is "preferred"

## Considerations

- Most mass models do not come with uncertainty estimates
  - Typical BMA is not applicable



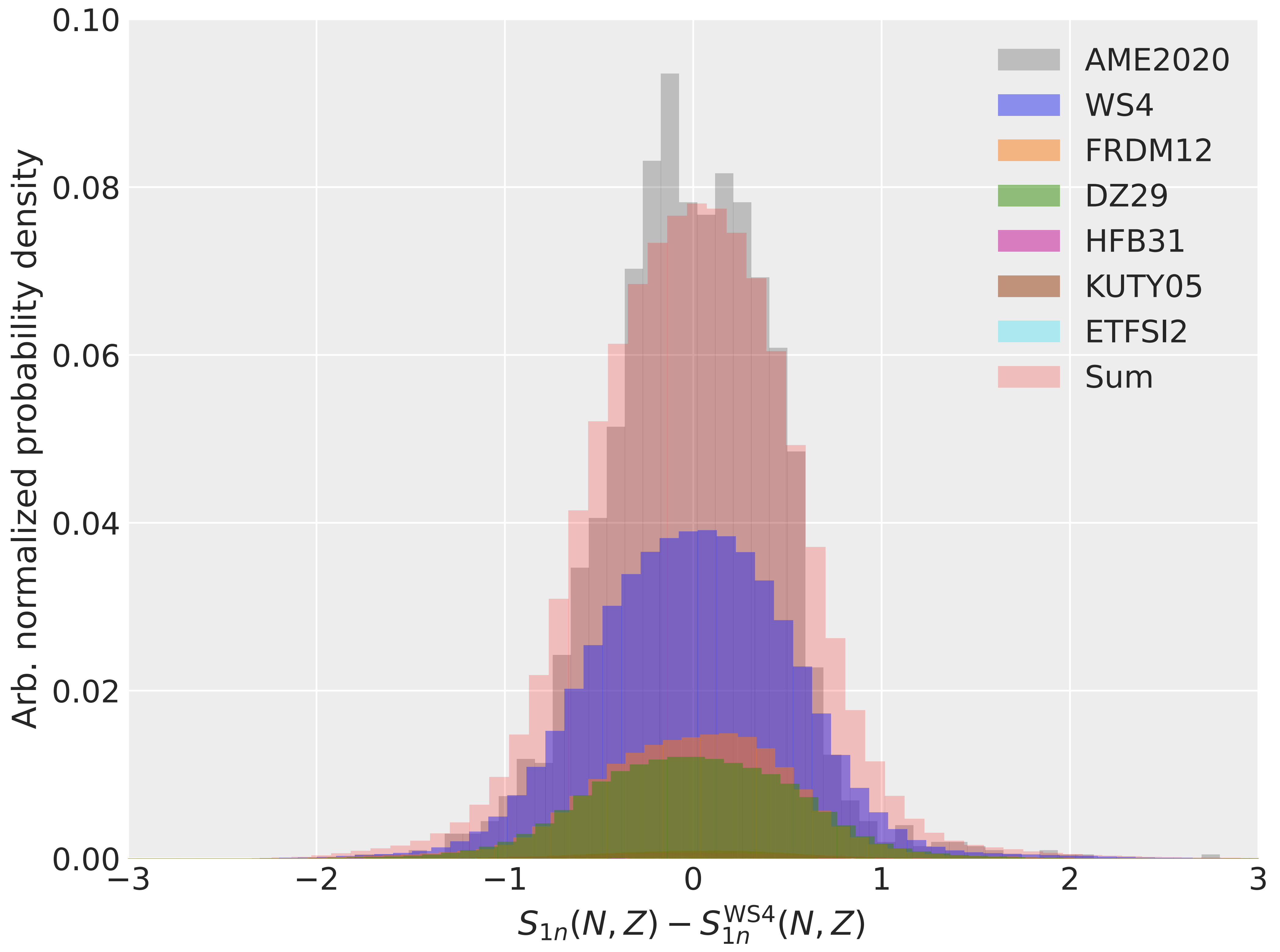
# Uncertainty quantification of one neutron separation energy ($S_{1n}$)

YS, Dillmann, Kruecken, Mumpower, and Surman, Phys. Rev. C 109, 054301 (2024)



- $S_{1n}$ is directly relevant to $(\gamma, n)$ rates
- Mass models are expressed as a superposition of Gaussians (Gaussian mixture model)
- Weights and $\sigma$ are inferred from experimental data through MCMC

| Mass model (raw) | Weight | Standard deviation | $\sigma_{\mathrm{RMS}}$ [MeV] |
|---|---|---|---|
| WS4 [6] | (0.459, 0.596) | (0.183, 0.214) | 0.239 |
| FRDM12 [2] | (0.143, 0.251) | (0.129, 0.174) | 0.312 |
| DZ29 [7] | (0.113, 0.229) | (0.125, 0.245) | 0.271 |
| KUTY05 [44] | (0.034, 0.130) | (0.140, 0.322) | 0.753 |
| HFB31 [10] | (0.000, 0.027) | (0.183, 0.214) | 0.428 |
| ETFSI2 [45] | (0.000, 0.027) | (0.026, 0.761) | 0.828 |



# Properties of the model



- Gaussian (scale) mixture model

$$p(S_{1n} \mid M_1, \ldots, M_K) = \sum_{k=1}^{K} w_k \, \mathcal{N}(\mu_k, \sigma_k)$$

Predictive quantity — Mass models — Weight — Gaussians representing mass models and errors

- $\sigma_k$ is the width of the Gaussian as a component of the mixture model

- Model variance = inter-model variance + within-model variance

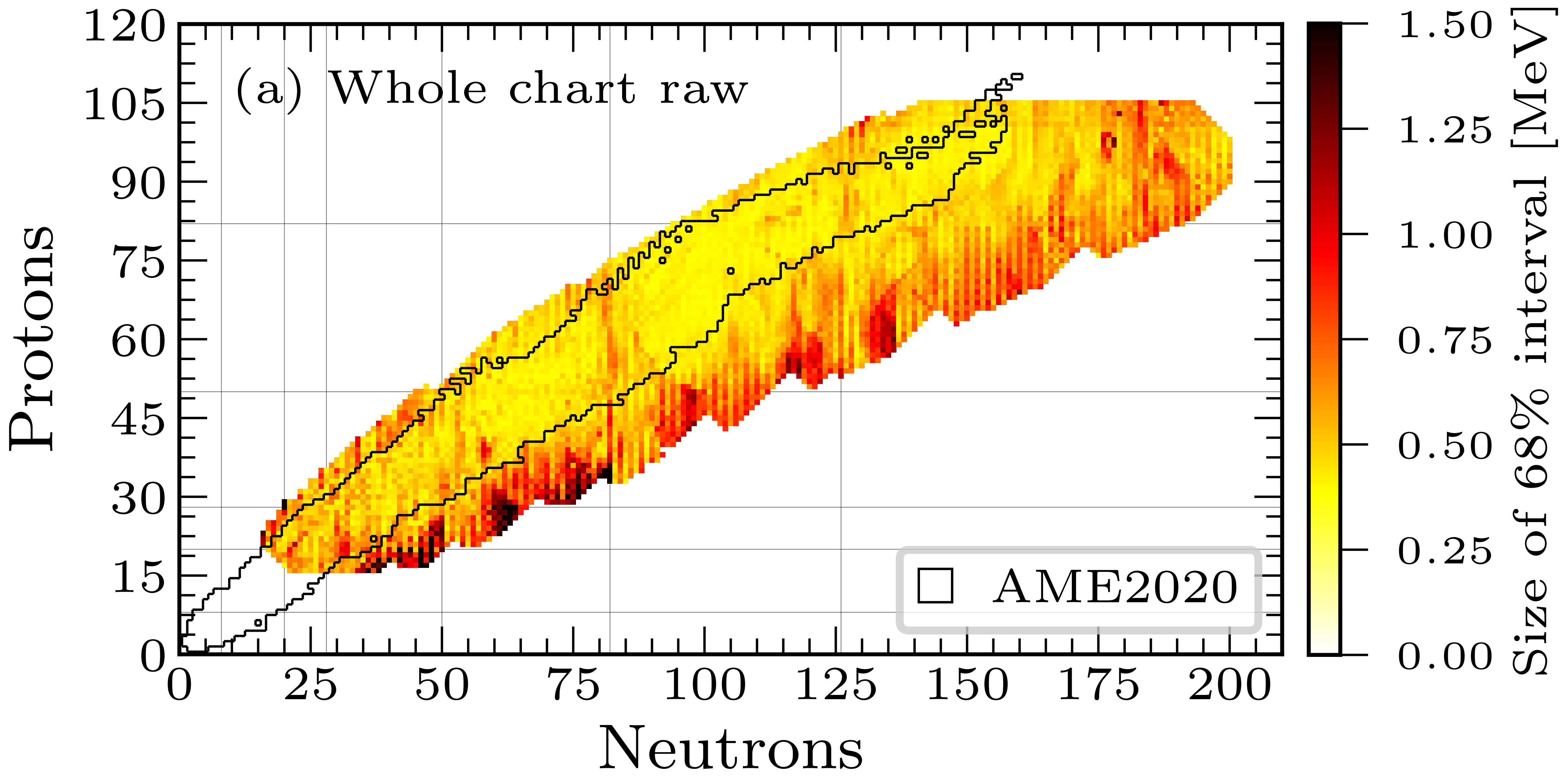
$$\mathrm{Var}(S_{1n} \mid M_1, \ldots, M_K) = \sum_{k=1}^{K} w_k \left( M_k - \sum_{l=1}^{K} w_l M_l \right)^2 + \sum_{k=1}^{K} w_k \sigma_k^2$$

