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D. Rochman

TENDL-2017: better cross sections, better covariances

Workshop on TALYS/TENDL Developments, 13-15 November 2017, Prague, Czech Republic

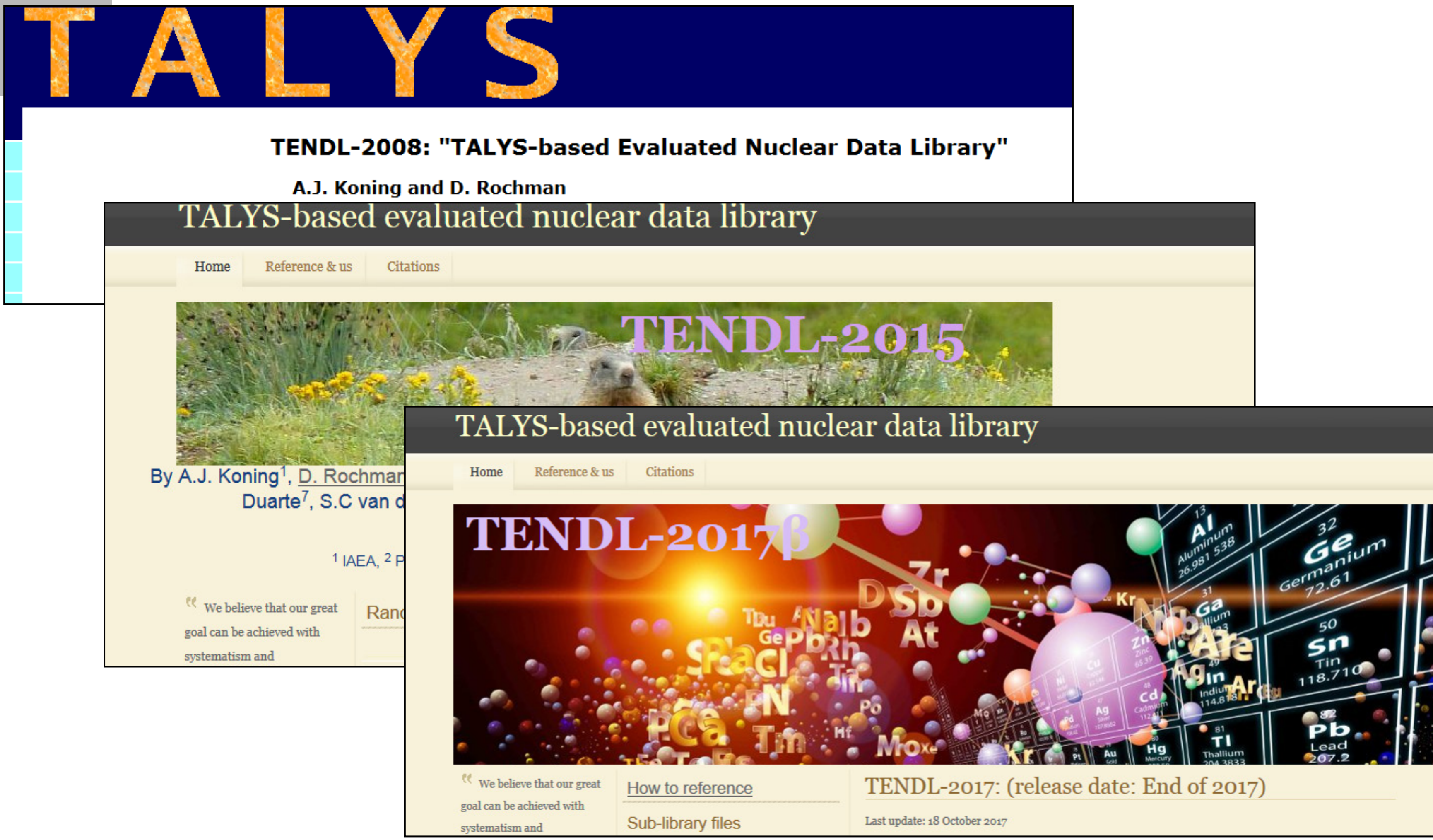
Summary

- Short history, background
- TENDL-2017, plans, schedule
  - Better cross sections
  - Bayesian Monte Carlo with isotopic EXFOR data
- Beyond TENDL-2017
  - Bayesian Monte Carlo with natural element EXFOR data
  - BMC with integral data
  - Cross-isotope correlations

