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Covariances from model variation: Application to quantities for astrophysics

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Summary

- Background, Goal and Method
- Model variation
- Examples
- Future

Background

- Current evaluated covariances are usually based on
  - Dedicated assessment of experimental/theoretical uncertainties + biases
  - Default theoretical calculations

- In TENDL (and partly in JEFF-3.3), covariances are based on
  - BMC when experimental data are available
  - TMC when experimental data are not available

- In case of covariances based on theoretical calculations
  - Parameter pdf are assumed
  - A set of models is fixed

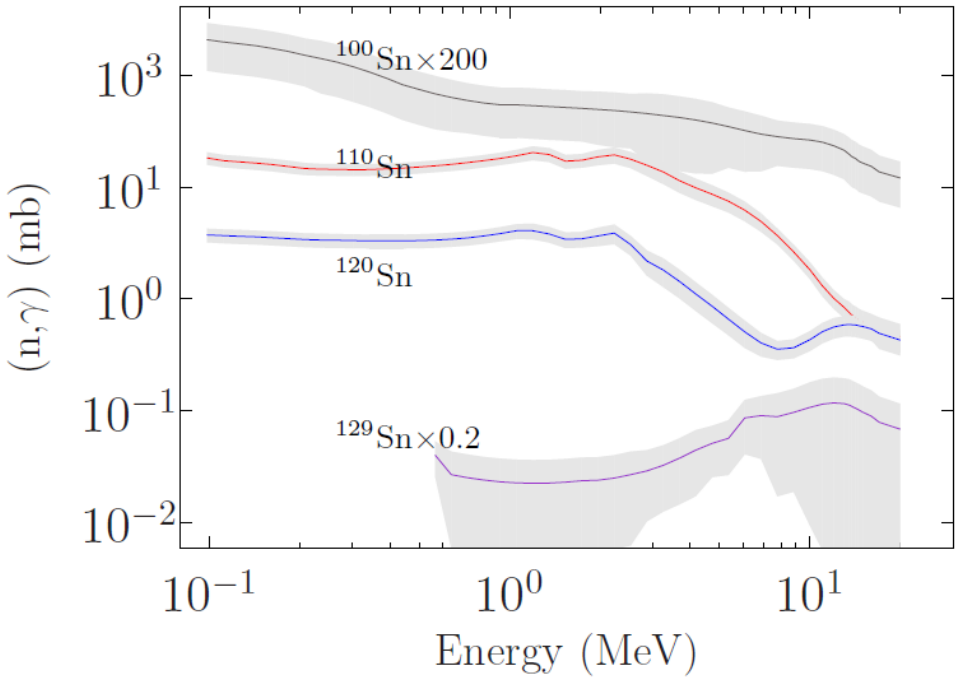
- This is fine when model predictions are “good” compared to their parameter variations

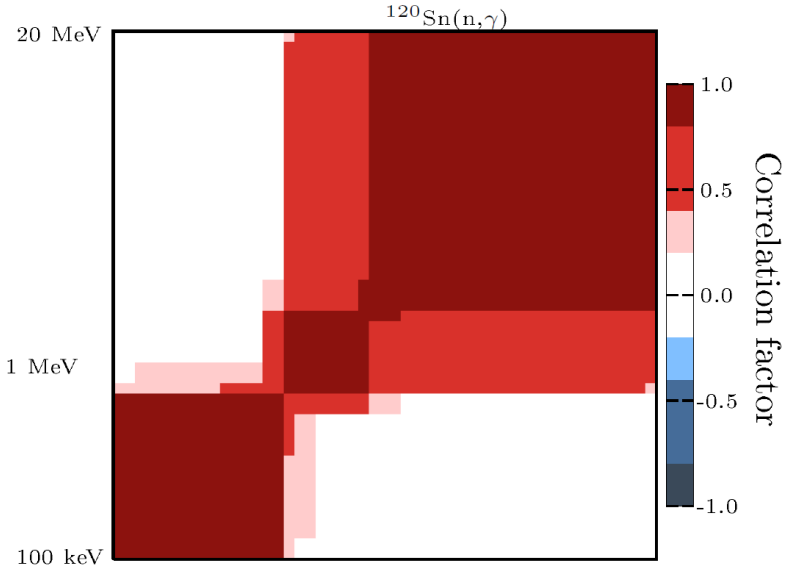
- What to do away from the stability line ?

Example on Sn isotopes

– From drip line to drip line: Sn 94 – [112-124] – 169.

– In TENDL-2021: Sn 100 – 134.
– Covariance obtained by variation of model parameters (OMP, LD, γ-str)





Background & Goal

- In astrophysics, more than 8800 isotopes can be considered
  - ≈ 270 with experimental data
  - ≈ 3500 with known masses (Audi masses)
  - ≈ 5400 with nothing

- Changing model parameters is not enough
- Changing models gives an indication of systematical effects

- Goal: Produce quantities as in BRUSLIB but with uncertainties:
  - Cross sections & Reaction rates (n,g), (n,p), (n,a) (p,a), (p,n), (p,g) (a,n), (a,p), (a,g)
  - MACS
  - Normalized partition functions

Method

- Systematical TALYS calculations for 8800 isotopes (ground state)
- For each isotopes, repeat calculations with different models and extract:
  - 9 cross sections from 0.01 eV to 20 MeV:

    (n,g), (n,p), (n,a)
    (p,a), (p,n), (p,g)
    (a,n), (a,p), (a,g)

  - 9 Reaction rates for all temperatures taking into account the thermal population of the target