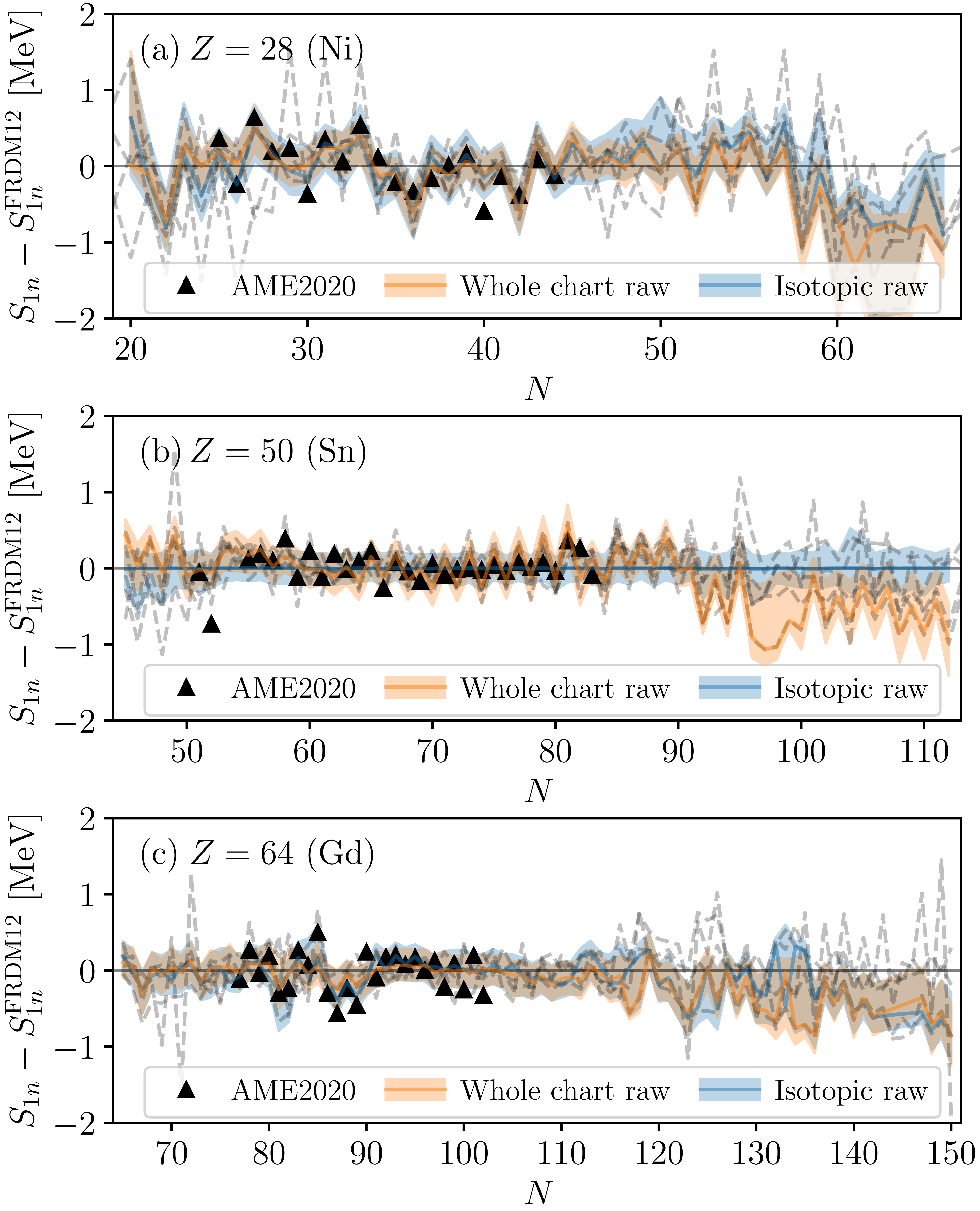
# Quantified uncertainty



- The Gaussian mixture can model the increasing uncertainty towards the neutron-rich region.

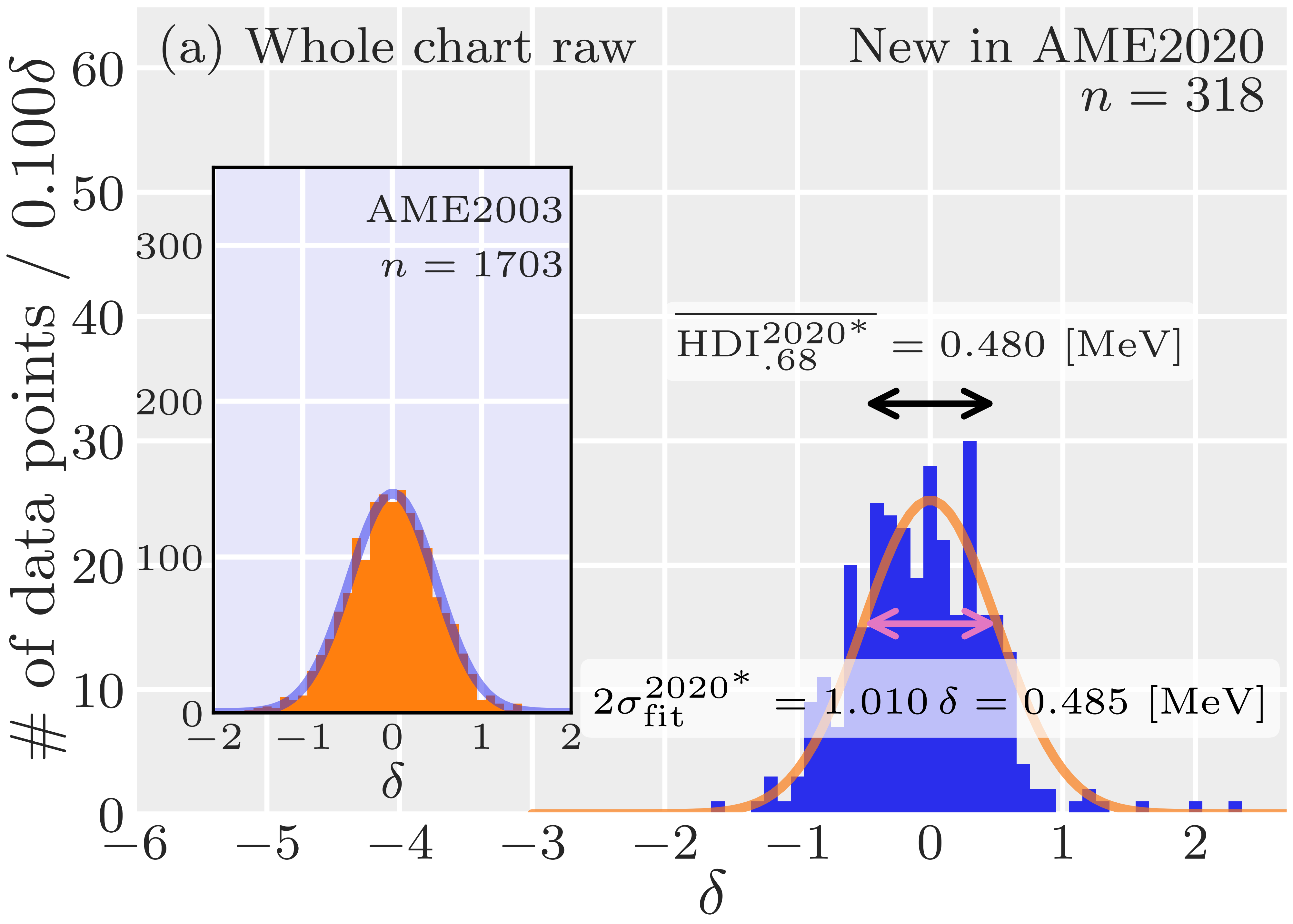
- Best result is obtained when the whole chart is used for inference.



# Discussion

- The method quantifies the uncertainty of the "choice" from a set of mass models you consider, based on the performance of the mass model.
- The model based on AME2003 provides adequate uncertainty estimates for new data in AME2020.




| | Training data (AME2003) | Test data (New data in AME2020) |
|---|---|---|
| Coverage of the 68% highest density interval | 71.5% | 69.5% |

