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TENDL and BMC evaluations: advantages and limits

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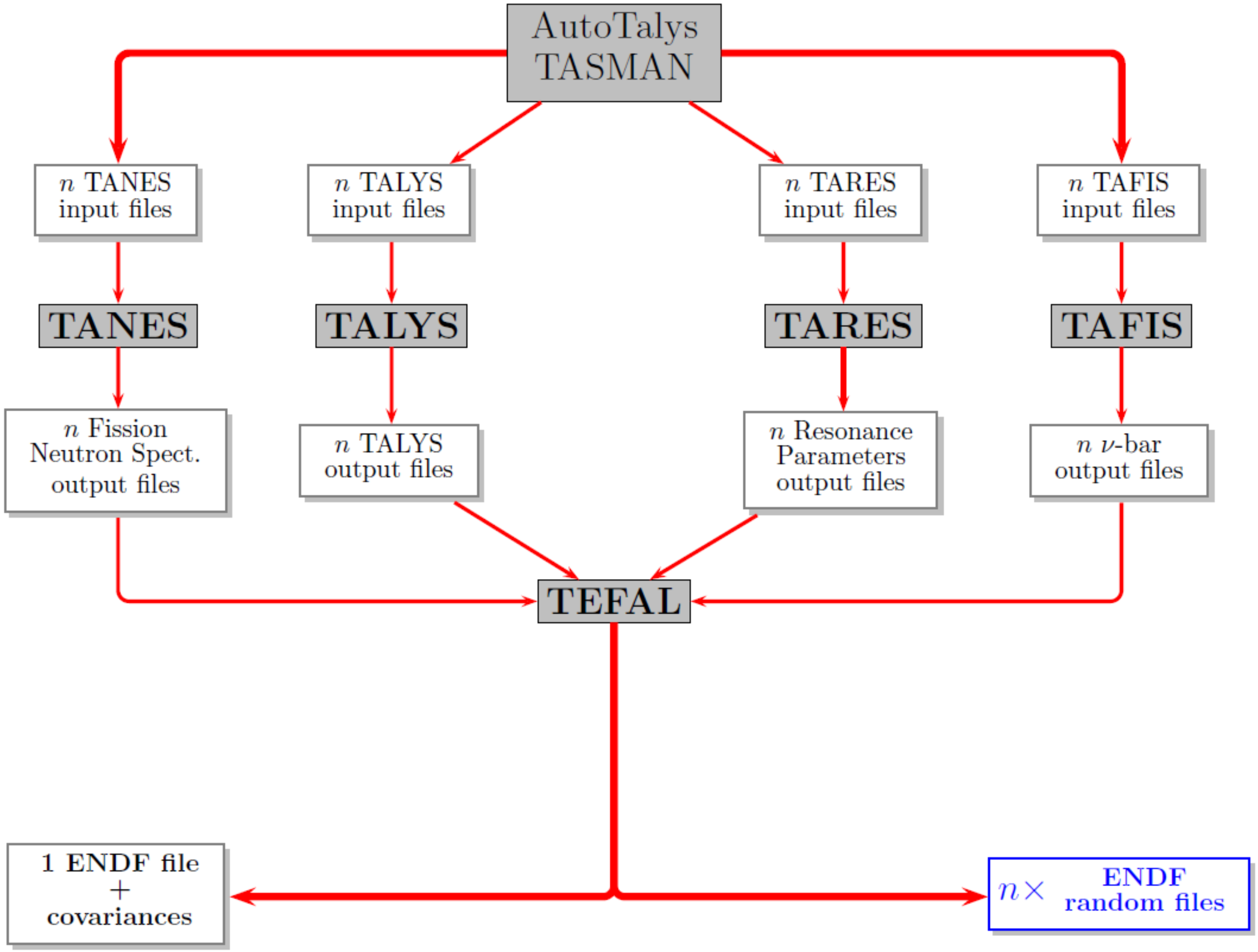
Summary

- The TENDL/T6 system, focus on RRR + fast range
- BMC/BFMC + integral data
- Mixing TALYS and EMPIRE: The beauty and the beast
- Application for INDEN

All slides can be found here: https://tendl.web.psi.ch/bib_rochman/presentation.html

TENDL-2008 to 2017: short history

- Method: Quality evaluation, production automation, open source

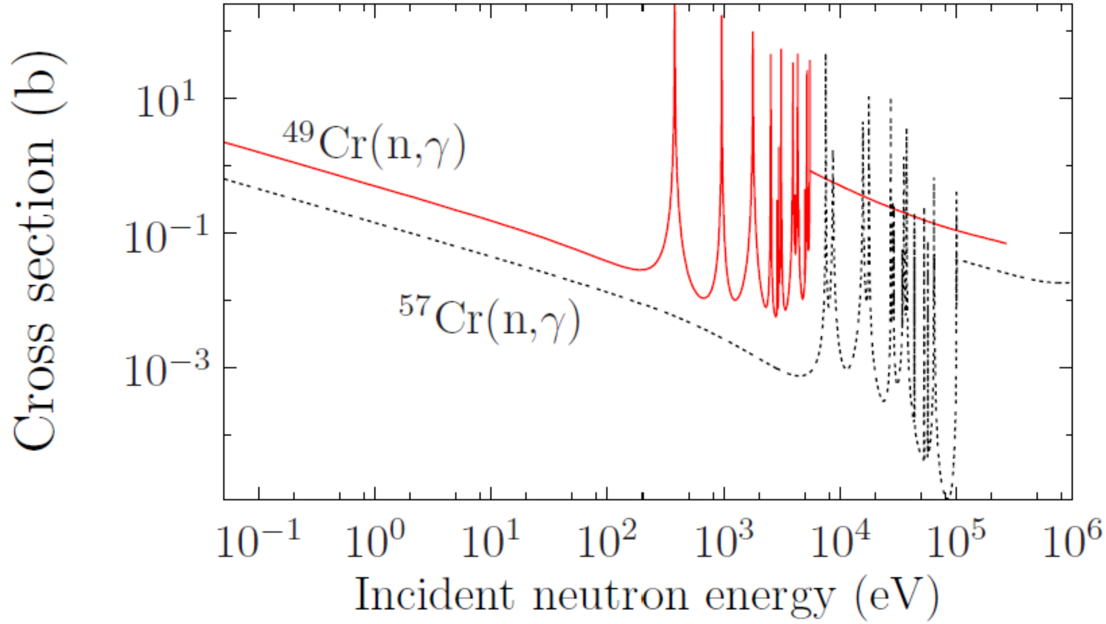


TENDL-2008 to 2017: short history

- Goal: improve simulations (C/E) for the European library and TENDL,
- Methods: reproducibility & completeness, development of a portable system (called T6) capable of producing TENDL + random nuclear data files and to process them for applications,
- Background:
  - Theoretical calculations (TALYS) with experimental inputs, and alternatively, TALYS normalization from other libraries
  - Resonances from experimental analysis, or the "HFR" approach (statistical resonances)
  - Covariances: Bayesian Monte Carlo
- Not from scratch: Make use of other libraries, such as JEFF, ENDF/B, and of course the EAF-2010 library with the JUKO/CCFE validation scheme

TENDL-2017: Resonance range

- Isotopes with measured resonances: all integrated in MF2
- For the other isotopes (no measurements):
  - HFR calculations:
    1. TALYS + specific ld + specific omp + specific γ-str
    2. TALYS output: average D_0, Γ_γ, Γ_n, Γ_f... as a function of E_n
    3. CALENDF + TALYS output in the form of an ENDF-6 file
       - generate random ladders of resonances using the statistical properties
       - Just like in the unresolved resonance range,
       - But this time from 0 to a few 10 or 100 keV.