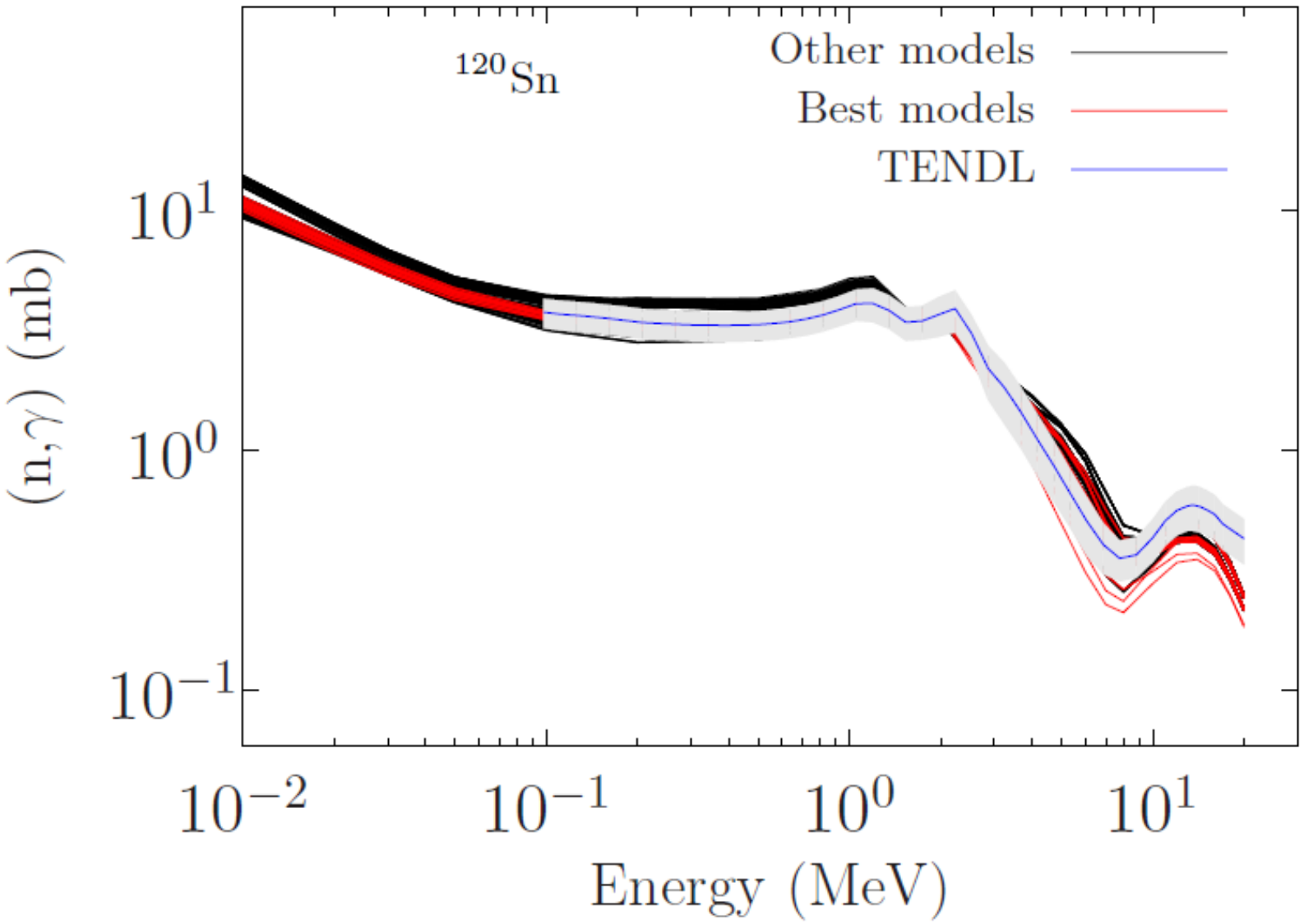
  - 1 Normalization partition function

  - 1 Laboratory (not stellar) MACS

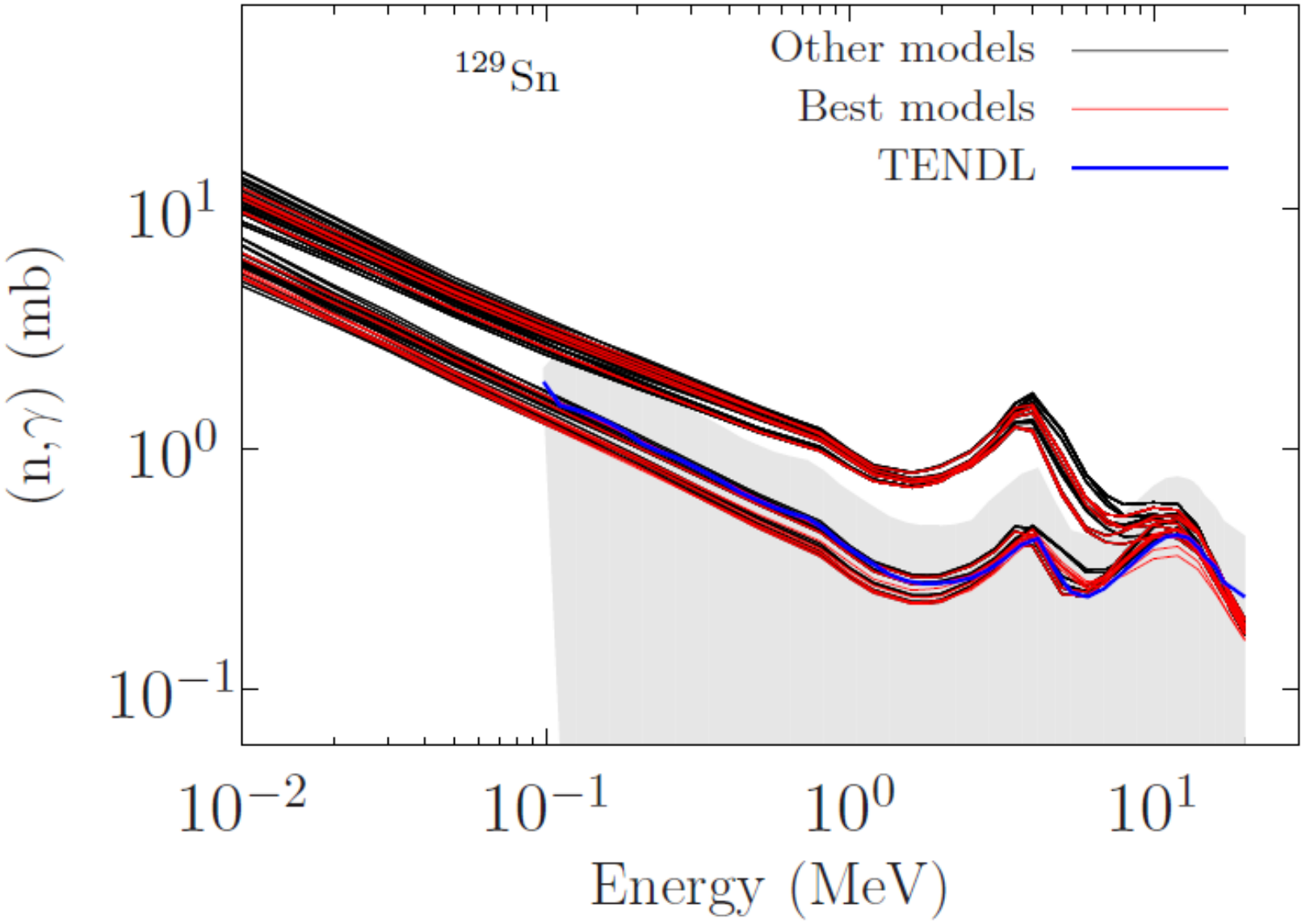
- For isotopes with experimental data (≈270): use adjusted parameters when possible