**Figure: Distribution of experimental data relative to quantified uncertainty band**

# Comparison of different methods



- This work: Modelling uncertainty with a Gaussian mixture model

➡ Average the **predictive densities**

➡ The model parameters (weights etc.) are global, i.e. same for all nuclei

# Comparison of different methods



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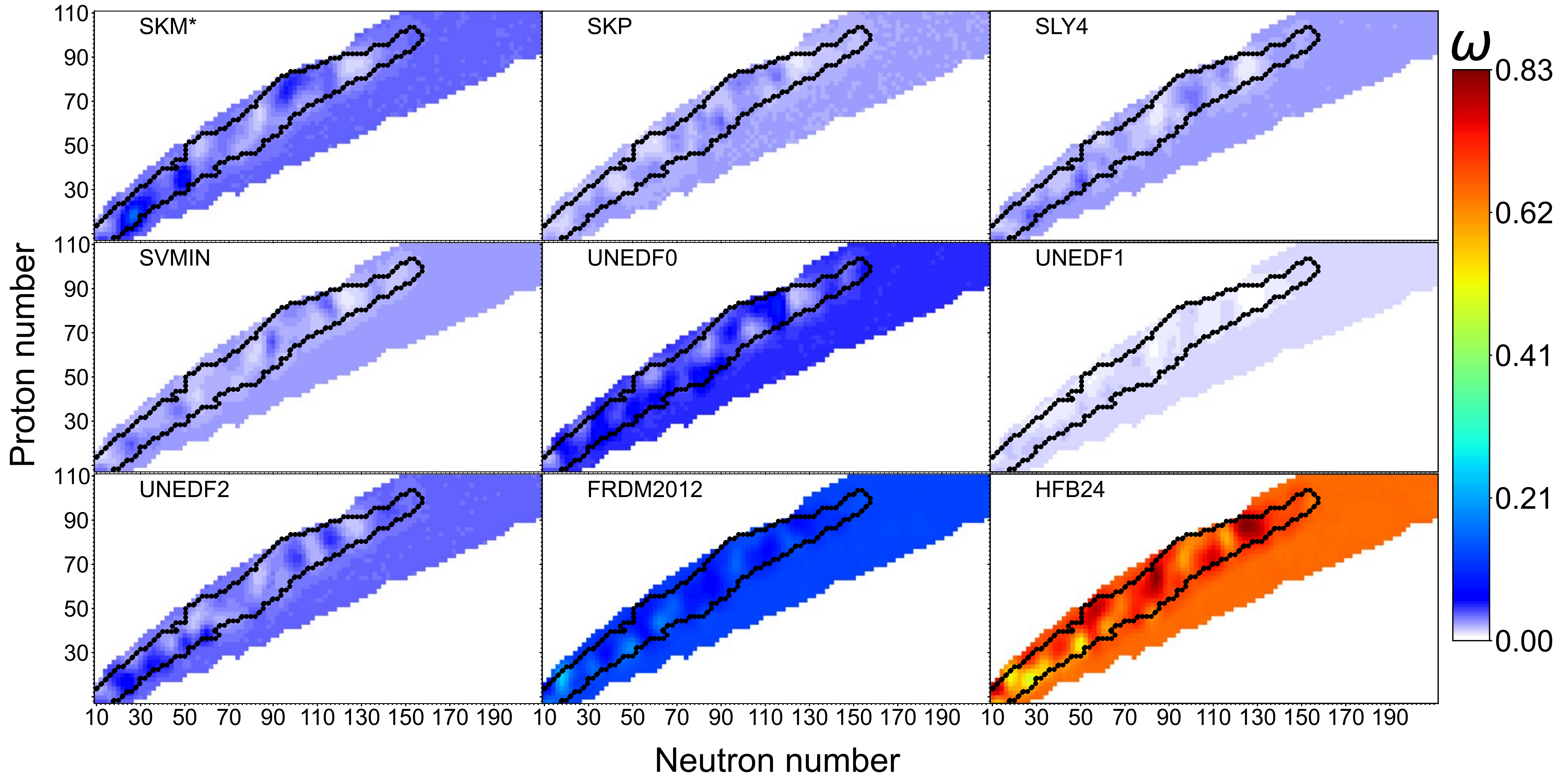
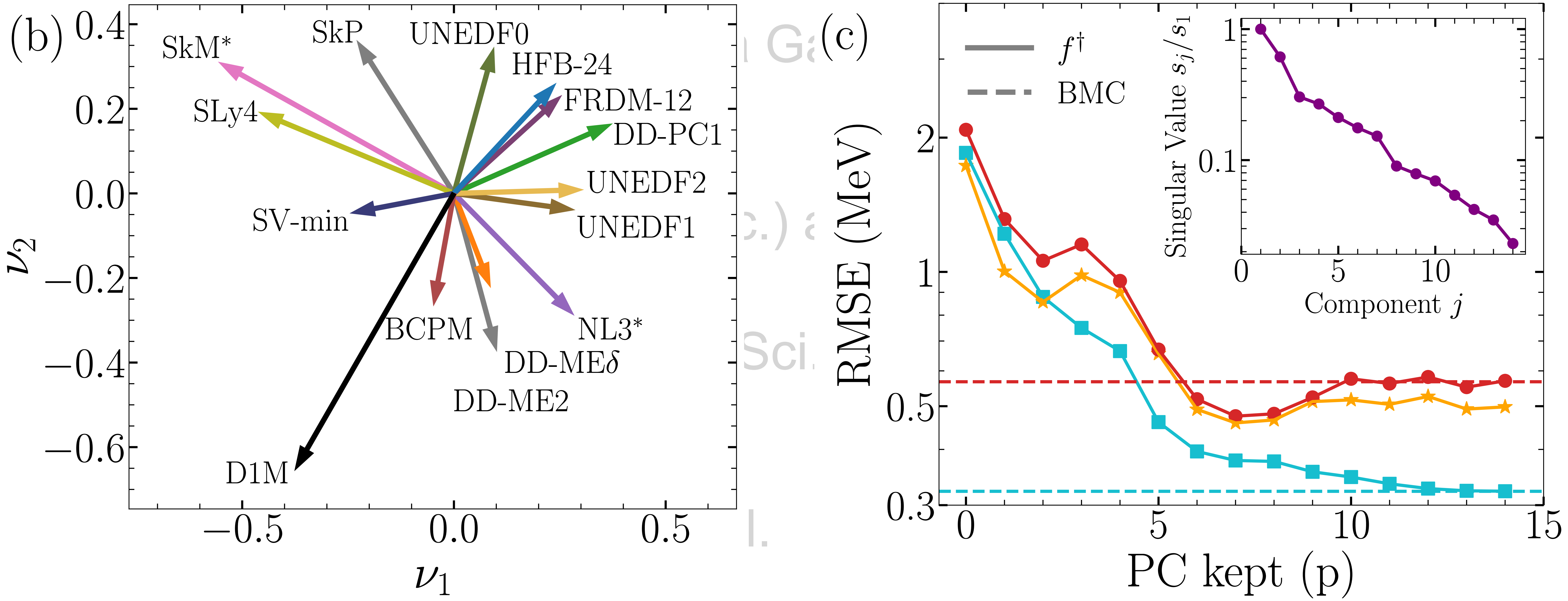
- Bayesian Model Mixing: Kejzlar et al., Sci. Rep. 13: 19600 (2023)
  - ➡ Average the **predictions**
  - ➡ The model parameters can be local.



# Comparison of different methods



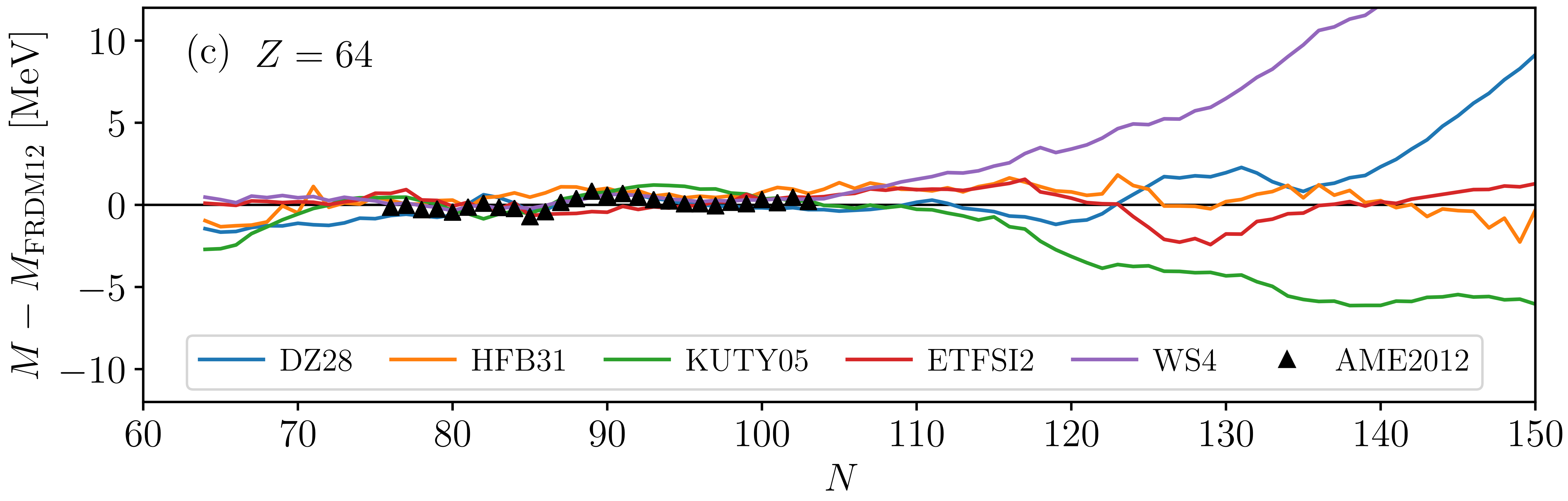

- Bayesian Model Combination: Giuliani et al. Phys. Rev. Res., 6: 033266 (2024)
  - ➡ Average the predictions
  - ➡ Redundant models are eliminated through PCA.

# Application to mass excess

- Uncertainty quantification of mass excess

➡ Propagation to $S_{1n}$, $Q_\beta$ and other relevant quantities for the *r*-process

➡ Challenging due to the large spread in the neutron-rich region.
(inter-model variance >> within-model variance $\sigma_k^2$)




➡ Parametric modelling of the within-model variance may be necessary.

# Summary and outlook



- Gaussian mixture model used to quantify the uncertainty of $S_{1n}$.
- This method averages the predictive densities, rather than the predictions.
- The variance can naturally incorporate
  the spread between the models into the uncertainty.
- There is still work to be done before it can be applied to the *r*-process.

# Nuclear Reaction Network

One-nucleus | Two-nucleus | Three-nucleus reaction

$$\frac{dY_i}{dt} = \sum_j P_j^i \; \lambda_j Y_j + \sum_{j,k} P_{j,k}^i \; \frac{\rho}{m_u} \langle j,k \rangle Y_j Y_k \; + \sum_{j,k,l} P_{j,k,l}^i \; \frac{\rho^2}{m_u^2} \langle j,k,l \rangle Y_j Y_k Y_l.,$$

- More than 5000 species involved for the rapid neutron capture process.
- Inputs:
  - Nuclear: reaction/decay rates, masses, etc.
  - Astro: Temporal evolution of $T$ and $\rho$, and initial $Y_i$
- Outputs:
  - Time evolution and final ($t \to \infty$) values of $Y_i$
  - energy release
- Typical computation time: **a few minutes to hours.**