BMC/BFMC + integral data

- Motivation 1: integral data are already used during adjustment
- Motivation 2: This should be done at the evaluation level
- Motivation 3: It leads to uncertainty reduction and cross-isotope correlations
- Motivation 4: nothing new: already done with GLLS by SG… at the OECD

BMC/BFMC + integral data

- Step 1 - Preliminary work: in-depth cross section evaluation (traditional method of parameters/models adjustment)

- Step 2 - BMC: Based on step 1,
  – Generate n=100 000 (or 1000) random files (TMC-way)
  – Calculate n times the benchmarks
  – Assign weights to all realizations *i* with a chi2 and update the parameter distributions

For a random file i and a set of p benchmarks:

$$\chi_i = \sum_j^p \left(\frac{\mathrm{k}^{(\mathrm{j})}_{\mathrm{eff,i}} - \mathrm{k}^{(\mathrm{j})}_{\mathrm{exp}}}{\Delta \mathrm{k}^{(\mathrm{j})}} \right)^2 \quad (1)$$

$$w_i = \exp(-\frac{\chi_i}{2}) \quad (2)$$

$$\begin{cases} \omega = \sum_i^n w_i \\ \omega_\sigma = \sum_i^n w_i \cdot \sigma_i / \omega \end{cases}$$

  – Update the cross sections with the weights.

- Some BMC/BFMC references:
  – EPJ/A 51 (2015) 184, Nucl. Data Sheets 123 (2015) 201, EPJ/N 3, 14 (2017)

BMC/BFMC + integral data: example 1/5

- Fast range:

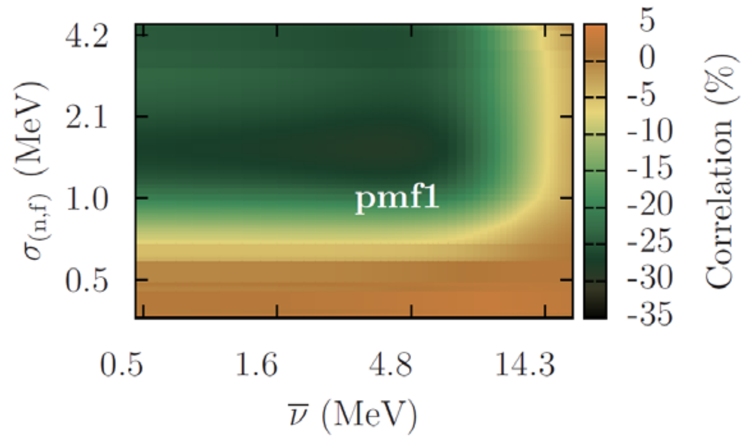


Fig. 3. Correlation matrix between ^{239}Pu ν and σ considering the fast pmf1 benchmark. The X- and Y-axis are in log scale.

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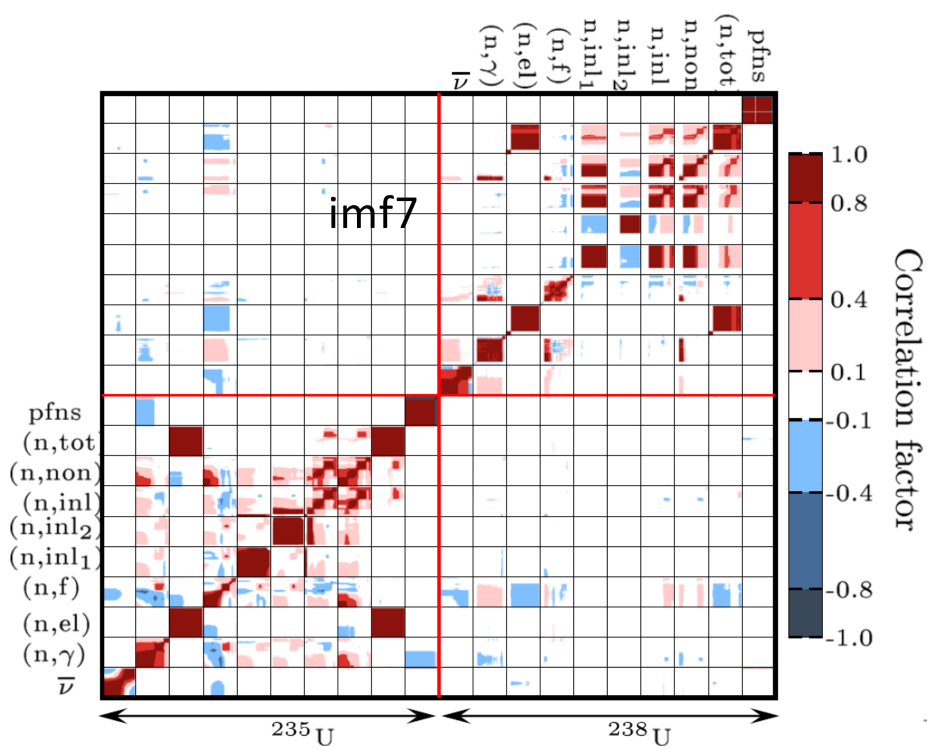