- See next slide for examples

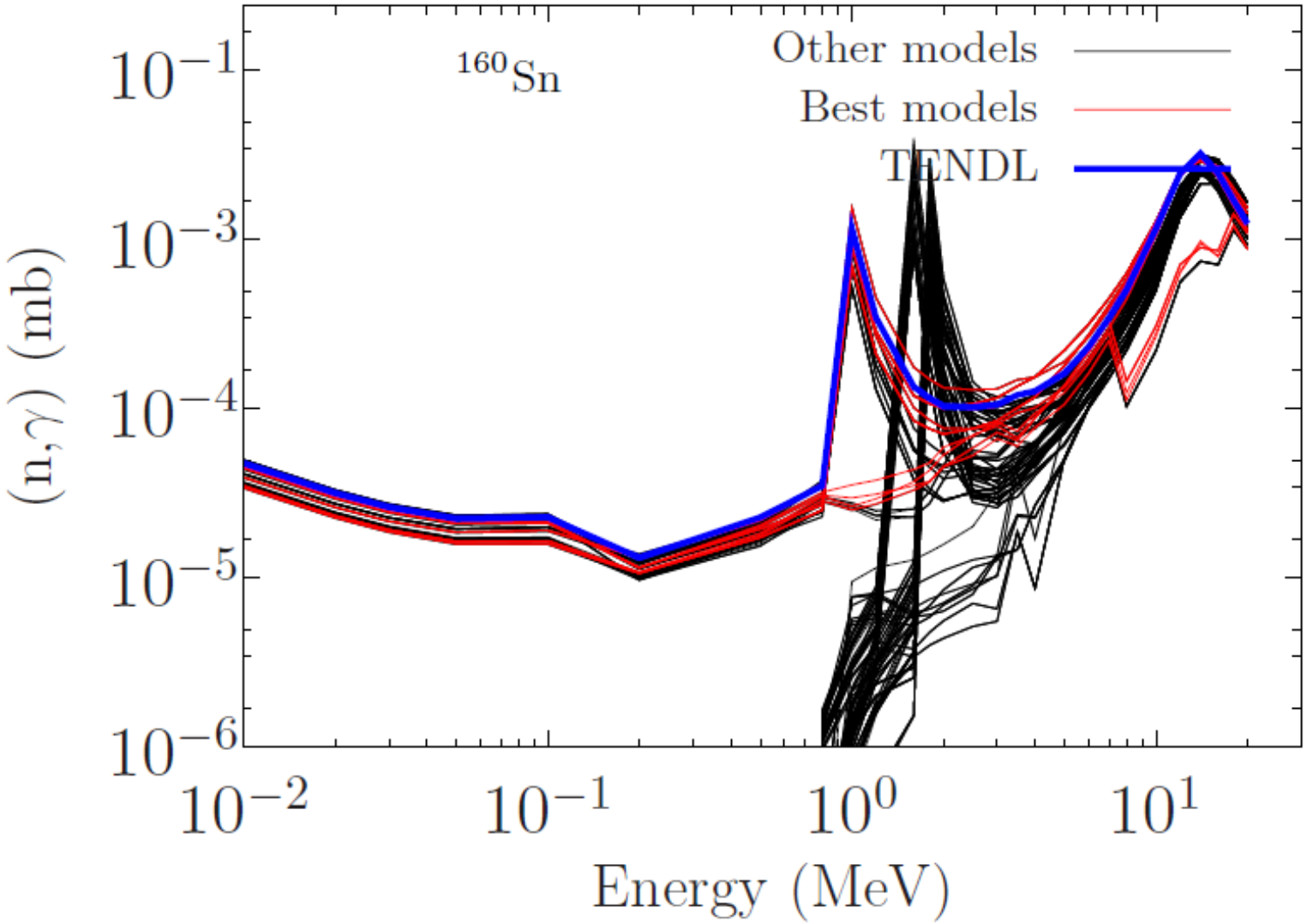
Example Sn-120 (stable)



Example Sn-129 (less stable)



Example Sn-160 (even less stable)