➡ **Still too costly for Bayesian inference**

# Reducing the computational cost of reaction network calculations with an ANN emulator

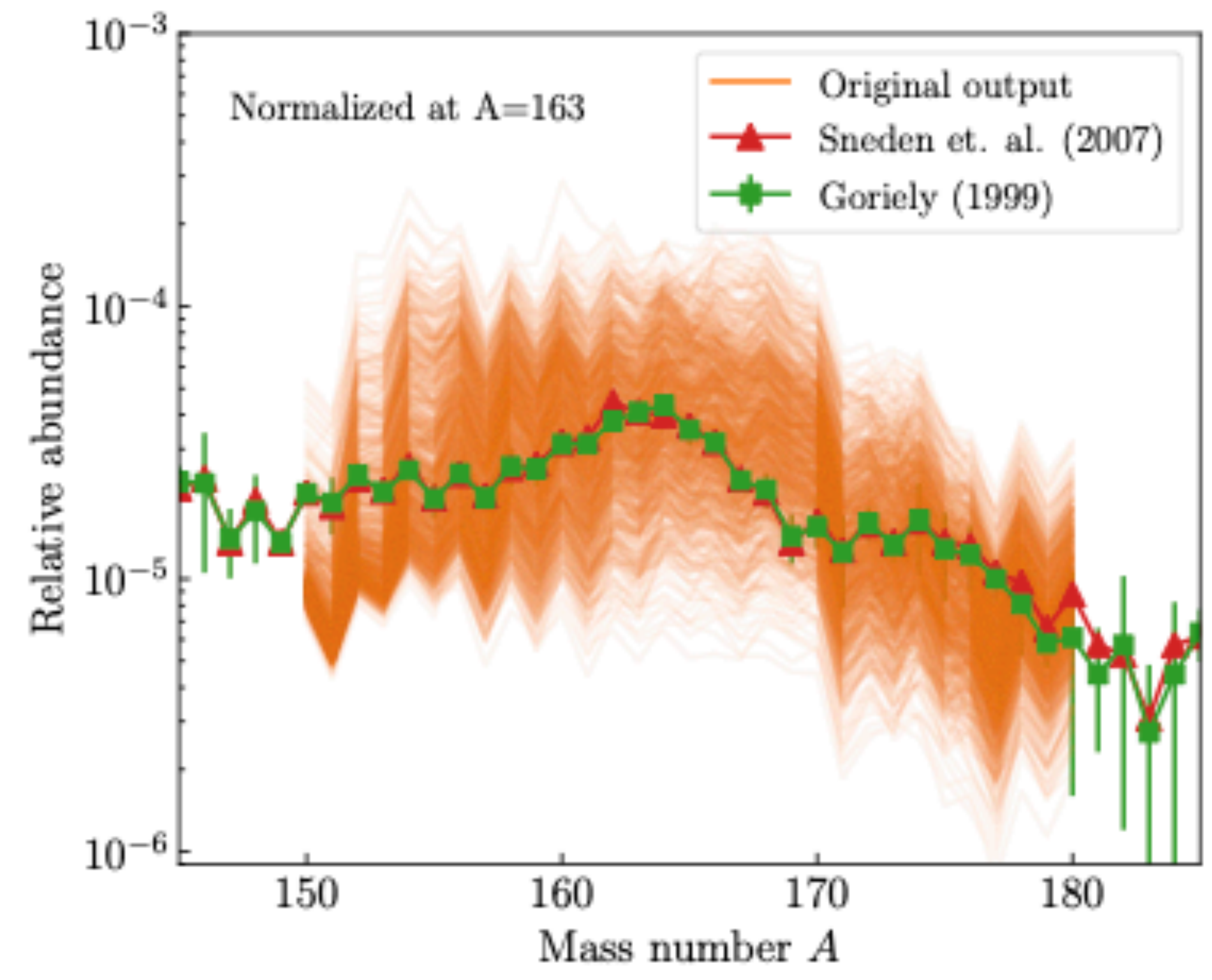


Simultaneously vary

- $\beta$-decay half-lives
- $S_n$ (propagated to $n$ capture rate)

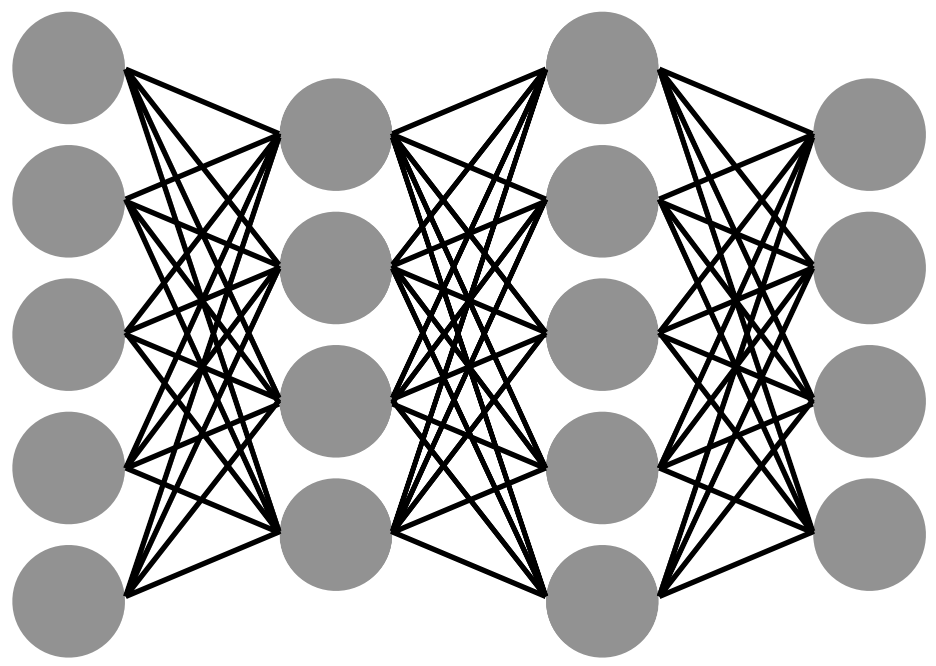
Solve nuclear reaction network ODE:

$$\frac{dY_i}{dt} = \sum_j P_j^i \ \lambda_j Y_j + \sum_{j,k} P_{j,k}^i \ \frac{\rho}{m_u} \langle j,k \rangle Y_j Y_k + \sum_{j,k,l} P_{j,k,l}^i \ \frac{\rho^2}{m_u^2} \langle j,k,l \rangle Y_j Y_k Y_l.,$$