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

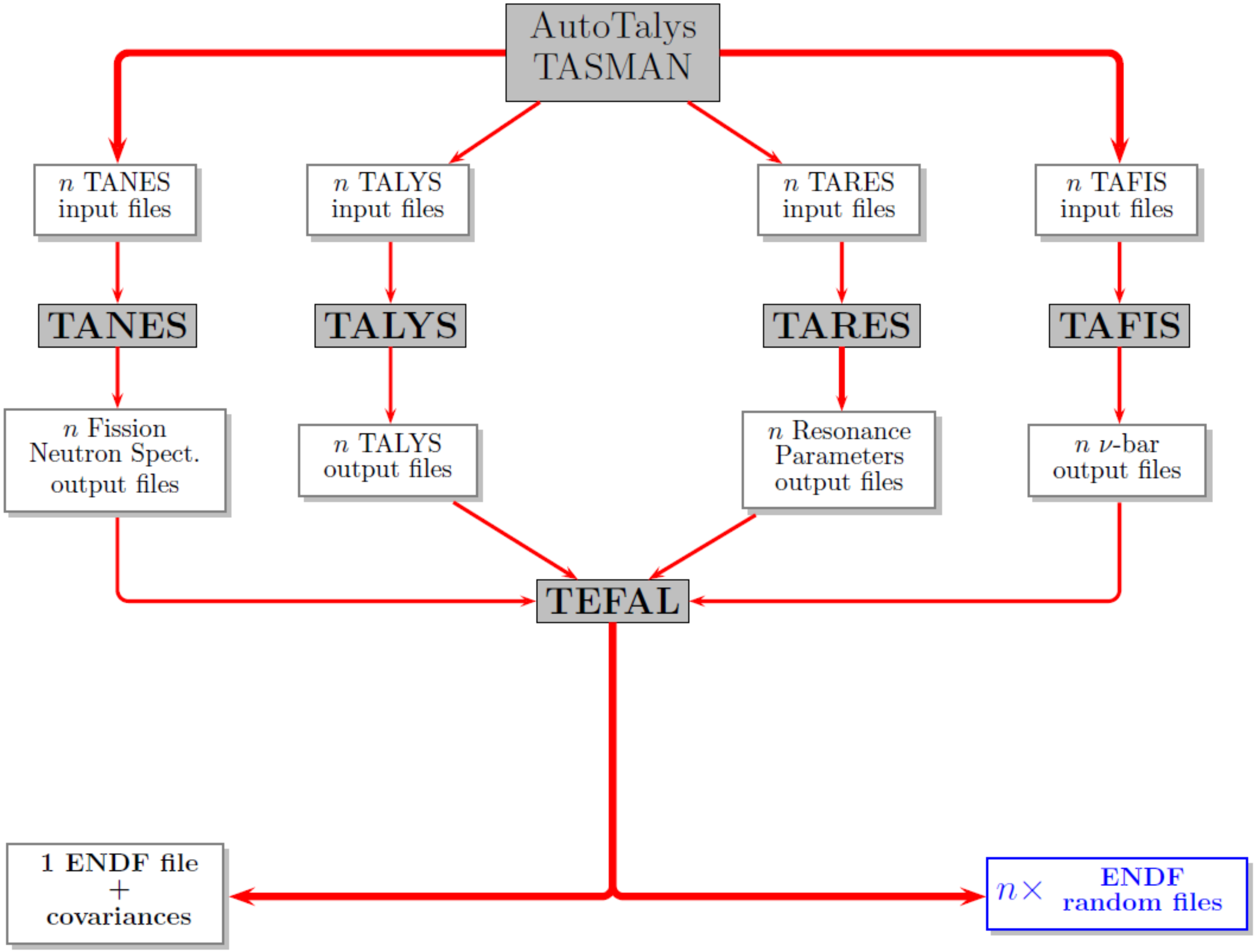
TENDL-2008 to 2017: short history

- Started in 2008 at NRG
- Released in 2008, 2009, 2010, 2011, 2012, 2013, 2014, 2015 and 2017.