Model variation

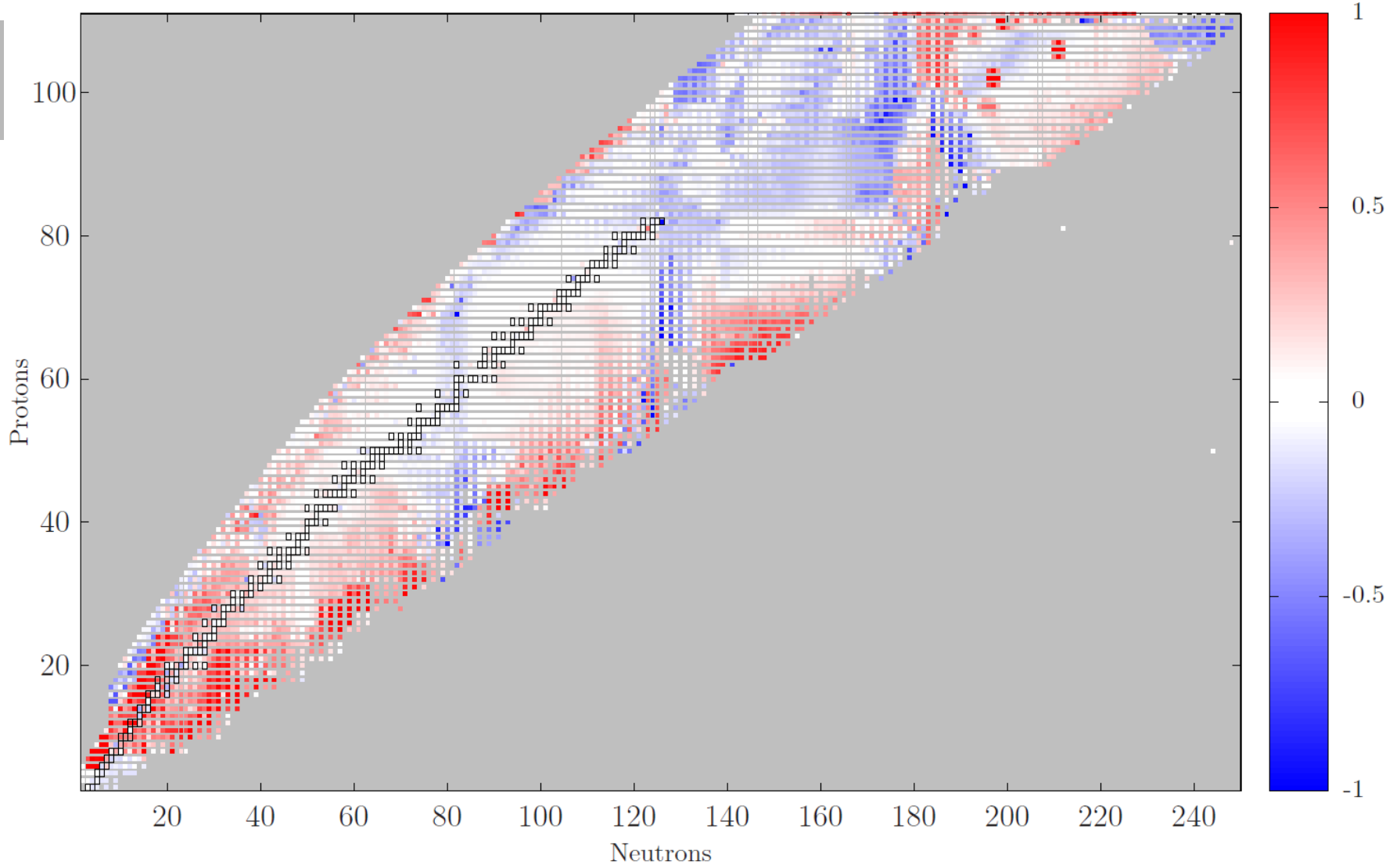
- In TALYS, a number of models can be changed:
  - Gamma strength function
  - Level density
  - Optical model
  - Gamma strength function for M1
  - Collective enhancement
  - Width fluctuation
  - Mass model
- Default TALYS is 91n3n12

```
85y8n01
|||||||
||||||massmodel (0,1,2, or 3)
|||||widthmode  (0,1 or 2)
||||colenhance  (y, n)
|||strengthM1   (3, 8)
||jlmomp        (y, n)
|ldmodel        (1, 2, 5)
strength        (8, 9)
```

```
(0: Duflo-Zuker formula,     1: Moeller table,  2: Goriely HFB-Skyrme table,
(0: no width fluctuation,    1: Moldauer model, 2: Hofmann-Richert-Tepel-Weidenmueller
(y: (yes) explicit collective enhancement of the level density)
(3: Hartree-Fock BCS tables, 8:Gogny D1M HFB+QRPA
(y: (yes) JLM microscopic optical model potential)
(1: Constant temperature + Fermi gas model,  2: Back-shifted Fermi gas model,
(8: Gogny D1M HFB+QRPA,      9: SMLO
```

Model variation: example

- Ratio for (n,g) cross section at 30 keV from models log(81n8n12/91n3n12)



Correlations

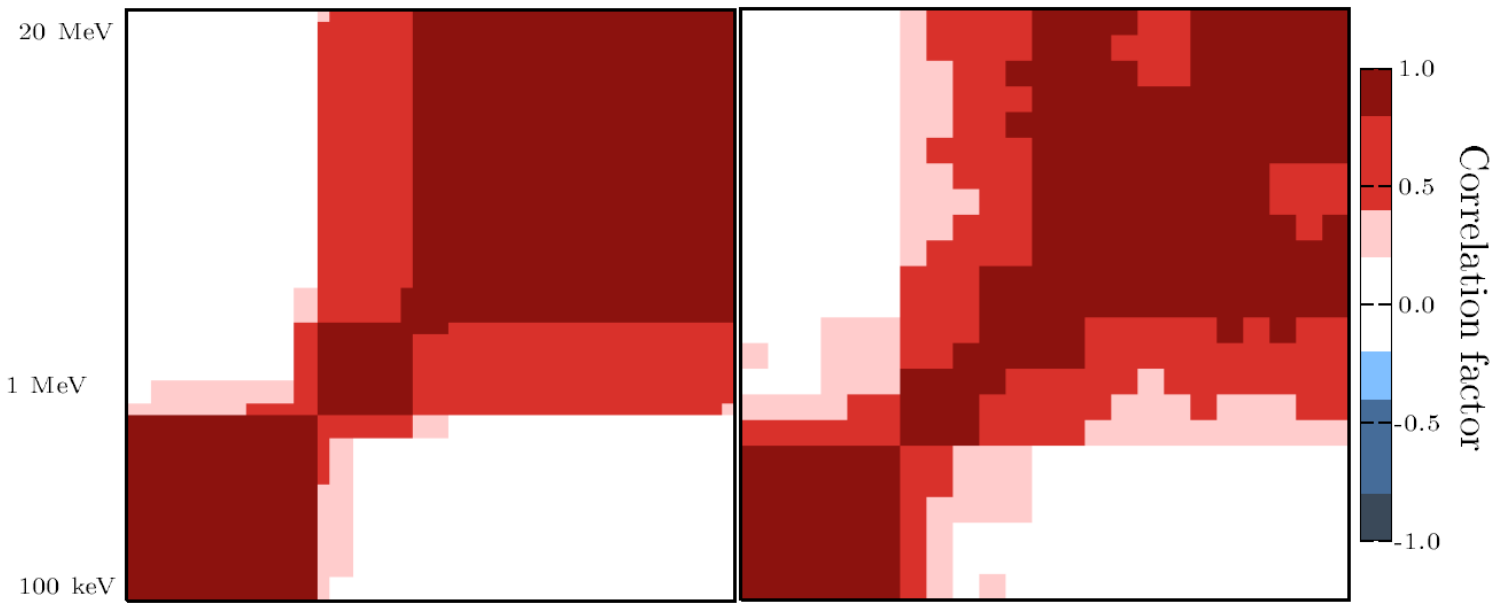


Figure 2: Correlation matrices for ^{120}Sn based on variation of model parameters (left) and models (right)