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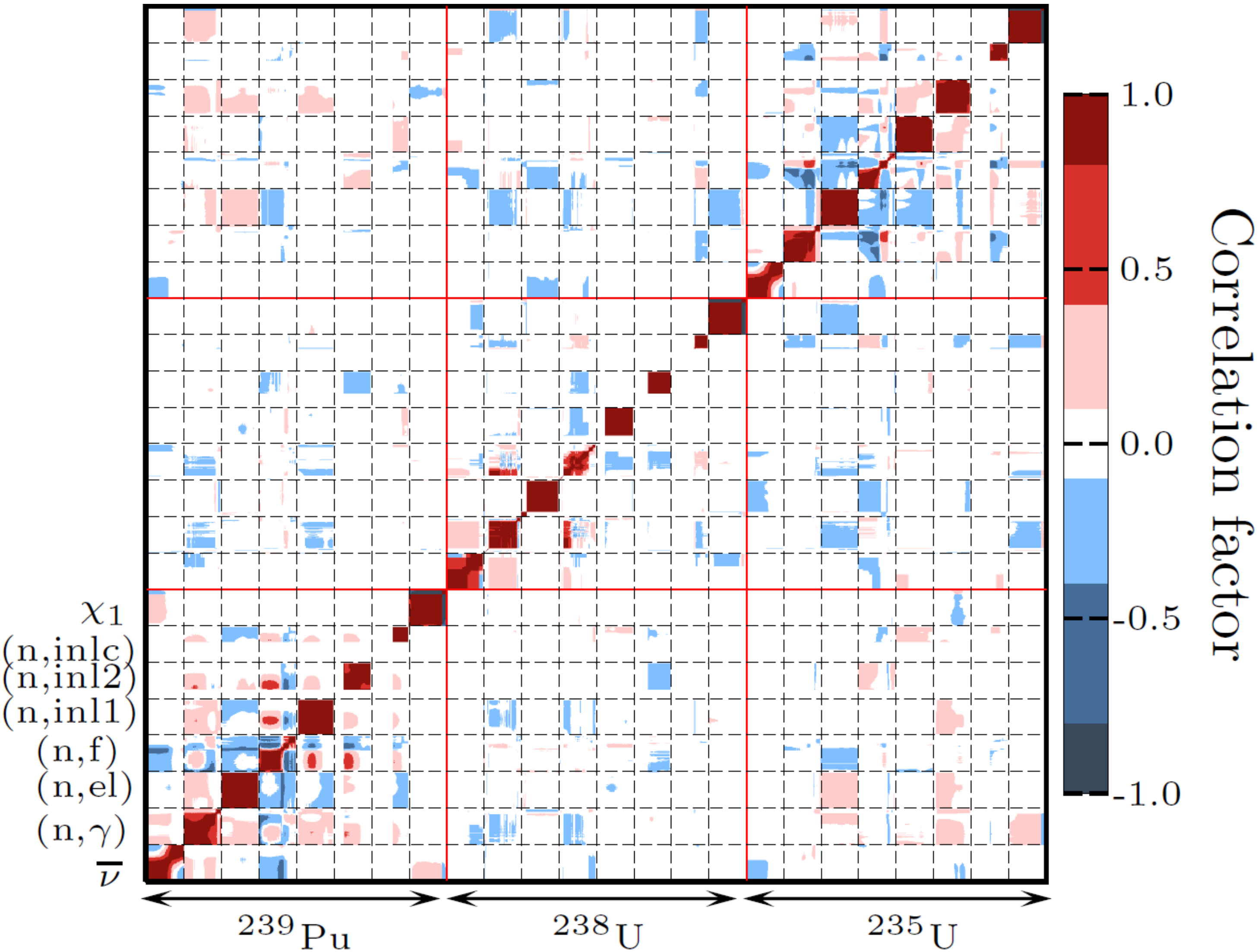
BMC/BFMC + integral data: example 2/5

- Fast range: 14 reactions together (k_{eff} and reaction rates)



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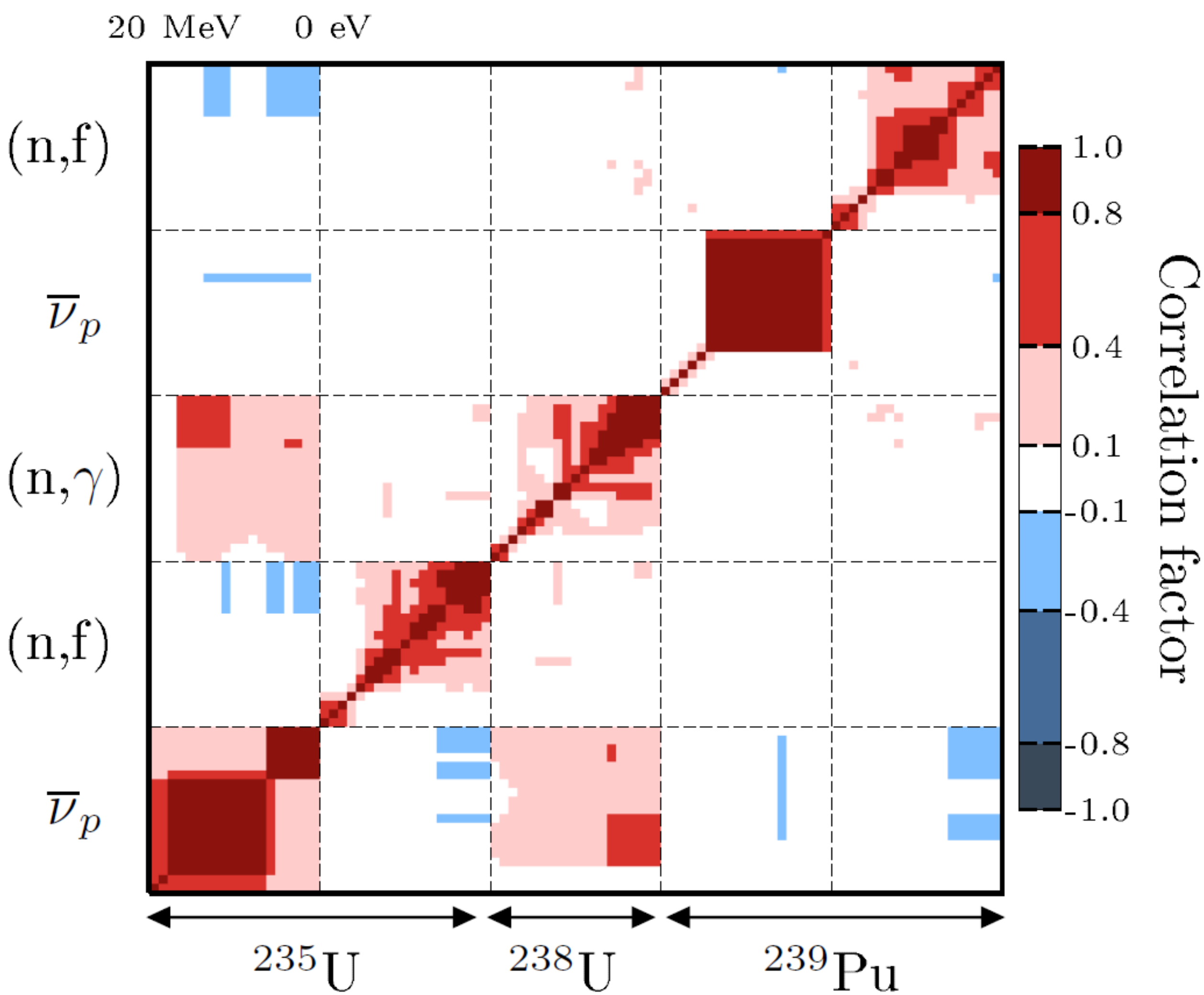
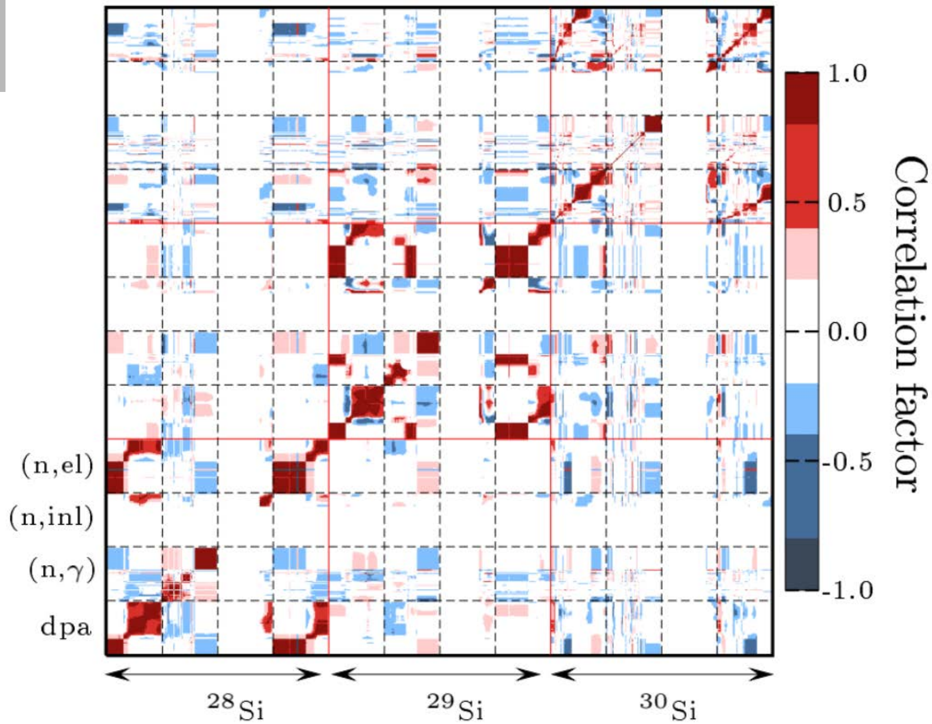
BMC/BFMC + integral data: example 3/5