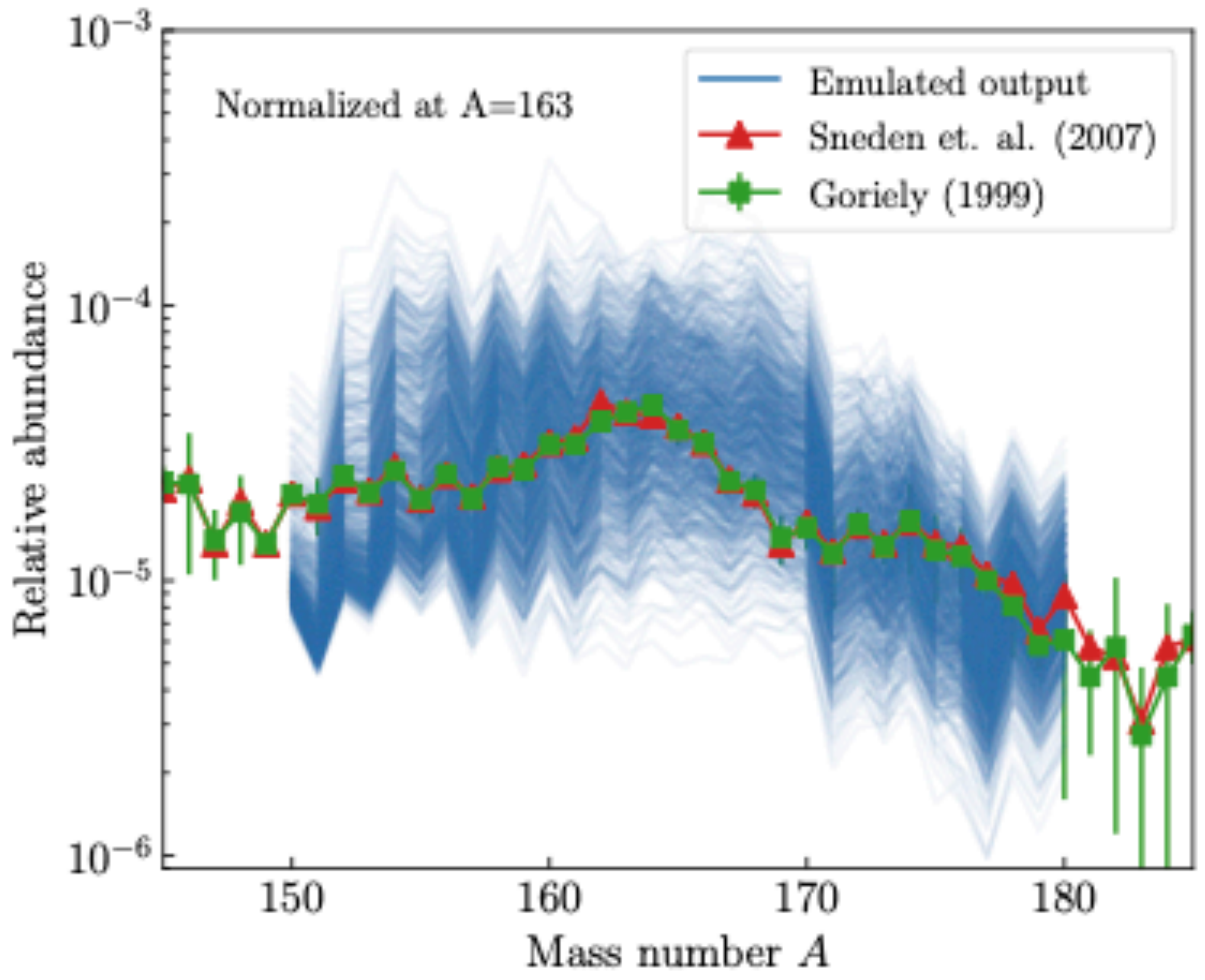



**Train**

ANN Emulator

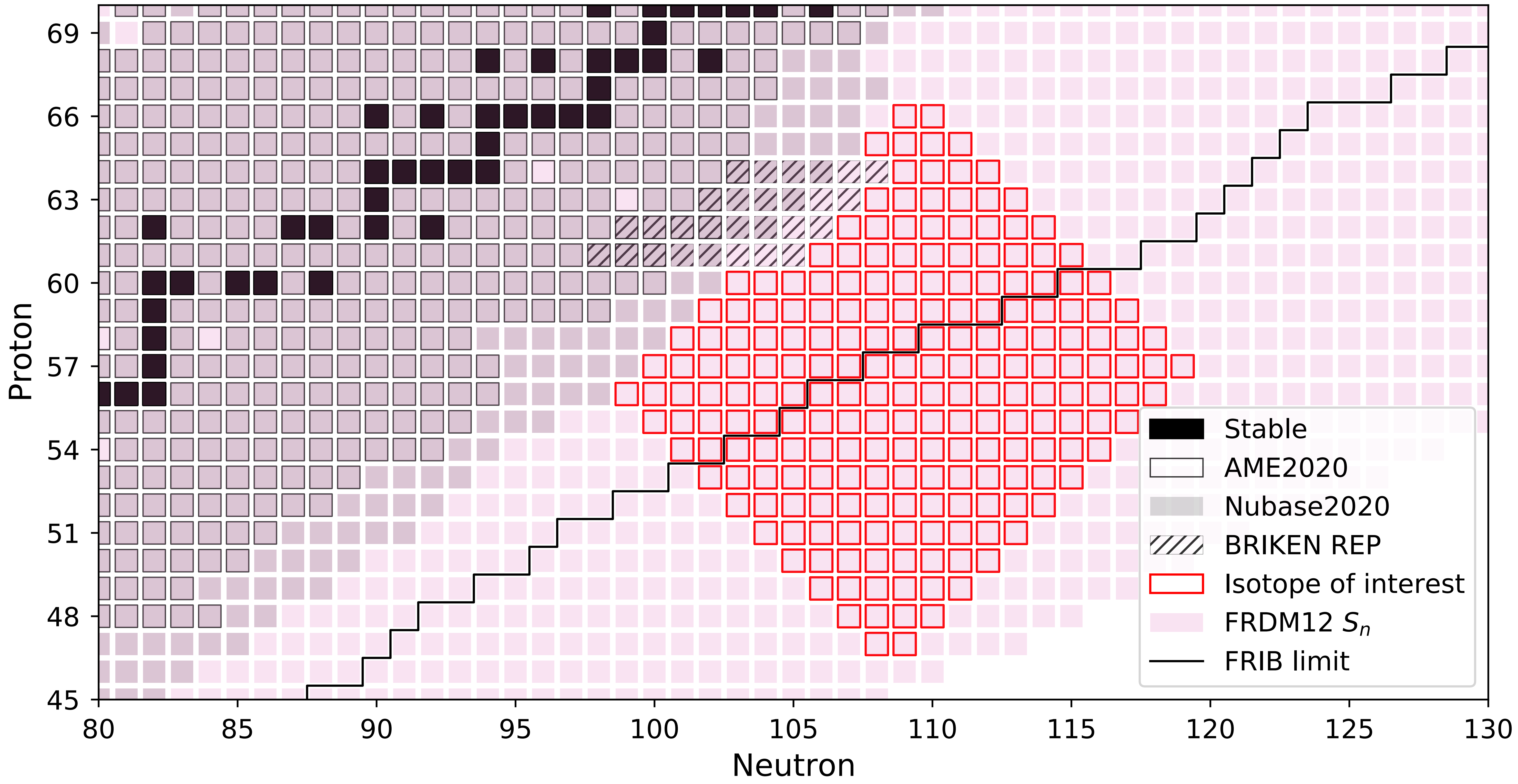


**Predict**

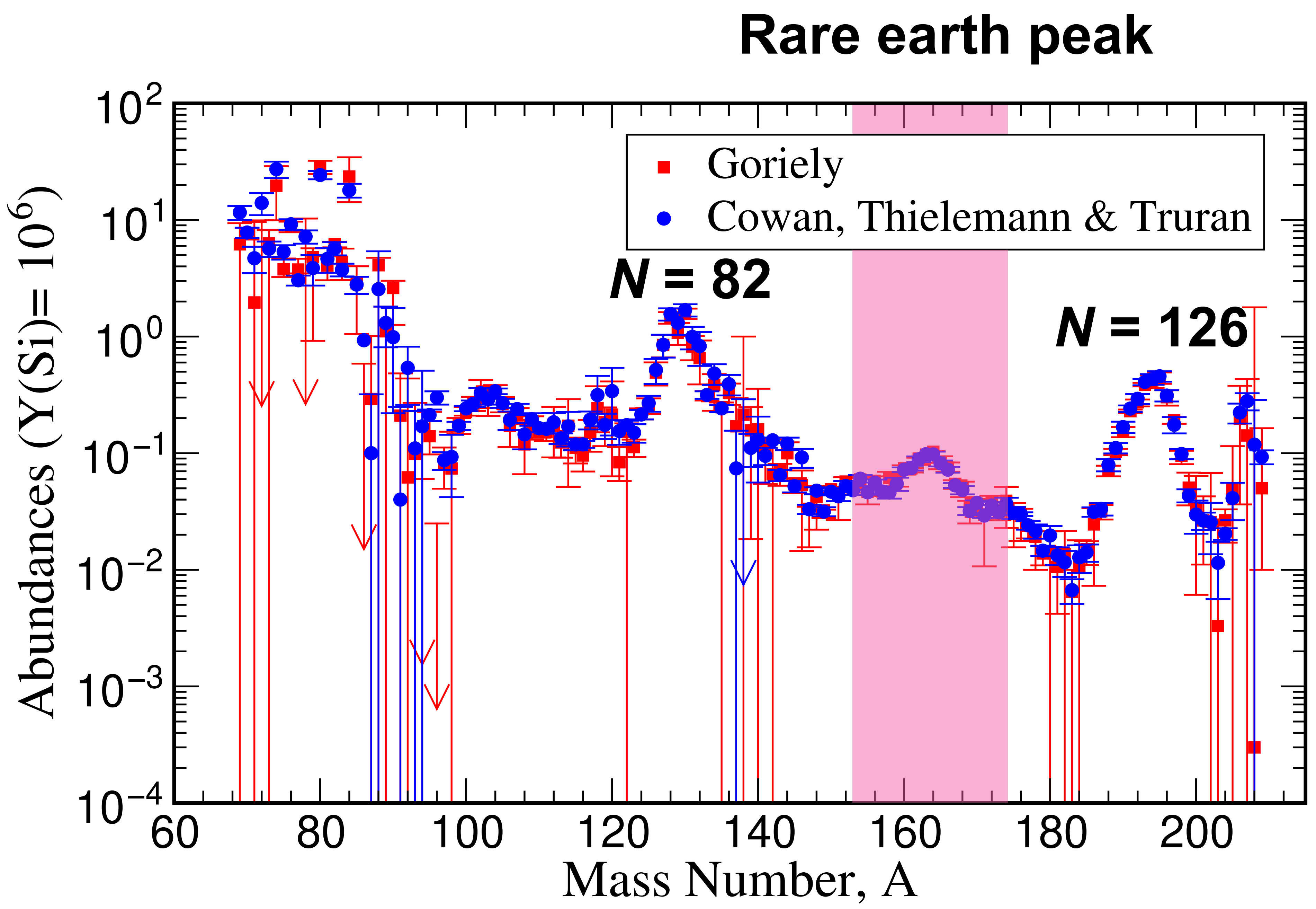


# Reducing the computational cost of reaction network calculations with an ANN emulator






BRIKEN REP $\beta$-decay measurement: G. Kiss, A. Vitéz-Sveiczer, YS, et al. (2022) APJ, 936:107




From Cowan et al. (2021), Rev. Mod. Phys. **93**, 015002

# ANN architecture



- Neural architecture search (NAS) + manual tuning to find the optimal architecture.

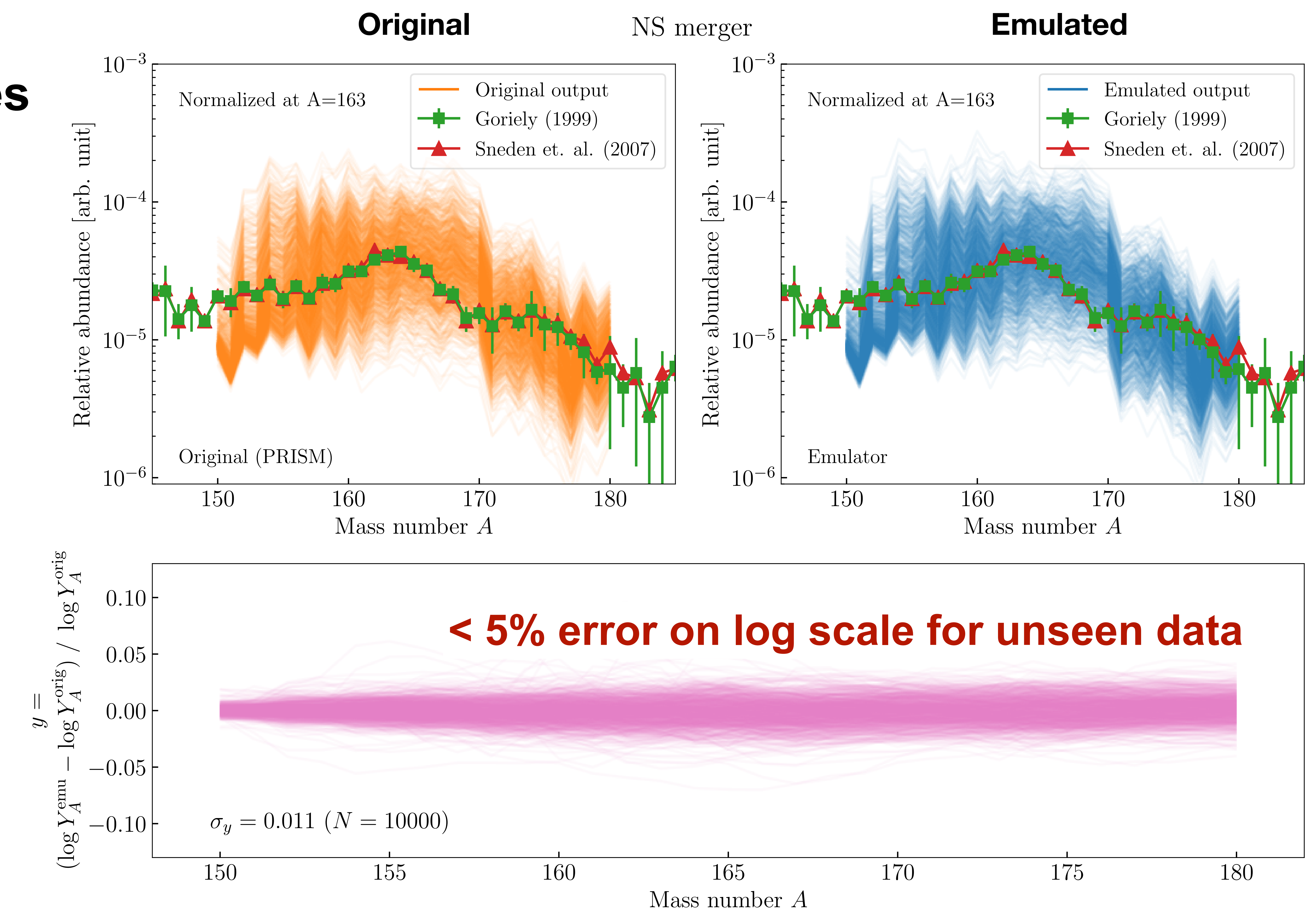
| Layer No. | Layer type | Activation | Kernel size | No. of filters | No. of units |
|---|---|---|---|---|---|
| 1 | Convolutional | ReLU | (3,3) | 128 | — |
| 2 | Convolutional | ReLU | (3,3) | 128 | — |
| 3 | Convolutional | ReLU | (3,3) | 128 | — |
| 4 | Convolutional | ReLU | (3,3) | 128 | — |
| 5 | Flatten | — | — | — | — |
| 6 | Fully connected | ReLU | — | — | 1024 |
| 7 | Fully connected | Linear | — | — | 31 |

- Trained on 300k samples.