Correlations

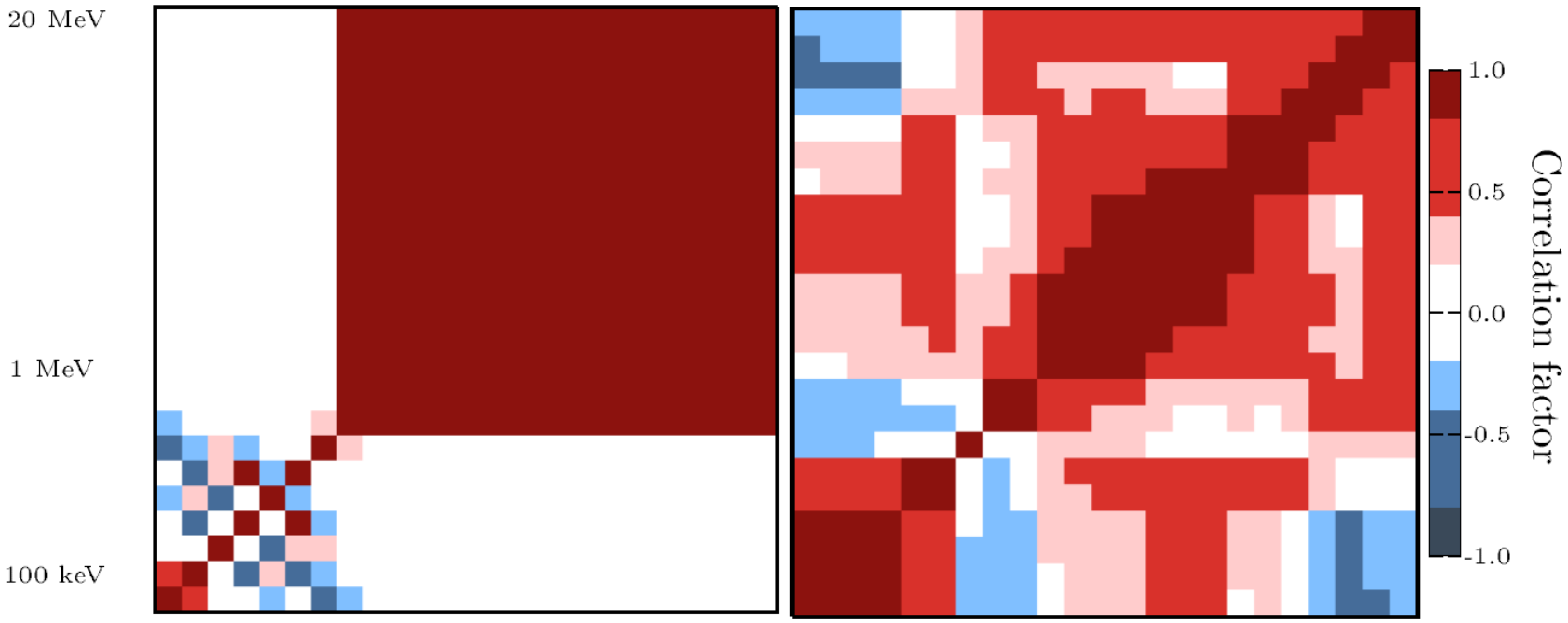
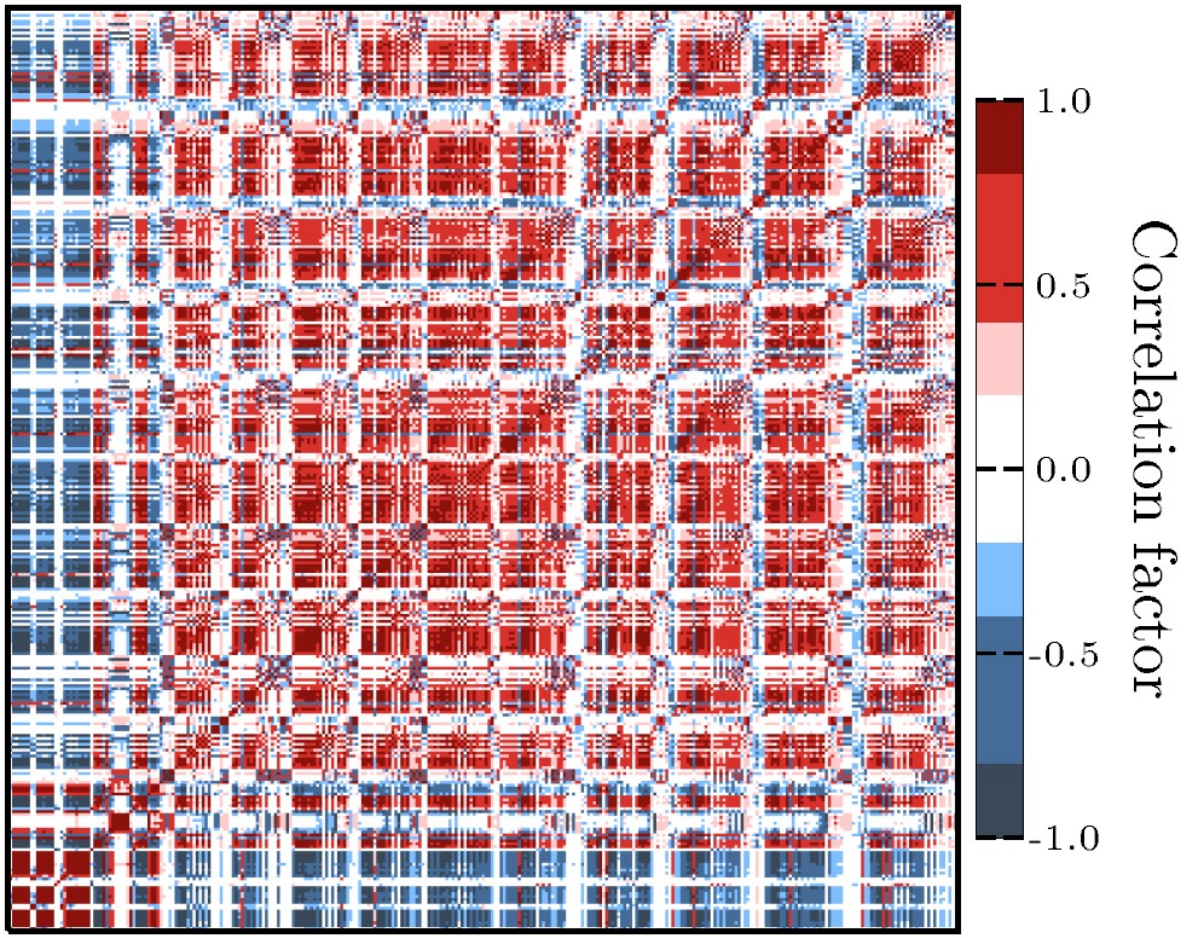