- Thermal range: due to the measured boron concentration in a PWR

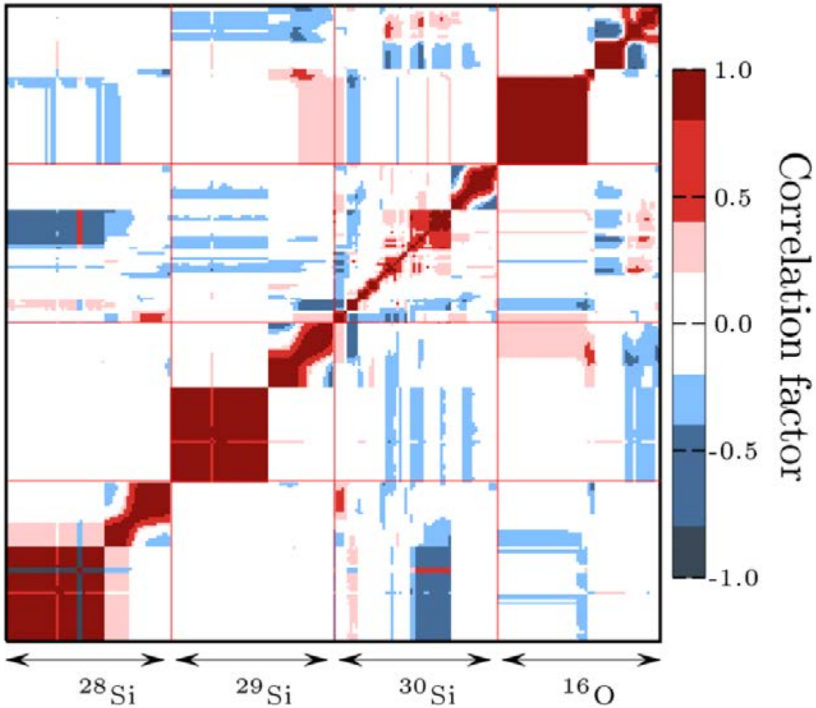


BMC/BFMC + integral data: example 4/5

- Based on EXFOR only: Si + SiO_2 + ^{16}O



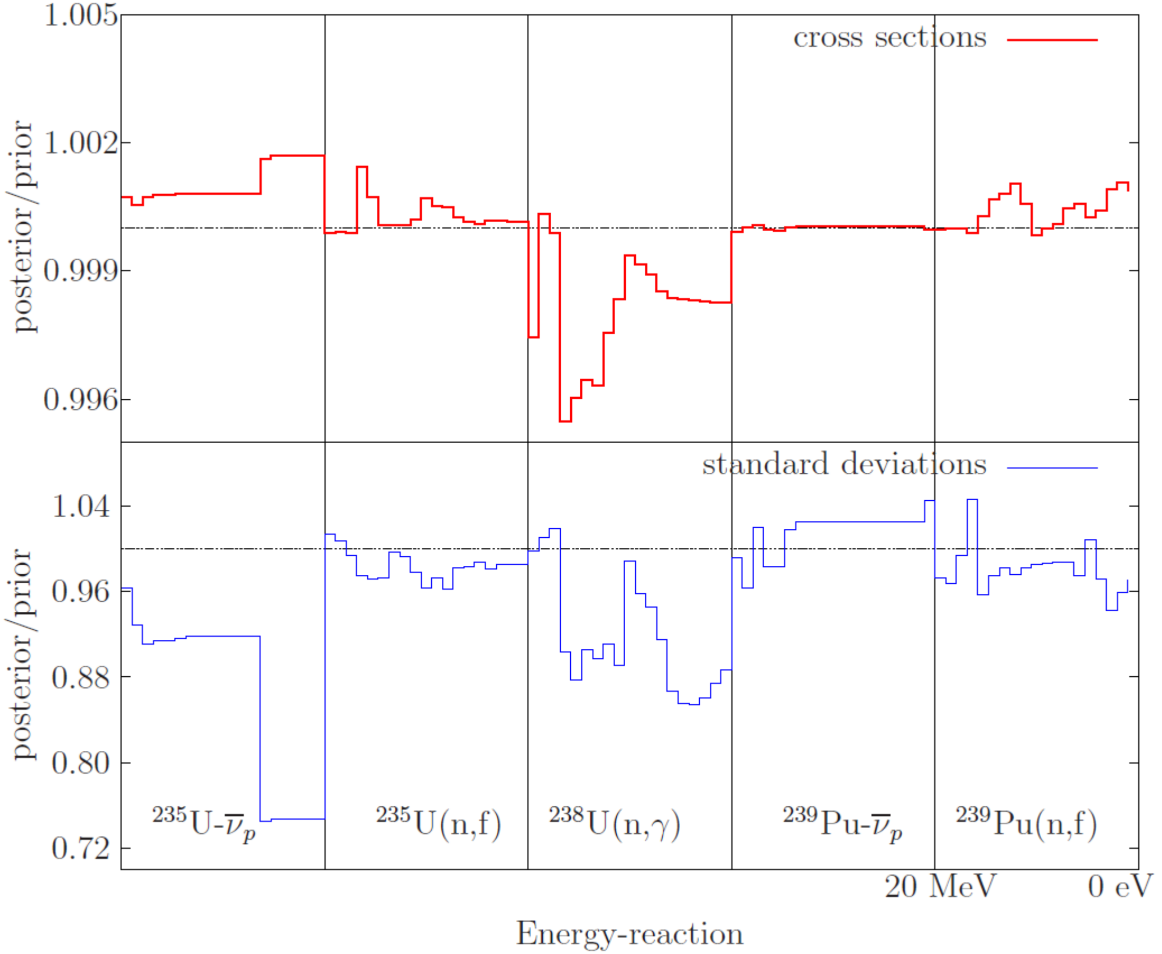
with SiO_2



(n,tot) only

BMC/BFMC + integral data: example 5/5

- Thermal range: due to the measured boron concentration in a PWR (uncertainty reduction)



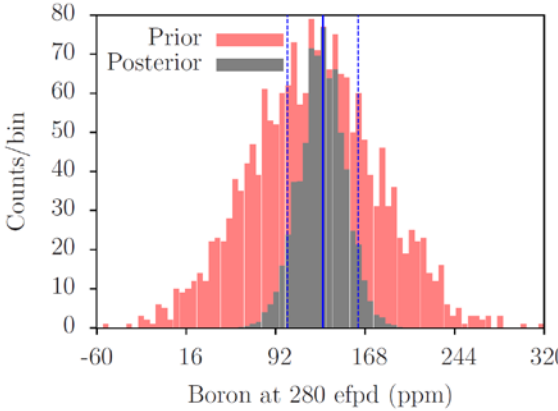


Fig. 5. Top: Ratios of posterior over prior nuclear data (cross sections and $\overline{\nu}_p$). Bottom: same for standard deviations.

Mixing TALYS and EMPIRE: The beauty and the beast

- Goal: Evaluations with best C/E for differential and integral data (not *toy models*)

- Bayesian methods are powerful to combine different sources of information:
  – Models
  – Differential data
  – Integral data

- As we consider many differential data, many integral data, many model parameters, we should also consider many models. It helps to
  – broaden the prior
  – avoid user selection of “best model”