# Performance of the emulator

- **~8 seconds to generate 10k samples with a NVIDIA P100 GPU**

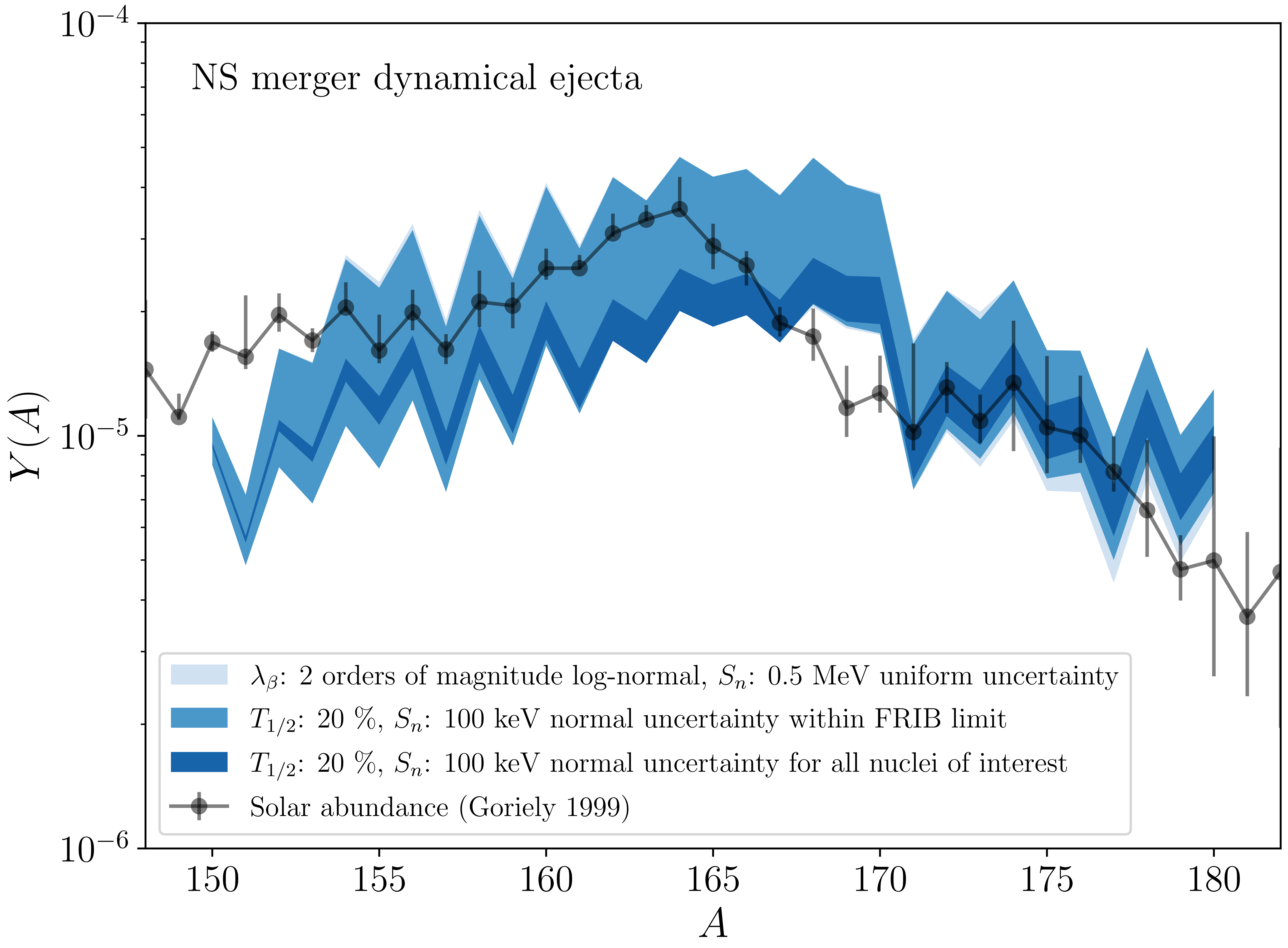
- It can be used in various tasks
  - Uncertainty propagation
  - Sensitivity analysis with correlated effect
    e.g. Kiss, Vitéz-Sveiczer, YS, et al. (2022) APJ, 936:107
  - Inverse problems
    e.g.
    Mumpower et al. (2017)
    J. Phys. G: Nucl. Part. Phys. 44 034003
    Vassh et al. (2021)
    ApJ 907 98

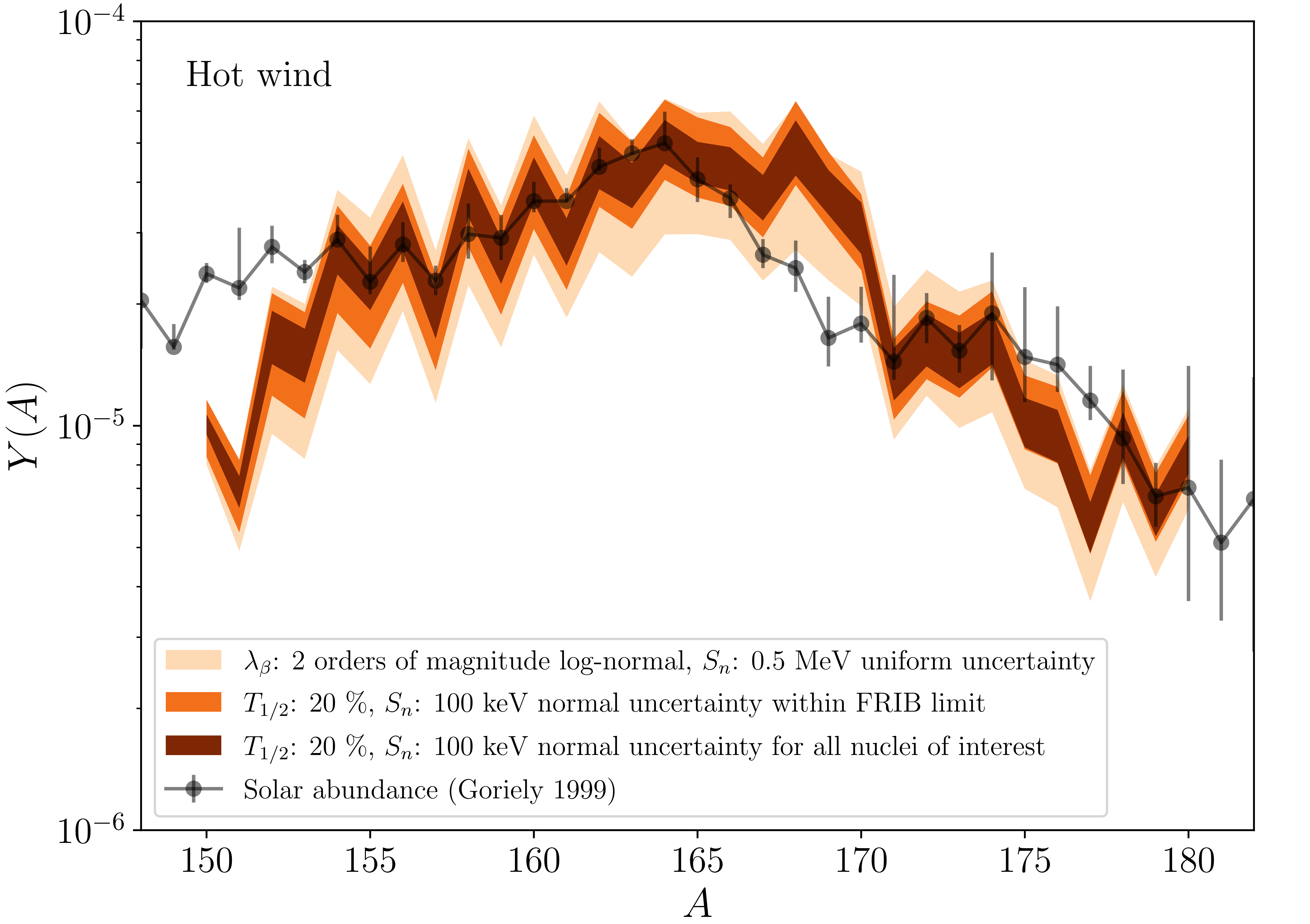



**YS et al. arXiv 2412.17918 (2025), submitted to J. Phys. G**

# Hypothetical uncertainty reduction with FRIB

The bands represent $\pm 1\sigma$ intervals




**YS et al. arXiv 2412.17918 (2025), submitted to J. Phys. G**

# Towards a more complete emulator



- Emulation of the complete abundance pattern
- Emulation of the time evolution of abundances

- Handle a wider variety of nuclear physics inputs
- Astrophysical conditions as input

- Development underway

# Summary

- Bayesian methods for uncertainty quantification in the presence of multiple models
- Emulators for *r*-process calculations

# Long-term goals

- Development of uncertainty-quantified, microscopic datasets for the *r*-process studies
- Development of a suite of emulators to enable uncertainty quantification, sensitivity analyses, and inverse problems
- Inference of neutron-rich nuclear properties from the *r*-process observables

**Thank you for your attention!**

NP3M FRIB UNIVERSITY OF NOTRE DAME THE UNIVERSITY OF TENNESSEE KNOXVILLE TRIUMF

# Backup slides

# The EBMA model (1)



- Prior for weights: $p(w_1, w_2, \ldots, w_k) = \mathrm{Dirichlet}(w_1, w_2, \ldots, w_k \mid \alpha_1, \alpha_2, \ldots, \alpha_k)$

$$= \frac{\Gamma\left(\sum_{k=1}^{K} \alpha_k\right)}{\prod_{k=1}^{K} \Gamma(\alpha_k)} \prod_{k=1}^{K} w_k^{\alpha_k - 1}, \quad \text{with } \alpha_1, \ \ldots, \alpha_k = 1$$

- Prior for variance: $p(\sigma_k) = \lambda \exp(-\lambda \sigma_k), \quad k = 1, \ \ldots, K$

- Likelihood: $L(w_1, \ldots, w_K, \sigma_1^2, \ldots, \sigma_K^2)$

$$= \prod_{n,p} \left( \sum_{k=1}^{K} w_k g_k(\Delta_{n,p} \mid m_{k,n,p}) \right),$$

- Posterior: $p(\boldsymbol{w}, \boldsymbol{\sigma}^2 \mid D) \propto L(\boldsymbol{w}, \boldsymbol{\sigma}^2)\ p(\boldsymbol{w})\ p(\boldsymbol{\sigma}^2),$

# The EBMA model (2)



- Predictive variance:

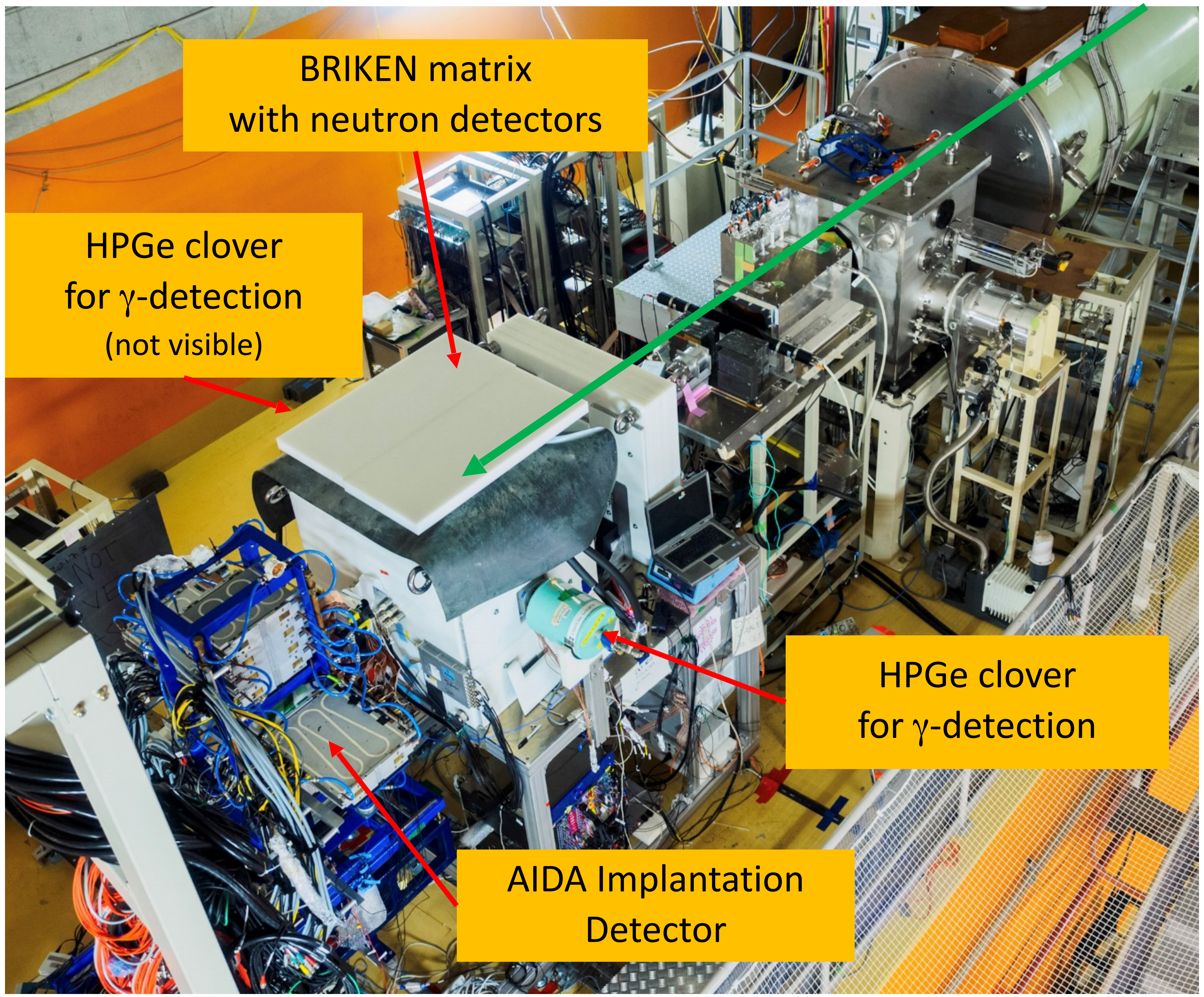
$$\mathrm{Var}(\Delta \mid m_1, m_2, \ldots, m_K) = \sum_{k=1}^{K} w_k \left( (m_k) - \sum_{i=1}^{K} w_i (m_i) \right)^2 + \sum_{k=1}^{K} w_k \sigma_k^2,$$

  - First term: spread of predictions by the member mass models of the ensemble,

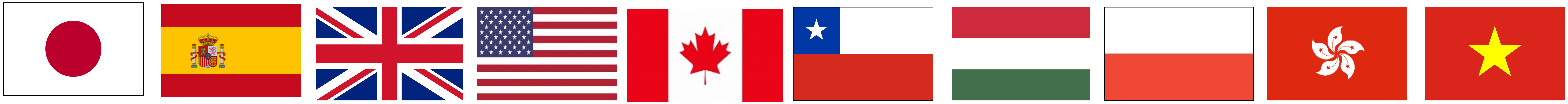
  - Second term: deviation from the observations of each mass model within the ensemble, weighted by the posterior weights.

# BRIKEN Experimental setup at RIKEN Nishina Center





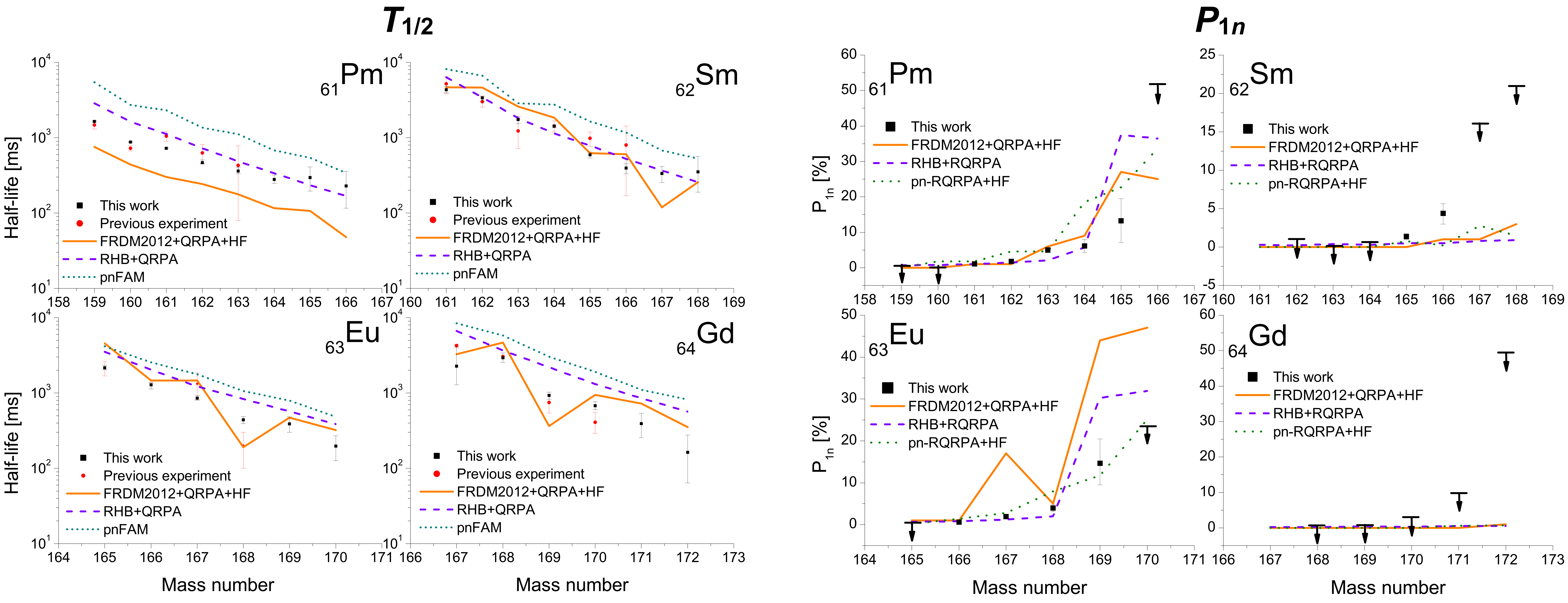

- Experimental campaign from 2016-2021
- Goal: measure half-lives and neutron-branching ratios of the most neutron-rich isotopes
- Physics results published so far:
  153 isotopes between $^{75}$Ni – $^{172}$Gd
  29 new $T_{1/2}$, 77 new $P_{1n}$ values,
  36 new $P_{2n}$ values



# BRIKEN experimental data

$P_{1n}$ and $T_{1/2}$ of $^{159-166}$Pm, $^{161-168}$Sm, $^{165-170}$Eu, and $^{167-172}$Gd measured with the BRIKEN detector system (28 isotopes, **9 new** $T_{1/2}$ and **28 new** $P_{1n}$)

## New experimental data from BRIKEN




G. Kiss, A. Vitéz-Sveiczer, YS, et al. (2022) APJ, 936:107

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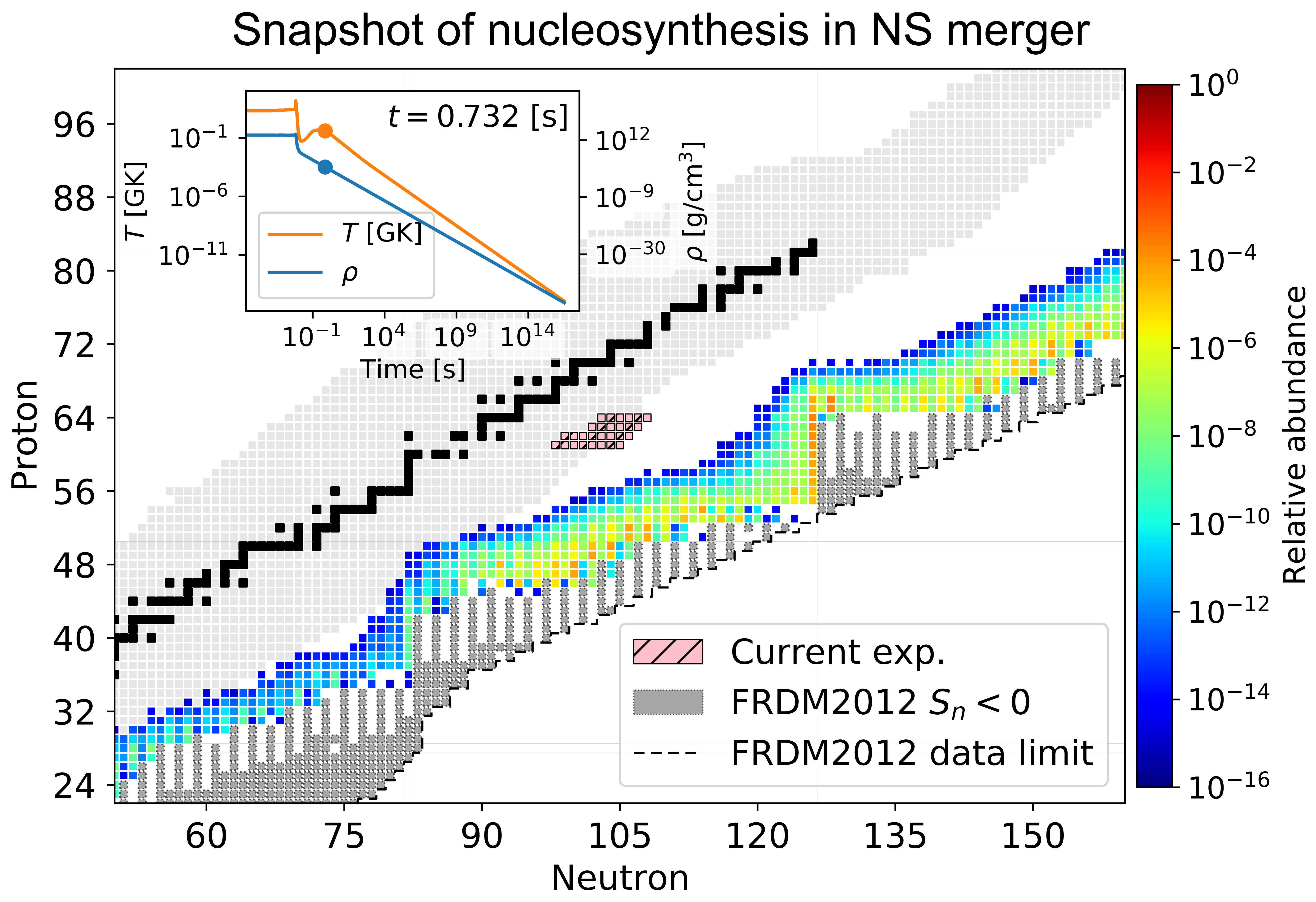