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

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TENDL-2008 to 2017: short history

- Impact:
  - More than 2800 isotopes,
  - 80 isotopes in JEFF-3.2, many in FENDL-3.1
  - >150 isotopes in JEFF-3.3 (=TENDL-2015)
  - 28 isotopes in ENDF/B-VIII.0 (=TENDL-2015)
  - Citations (by Google Scholar):

2009	2010	2011	2012	2013	2014	2015	2016	2017 (as of today)
5	15	50	48	56	86	103	103	110

  - Main paper: 2012

2018

New paper planned in NDS

ELSEVIER

Available online at www.sciencedirect.com

SciVerse ScienceDirect

Nuclear Data Sheets 113 (2012) 2841–2934

Nuclear Data Sheets

www.elsevier.com/locate/nds

Modern Nuclear Data Evaluation with the TALYS Code System

A.J. Koning* and D. Rochman

Nuclear Research and Consultancy Group NRG, P.O. Box, 1755 ZG Petten, The Netherlands

(Received 13 July 2012; revised received 15 September 2012; accepted 24 September 2012)

TENDL-2008 to 2017: validation

- **Criticality:** S. van der Marck criticality and shielding benchmarks
- **Activation:**

CCFE
CULHAM CENTRE FOR FUSION ENERGY

CCFE-R(15)25
January 2015

Jean-Christophe Sublet
Mark R. Gilbert

Decay heat validation, FISPACT-II & TENDL-2014, JEFF-3.2, ENDF/B-VII.1 and JENDL-4.0 nuclear data libraries

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JUKO Research

EAF-Doc-54

VALIDATION OF TENDL-2009 USING INTEGRAL MEASUREMENTS

(Draft Release 1)

CCFE-R(15)27
March 2015

Michael Fleming
Jean-Christophe Sublet
Jiri Kopecky

Integro-Differential Verification and Validation, FISPACT-II & TENDL-2014 nuclear data libraries

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EPJ Web of Conferences **146**, 02033 (2017) DOI: 10.1051/epjconf/201714602033
ND2016

TALYS/TENDL verification and validation processes: Outcomes and recommendations

Michael Fleming[1,a], Jean-Christophe Sublet[1], Mark R. Gilbert[1], Arjan Koning[2], and Dimitri Rochman[3]

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[3] Reactor Physics and Systems Behavior Laboratory, Paul Scherrer Institute, Villigen, Switzerland

TENDL-2017

- To be released “end of 2017”,
- As previously, about 2800 isotopes, from 0 to 200 MeV, fixed bugs,
- Incident particles: n,p,d,t,h,g,a
- With covariances, new: MF33 from 0 to 200 MeV (previously: MF32 + MF33),
- New: improved cross sections for fusion (thanks to N. Dzysiuk NRG and EUROfusion), (and possibly for fission products ?)
- Yes, TENDL will be great, again.

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TENDL-2017: Improved automation in T6

- New code versions to produce TENDL-2017: improved T6
- Effort at PSI and IAEA

```
|-- autonorm
|-- bin
|-- endftables
|-- libraries
|-- samples
|-- tafis-1.1
|-- talys
|-- tanes-1.1
|-- tares-1.3
|-- tasman
|-- tefal
`-- tools
```

- Tested in Linux, Mac, with many compilers,
- New “libraries” database for automatic comparison

```
|-- Er164
|-- Er166
|-- Er167
|-- Fe054
|-- Fe056
|-- Fe057
|-- Fe058
|-- Gd152
|-- Ge072
```