  – have a similar approach in “differential, integral and model spaces”.

- This presentation will show examples of mixing models, with random parameters within the Bayesian approach (BFMC)

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Models used for the calculations

- One single model might not be enough to “fit” all experimental data,

- Usually only one set of model is used for a full evaluation, e.g. in TENDL:
  - OMP Local Koning-Delaroche
  - Gamma-strength function: Kopecky-Uhl generalized Lorentzian
  - Level density model: Constant temperature + Fermi gas model

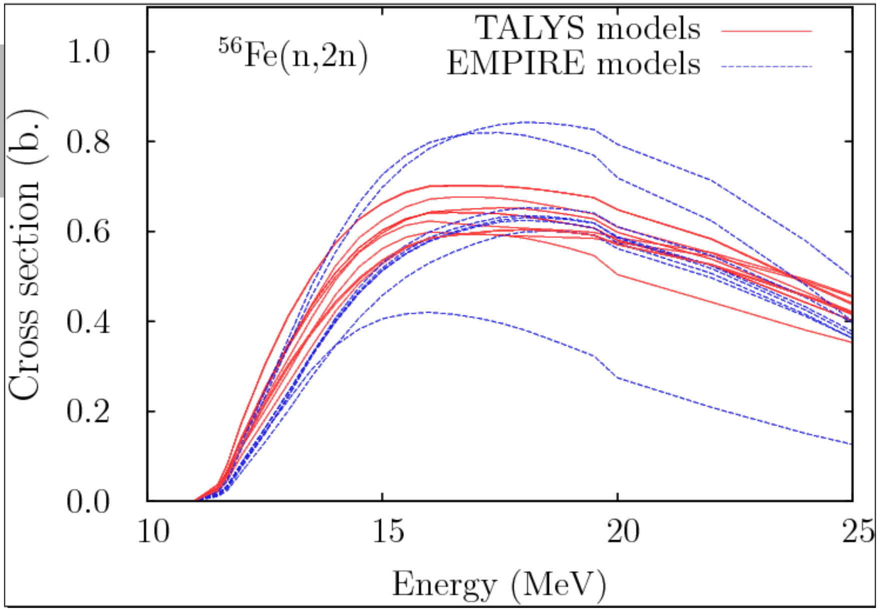
- Other options are available in TALYS:
  - 8 gamma-strength functions (called *i*)
  - 6 level density models (called *j*)
  - Different OMP (local, general, microscopic) (called *k*)

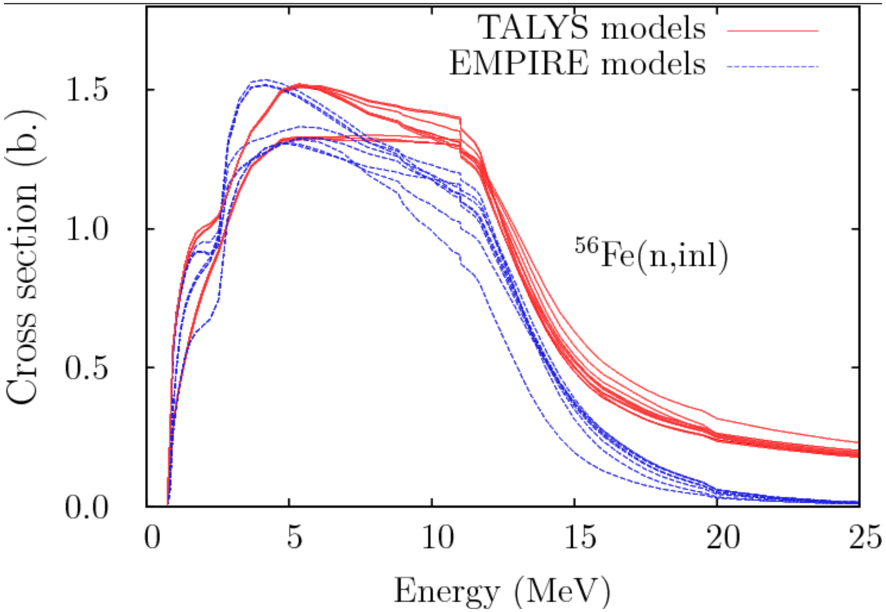
  - In total: *i* x *j* x *k* possibilities (11n, 12n, 58n…)
  - For each of these possibilities, one can sample model parameters

- Other extreme solution: EMPIRE.