Figure 3: Same as Fig. 2, but for for ^{160}Sn.

Correlation between isotopes

- Example of the 30 keV MACS values, from the variations of 288 models

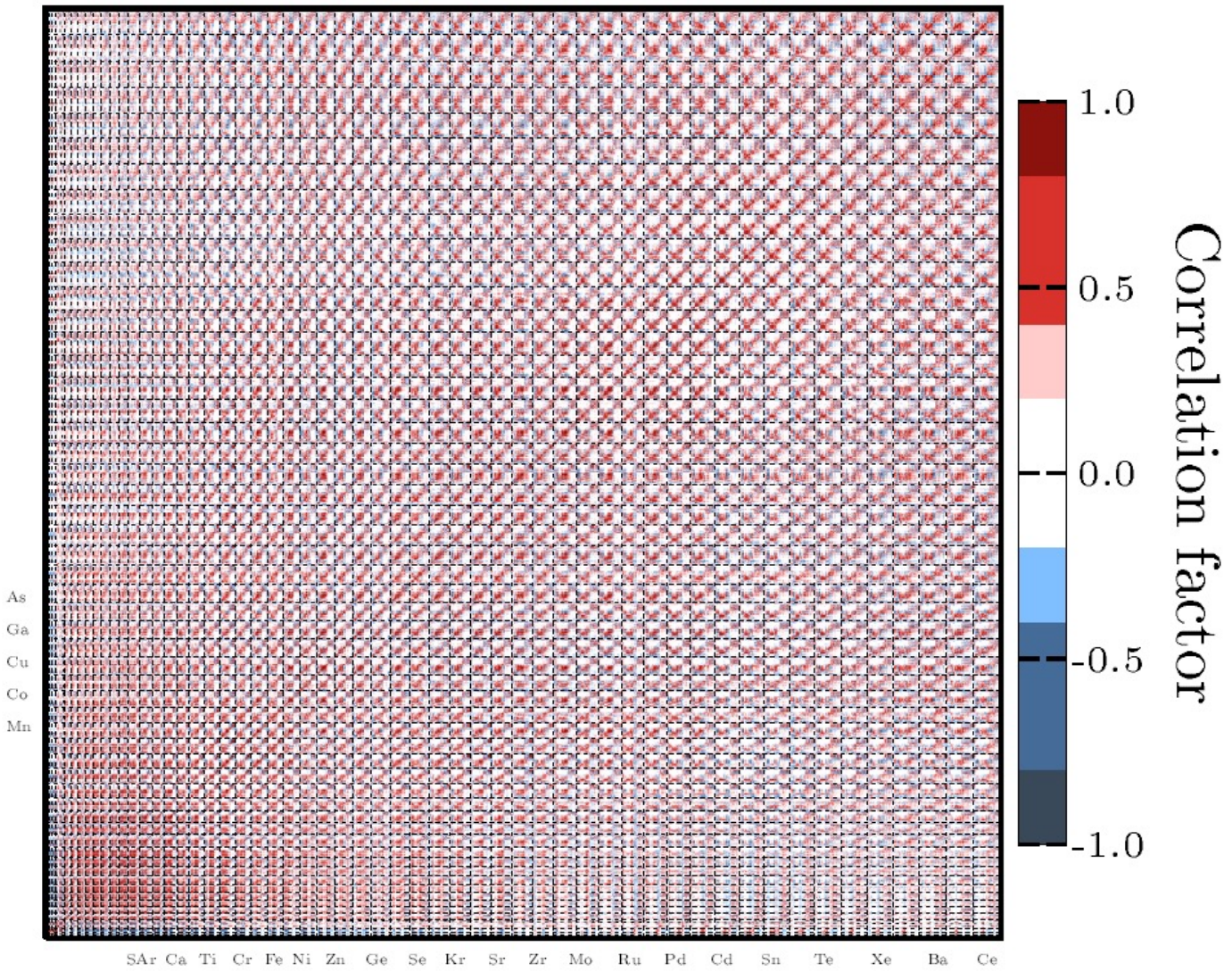
^{6}Li to ^{52}P



Correlation between isotopes

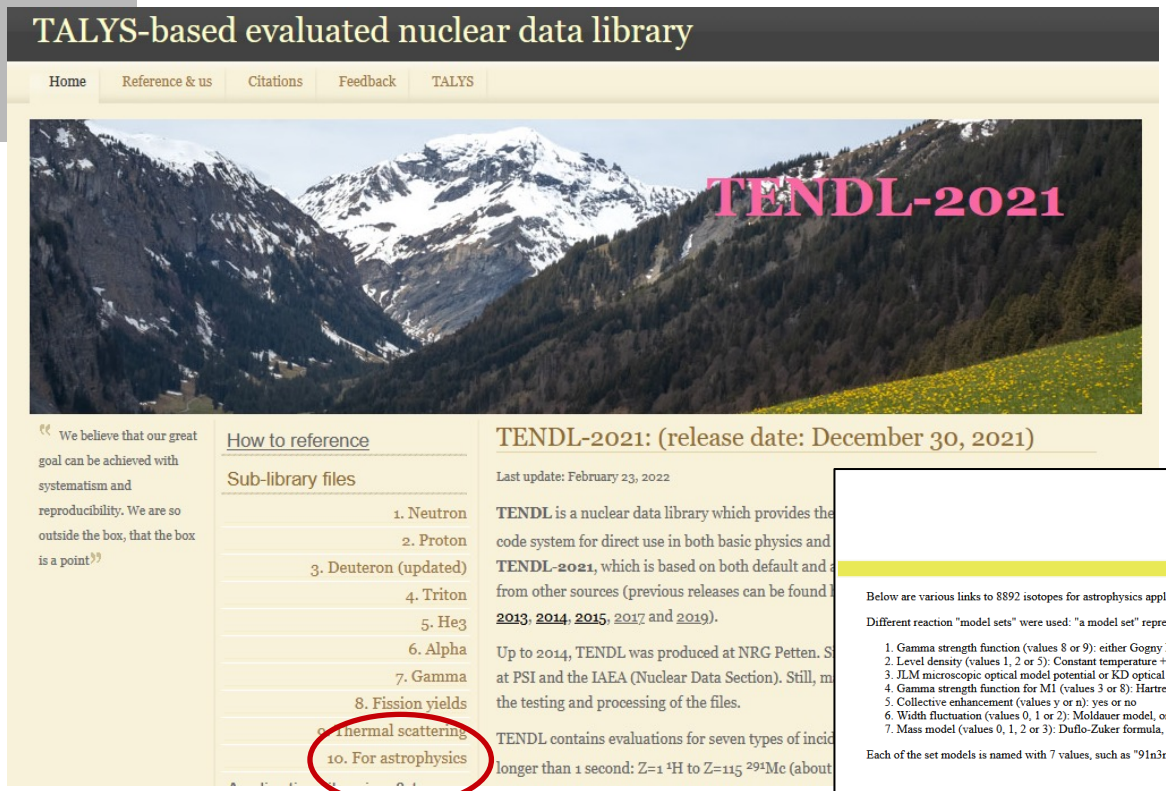
- Example of the 30 keV MACS values, from the variations of 288 models

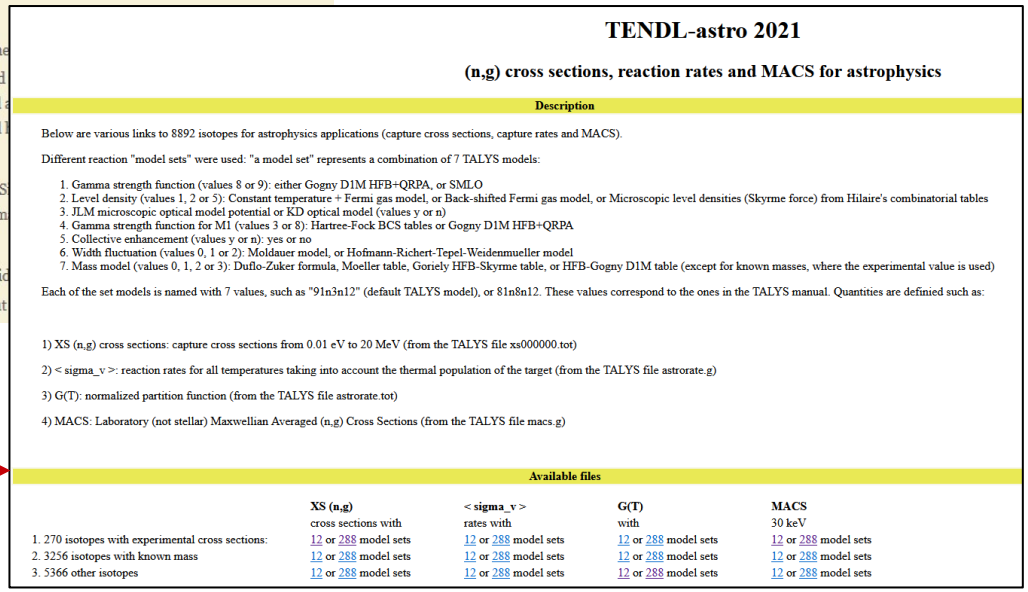
^{6}Li to ^{195}Ce



Model calculations available

- A large part of the model calculations are available in TENDL:
  https://tendl.web.psi.ch/tendl_2021/tendl2021.html





TENDL-astro 2021

(n,g) cross sections, reaction rates and MACS for astrophysics

Description

Below are various links to 8892 isotopes for astrophysics applications (capture cross sections, capture rates and MACS).

Different reaction "model sets" were used: "a model set" represents a combination of 7 TALYS models:

1. Gamma strength function (values 8 or 9): either Gogny D1M HFB+QRPA, or SMLO
2. Level density (values 1, 2 or 5): Constant temperature + Fermi gas model, or Back-shifted Fermi gas model, or Microscopic level densities (Skyrme force) from Hilaire's combinatorial tables
3. JLM microscopic optical model potential or KD optical model (values y or n)
4. Gamma strength function for M1 (values 3 or 8): Hartree-Fock BCS tables or Gogny D1M HFB+QRPA
5. Collective enhancement (values y or n): yes or no
6. Width fluctuation (values 0, 1 or 2): Moldauer model, or Hofmann-Richert-Tepel-Weidenmueller model
7. Mass model (values 0, 1, 2 or 3): Duflo-Zuker formula, Moeller table, Goriely HFB-Skyrme table, or HFB-Gogny D1M table (except for known masses, where the experimental value is used)

Each of the set models is named with 7 values, such as "91n3n12" (default TALYS model), or 81n8n12. These values correspond to the ones in the TALYS manual. Quantities are definied such as:

1) XS (n,g) cross sections: capture cross sections from 0.01 eV to 20 MeV (from the TALYS file xs000000.tot)

2) < sigma_v >: reaction rates for all temperatures taking into account the thermal population of the target (from the TALYS file astrorate.g)

3) G(T): normalized partition function (from the TALYS file astrorate.tot)