→

```
|-- cendl3.1
|-- eaf.2010
|-- endfb8.0
|-- exfor
|-- irdff1.0
|-- jeff3.3
|-- jendl.2007.he
|-- jendl4.0
|-- jendl4.0.he
|-- plots
`-- tendl.2015
```

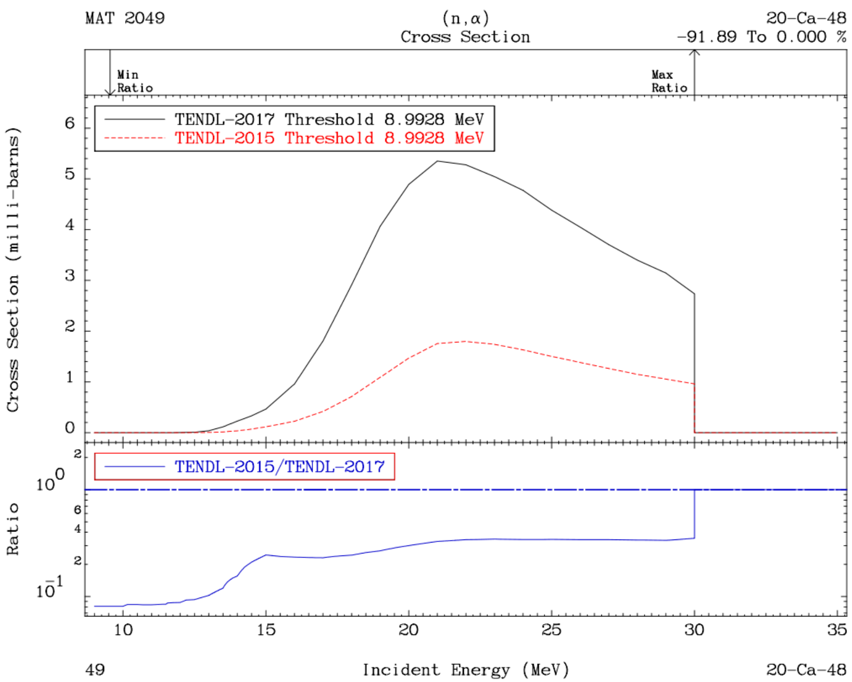
→

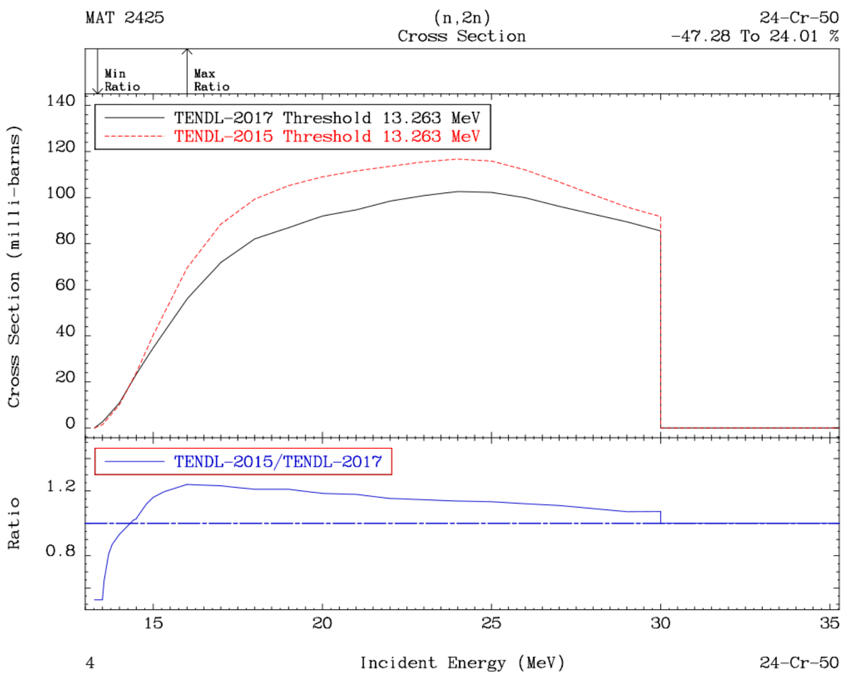
```
|-- eaf.2010
|    |-- check
|    |-- files
|    `-- tables
|-- endfb8.0
|    |-- check
|    |-- files
|    `-- tables
|-- exfor
|    |-- angle
|    |-- ddx
|    |-- eview
|    |-- ratio
|    |-- resonance
|    |-- spectrum
|    `-- xs
```