- In the following: -10 TALYS models (semi-empirical and microscopic)
  -8 EMPIRE models (semi-empirical and microscopic)

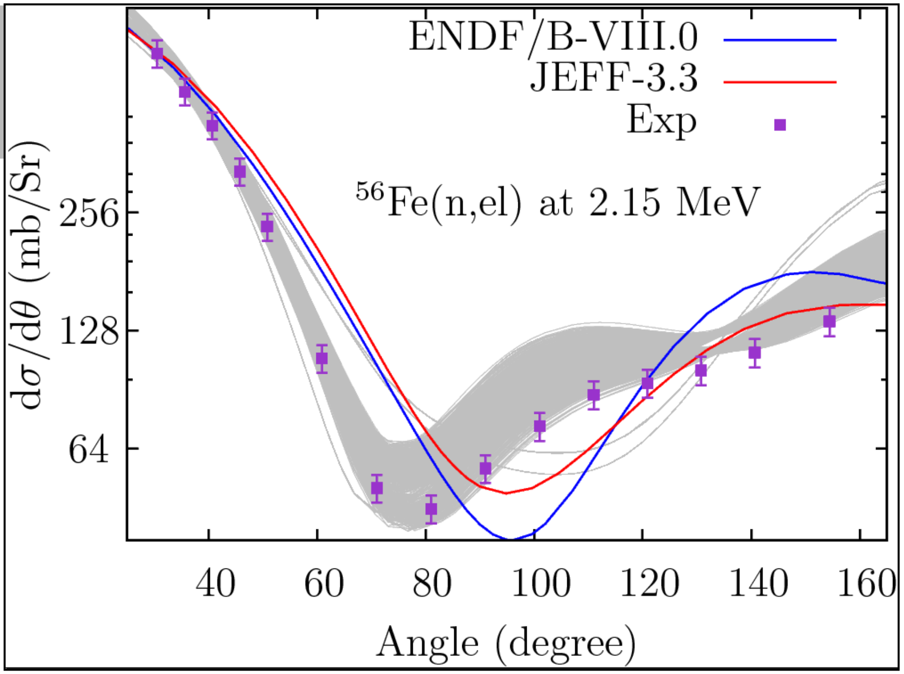
Example for ^{56}Fe(n,2n) and (n,inl)

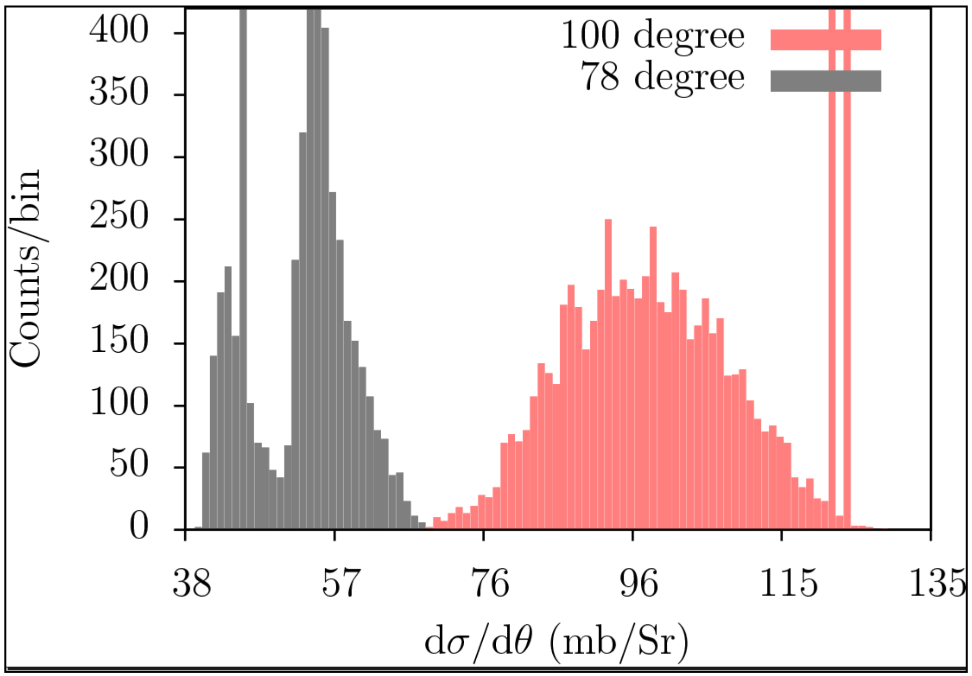




- All these models can be used as prior
- For each of these 18 models, 500 ENDF are produced by randomizing parameters.

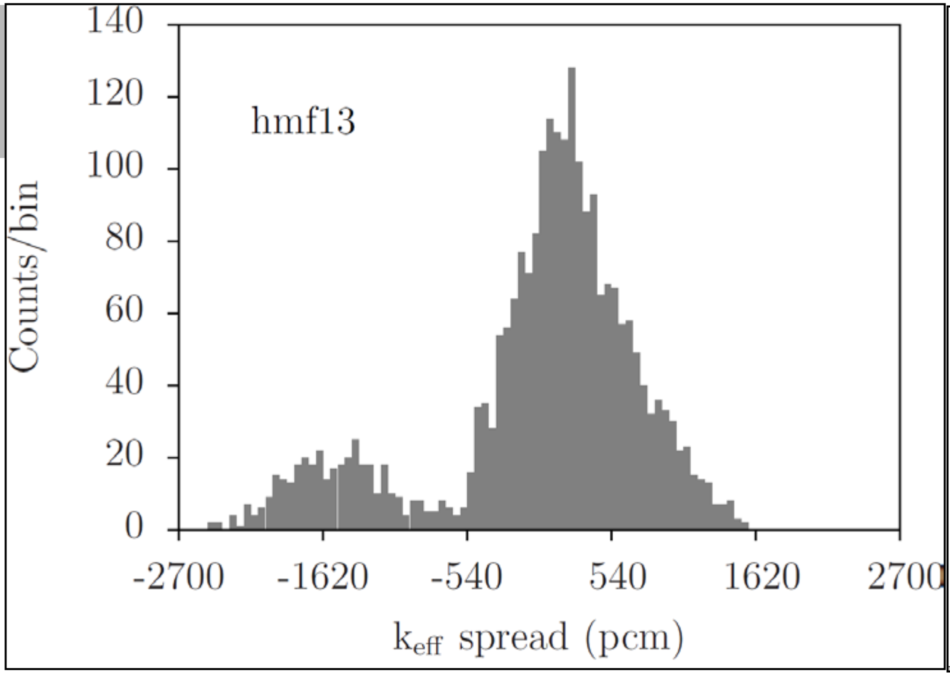
Example for ^{56}Fe angular distribution