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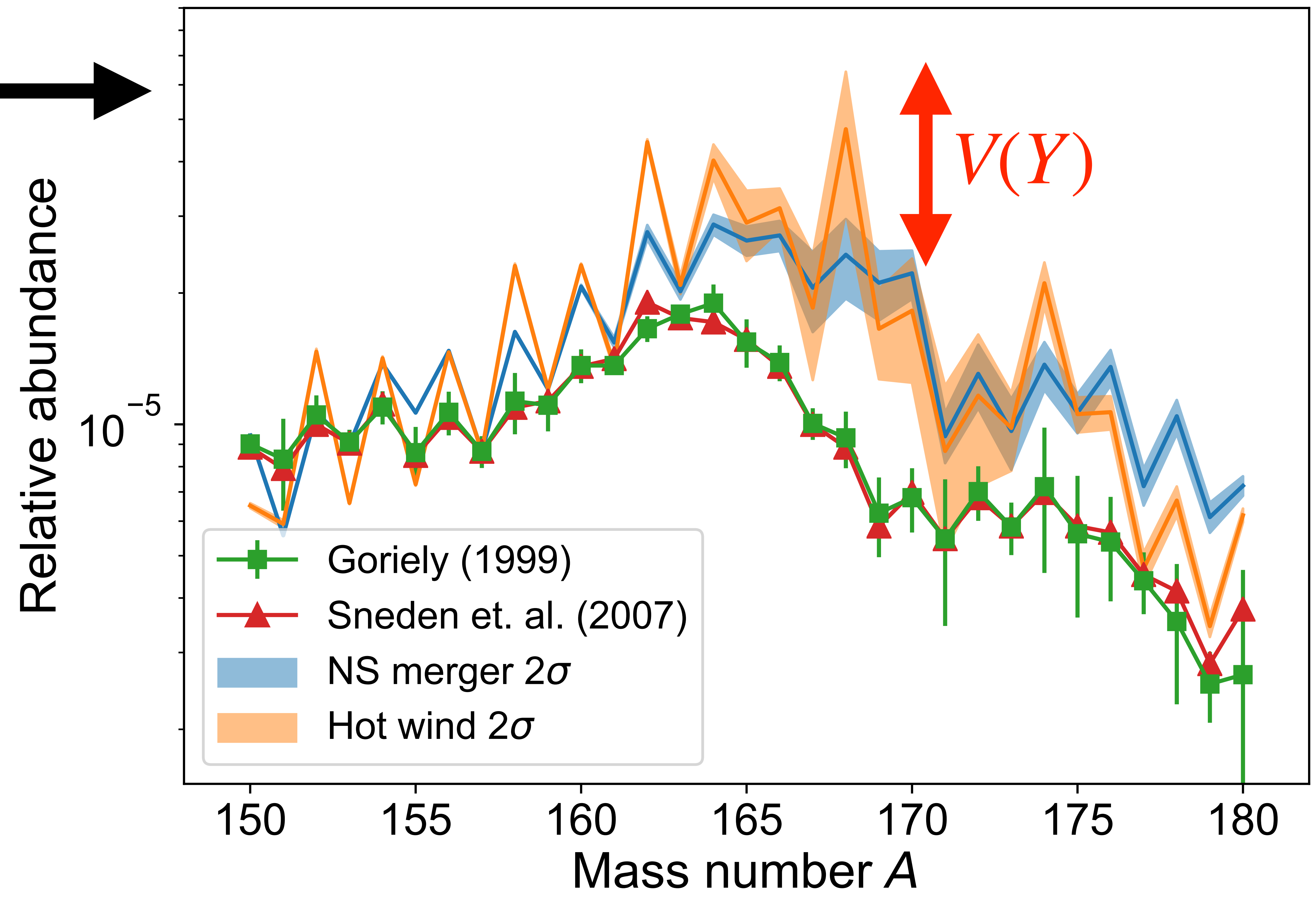
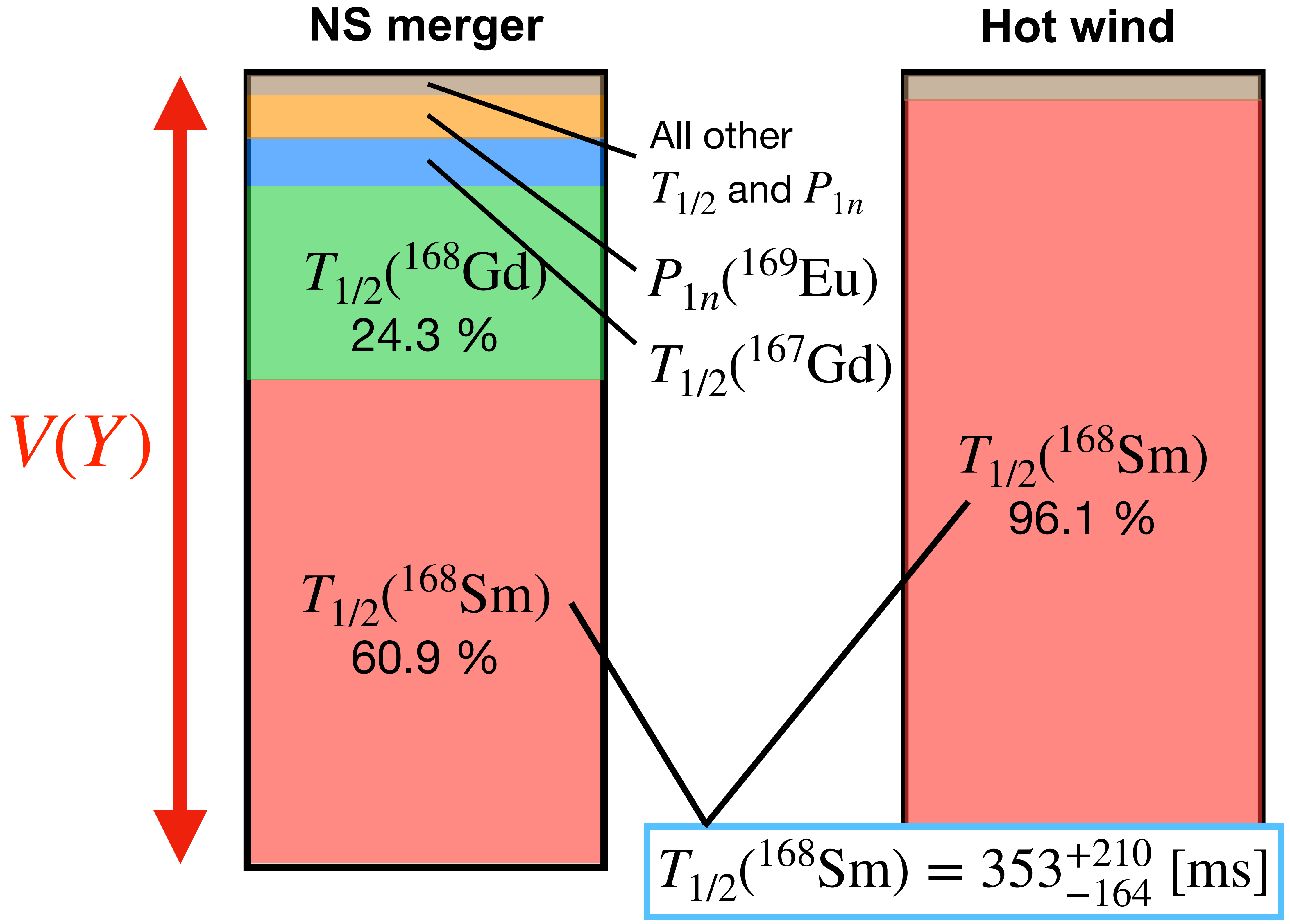
# Variance-based sensitivity analysis

Exp. uncertainty of $T_{1/2}$ and $P_{1n}$

**Monte Carlo sampling and abundance calculations**




**e.g. A=168**




**Variance decomposition**

G. Kiss, A. Vitéz-Sveiczer, YS, et al. (2022) APJ, 936:107

## $(n,\gamma) \leftrightarrow (\gamma,n)$ equilibrium

$$\frac{Y(N+1,Z)}{Y(N,Z)} = n_n \cdot \frac{G(N+1,Z)}{2G(N,Z)} \cdot \left(\frac{A+1}{A}\right)^{3/2} \cdot \left(\frac{2\pi\hbar^2}{m_u kT}\right)^{3/2} \cdot \exp\left(\frac{S_n(N+1,Z)}{kT}\right),$$

## Detailed balance

$$\lambda_{(\gamma,n)} = \langle\sigma v\rangle_{(n,\gamma)} \cdot \frac{G(N,Z)\cdot G_n}{G(N+1,Z)} \cdot \left(\frac{A}{A+1}\right)^{3/2} \cdot \left(\frac{m_u kT}{2\pi\hbar^2}\right)^{3/2} \cdot \exp\left(\frac{-S_n(N+1,Z)}{kT}\right),$$