TENDL-2017: fusion cross section from NRG

- N. Dzysiuk improved more than 90 reactions, such as capture, (n,2n), (n,p) and (n,a) (see N. Dzysiuk et al. (2017): Improving Activation Cross Sections for Fusion Applications, **Fusion Science and Technology**, DOI:10.1080/15361055.2017.1372682)

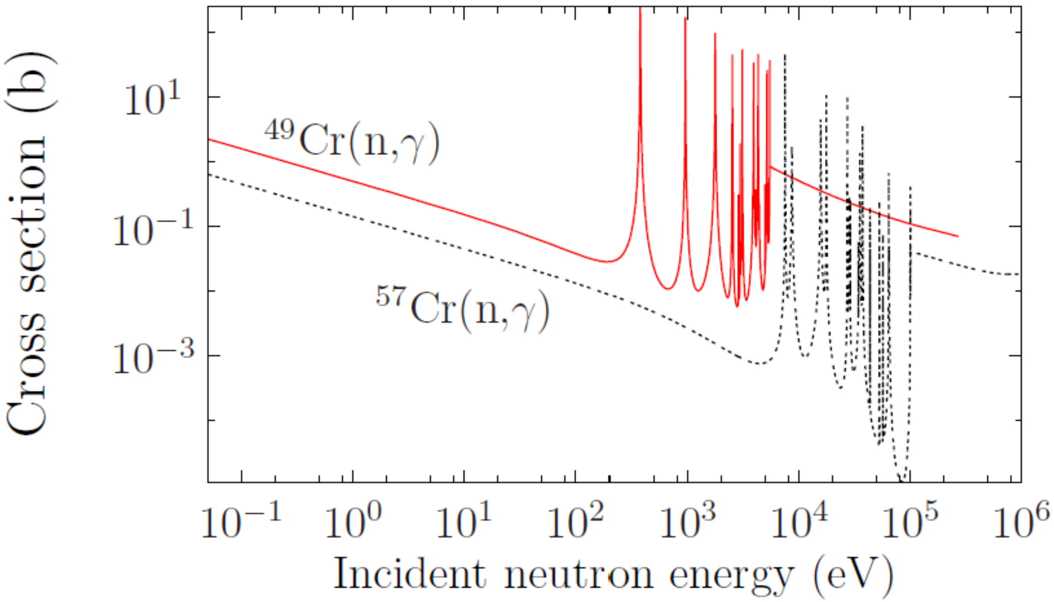
- About 78 of these reactions are now included in TENDL-2017





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.



TENDL-2017: Bayesian Monte Carlo

- Inclusion of experimental data (cross sections) with a Bayesian Monte Carlo method (BMC):
  - 1) General fitting process (by eyes, on isotopic EXFOR data)
  - 2) Sampling of all model parameters *i* times, *i=1…1000*
  - 3) Weighting of all realizations *i* with a chi2 and update the parameter distributions

$$\chi_i^2 = \left(\frac{\sigma_{\mathrm{i}} - \sigma_{\mathrm{exp}}}{\Delta\sigma_{\mathrm{exp}}}\right)^2$$