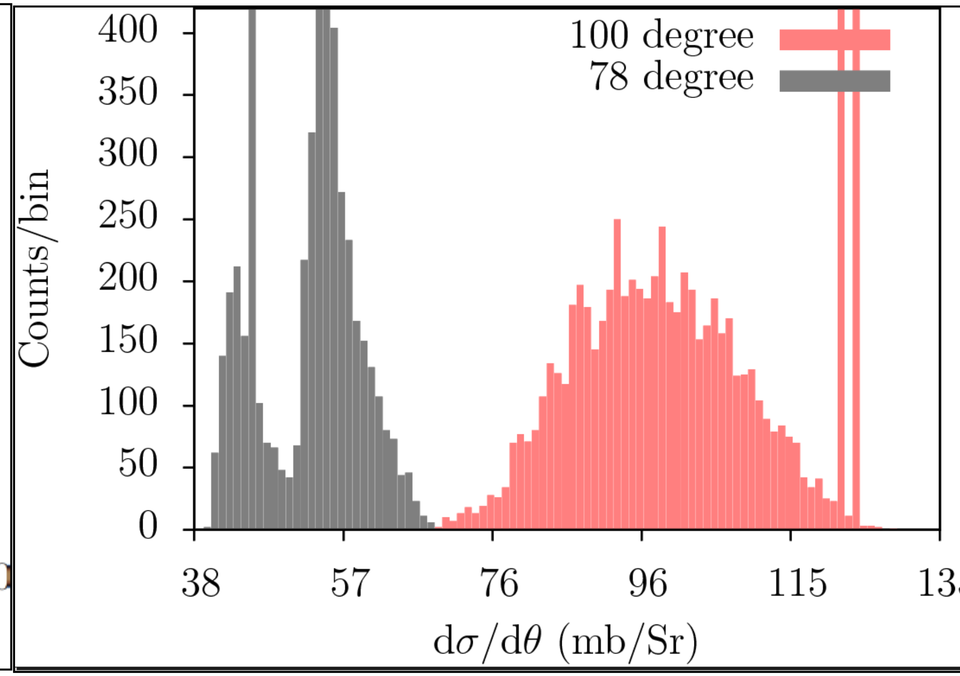




- Angular distributions are not normally distributed.
- Variations of models and parameters might not be enough to cover experimental data.
- Model defects might help in this case

Example for ^{56}Fe angular distribution



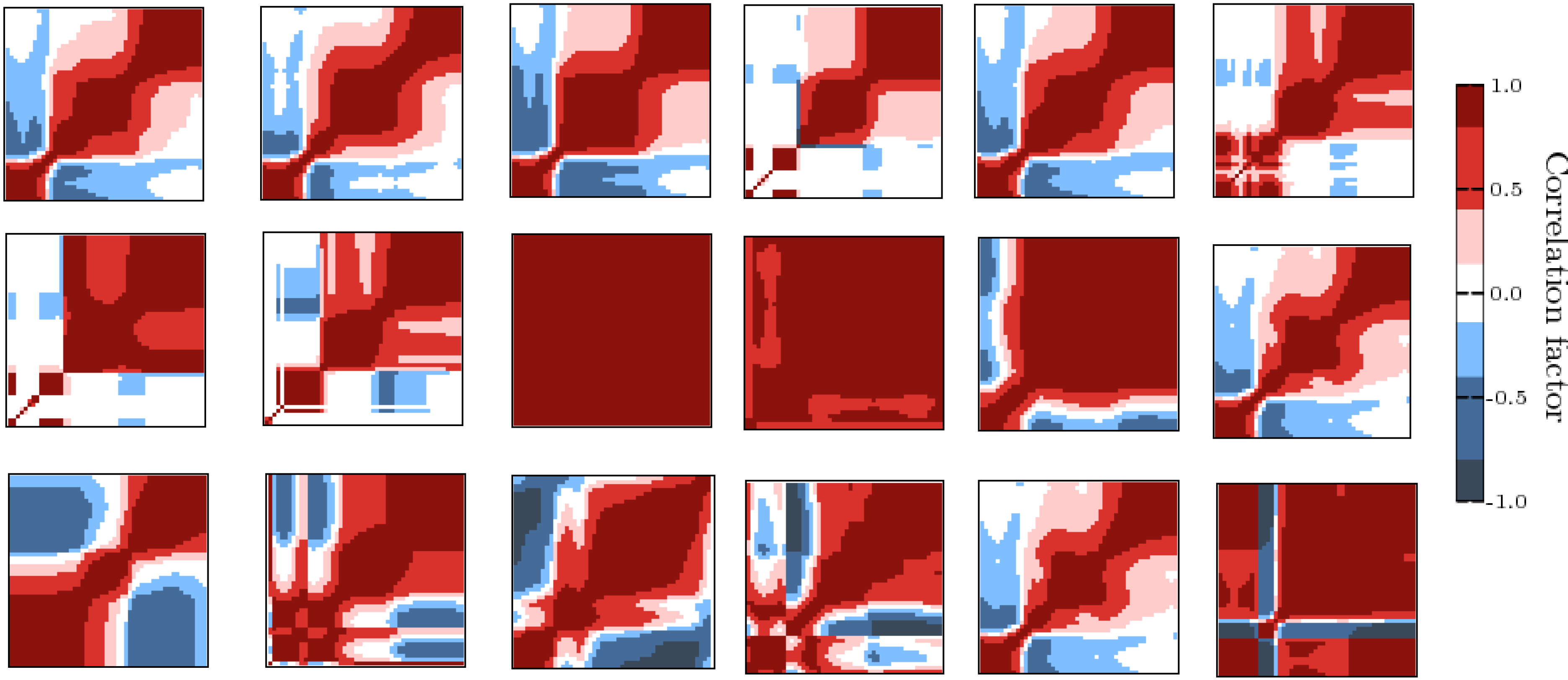


- Importance of angular distributions (n,el): same shape in the hmf13 benchmark

Example for ^{56}Fe(n,inl): TALYS+EMPIRE

- Many prior correlation matrices can be obtained depending on the models/combination, all for the same reaction