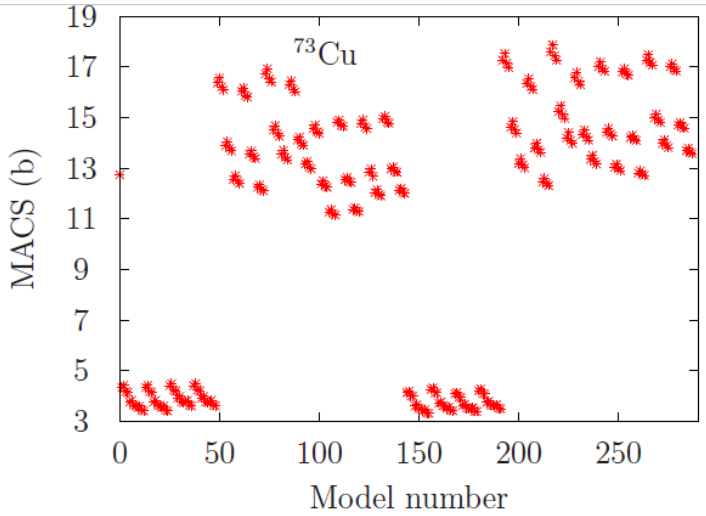
4) MACS: Laboratory (not stellar) Maxwellian Averaged (n,g) Cross Sections (from the TALYS file macs.g)

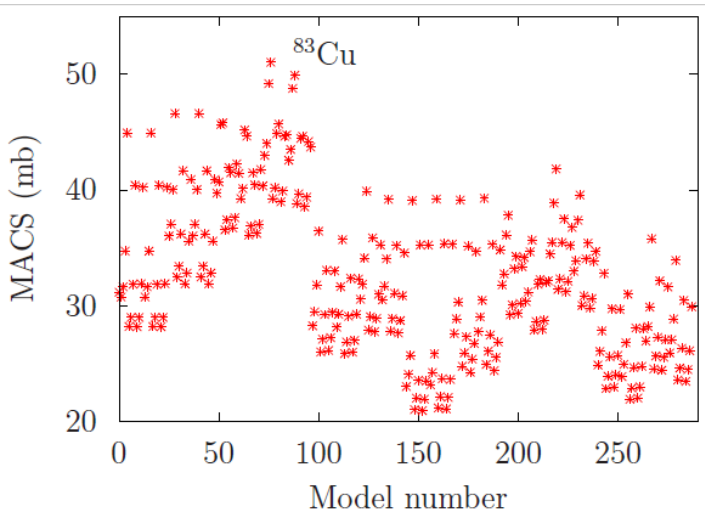
Available files

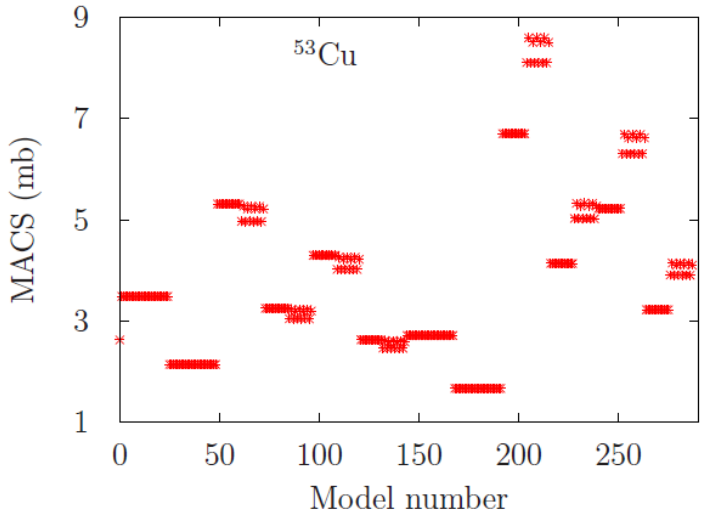
	XS (n,g) cross sections with	< sigma_v > rates with	G(T) with	MACS 30 keV
1. 270 isotopes with experimental cross sections:	12 or 288 model sets	12 or 288 model sets	12 or 288 model sets	12 or 288 model sets
2. 3256 isotopes with known mass	12 or 288 model sets	12 or 288 model sets	12 or 288 model sets	12 or 288 model sets
3. 5366 other isotopes	12 or 288 model sets	12 or 288 model sets	12 or 288 model sets	12 or 288 model sets

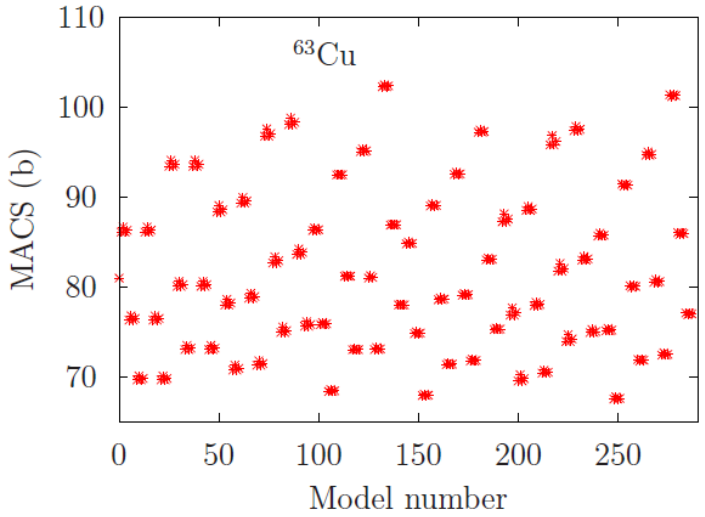
Model calculations: example

- Large variations and different distributions from stable to short-lives isotopes









Future and conclusions

- Systematical approach to various quantities for astrophysics
- Variation of models, and not model parameters
- Access to systematical uncertainties and correlations
- All available from the TENDL-2021 website

- Future: TENDL-2023 will include more model variations and more quantities, up to 960 model sets

Description of TALYS models

Below are various links to 8892 isotopes for astrophysics applications (cross sections, reaction rates and MACS) based on TALYS calculations (version 1.96).

Different reaction "model sets" were used: "a model set" represents a combination of 9 TALYS models:

1. Gamma strength function (values 8 or 9): either Gogny D1M HFB+QRPA, or SMLO
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8. Alpha optical model (values 5 or 6): Demetriou/Goriely, or Avrigeanu
9. Fission model (values 1 or 5): "experimental" fission barriers, or WKB approximation for fission path model.

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Wir schaffen Wissen – heute für morgen