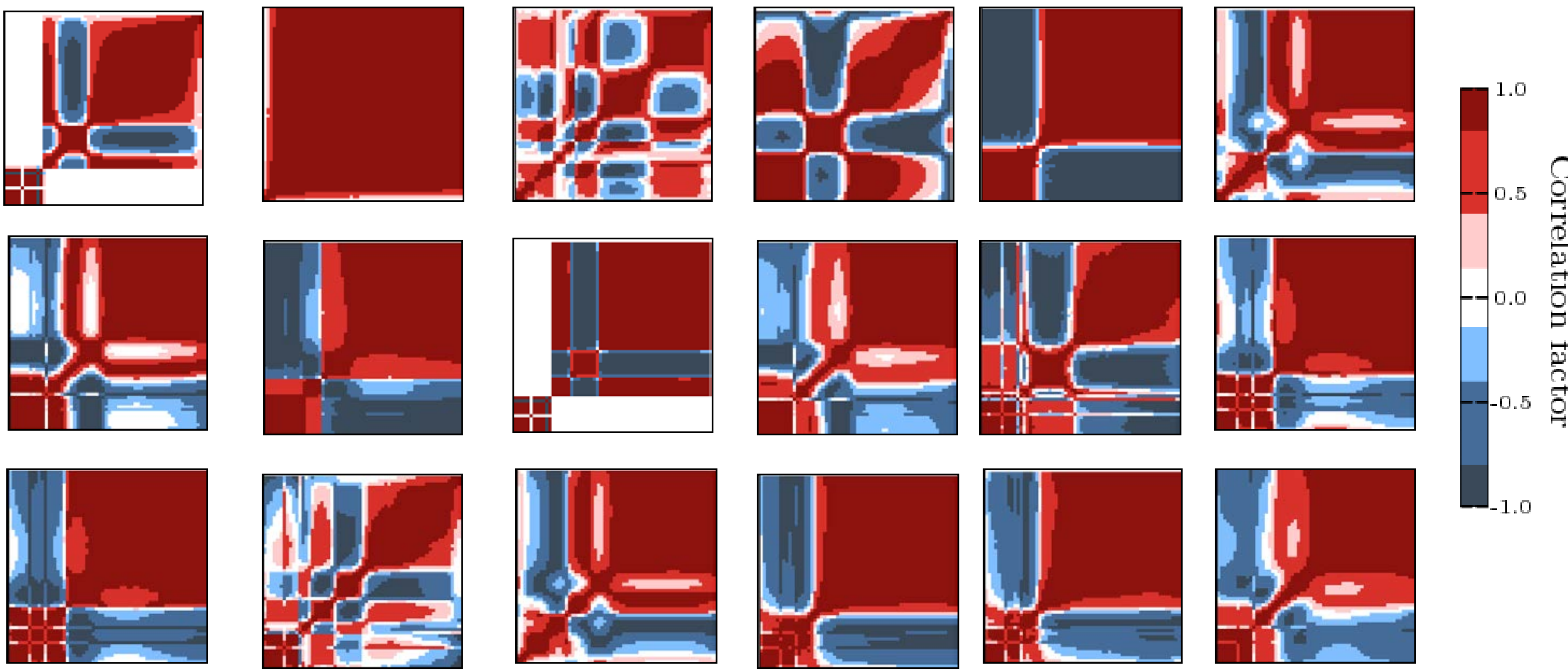
Examples for ^{56}Fe(n,inl)



Example for ^{56}Fe(n,tot): TALYS+EMPIRE

- Many prior correlation matrices can be obtained depending on the models/combination, all for the same reaction

Examples for ^{56}Fe(n,tot)



Application for INDEN

- <u>Some preliminary remarks</u>

  - Prior correlations can be anything,
  - There is no truth in “absolute covariance” (it is only an outcome of a method)
  - There is no general-purpose library (they all follow a set of choices)

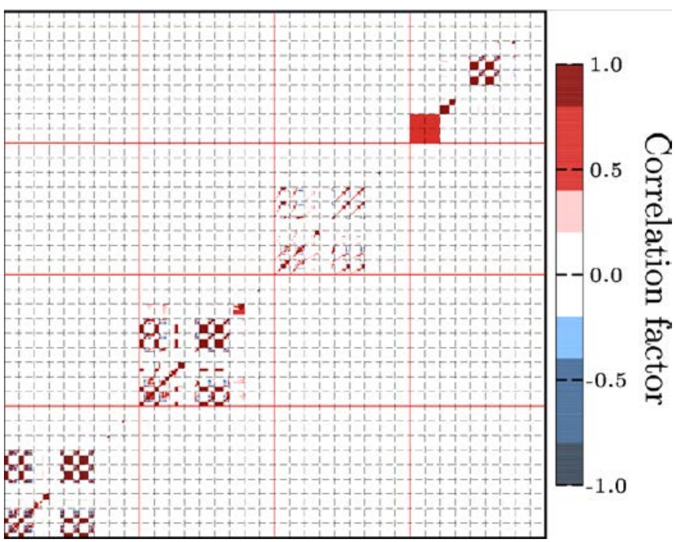
- <u>For future evaluations</u>, to be as general as possible (in terms of prior)

  - Integral/natural data helps to get cross-isotope correlations,
  - Integral/natural data helps to lower integral uncertainties,

  - Sampling models as well as model parameters is necessary,
  - But not enough (yet)
    - Models have to be improved, or
    - Some exp. data need to be discarded, or
    - Model defect needs to be included

Conclusions

- TENDL + BMC/BFMC + in-depth evaluation: power tool
- To compensate for model limitation: use model defects
- A necessity: use integral data during the evaluation process
- Outcome: more correlations, smaller uncertainties and less biaises



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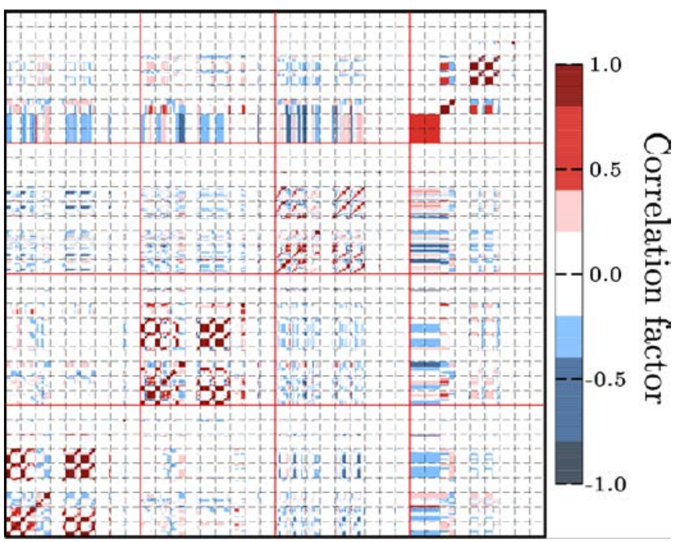

Tomorrow

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Wir schaffen Wissen – heute für morgen