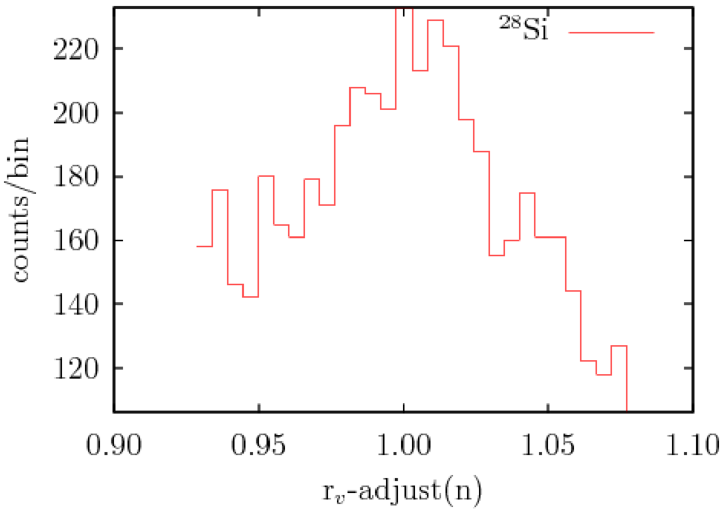
$$w_i = \exp(-\frac{\chi_i^2}{2})$$

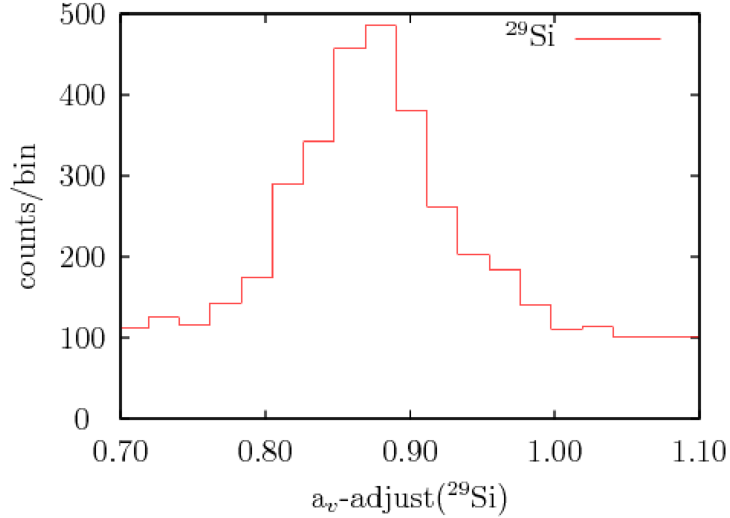
$$\begin{cases} \omega = \sum_i^n w_i \\ \omega_\sigma = \sum_i^n w_i \cdot \sigma_i / \omega \end{cases}$$

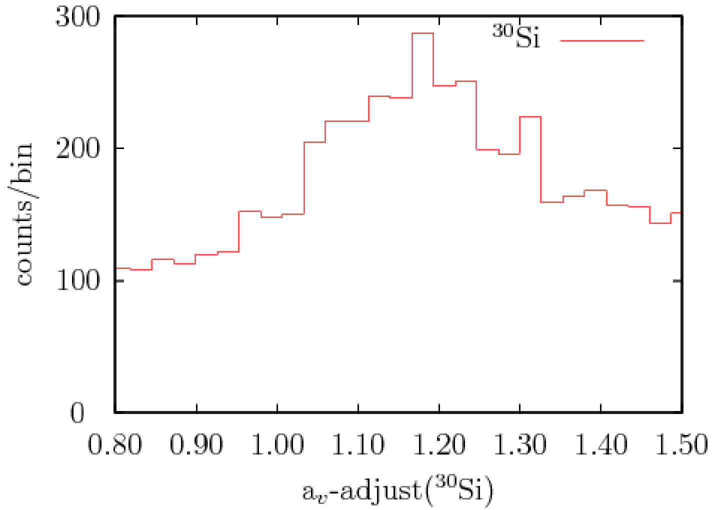
- Advantage: no assumptions on linearity and a priori Gaussian distributions
- Some BMC/BFMC references:
  - EPJ/A 51 (2015) 184,
  - Nucl. Data Sheets 123 (2015) 201,
  - EPJ/N 3, 14 (2017)

TENDL-2017

- Example of updated TALYS parameters with BMC, used for sampling in TENDL-2017: (prior: uniform distributions)

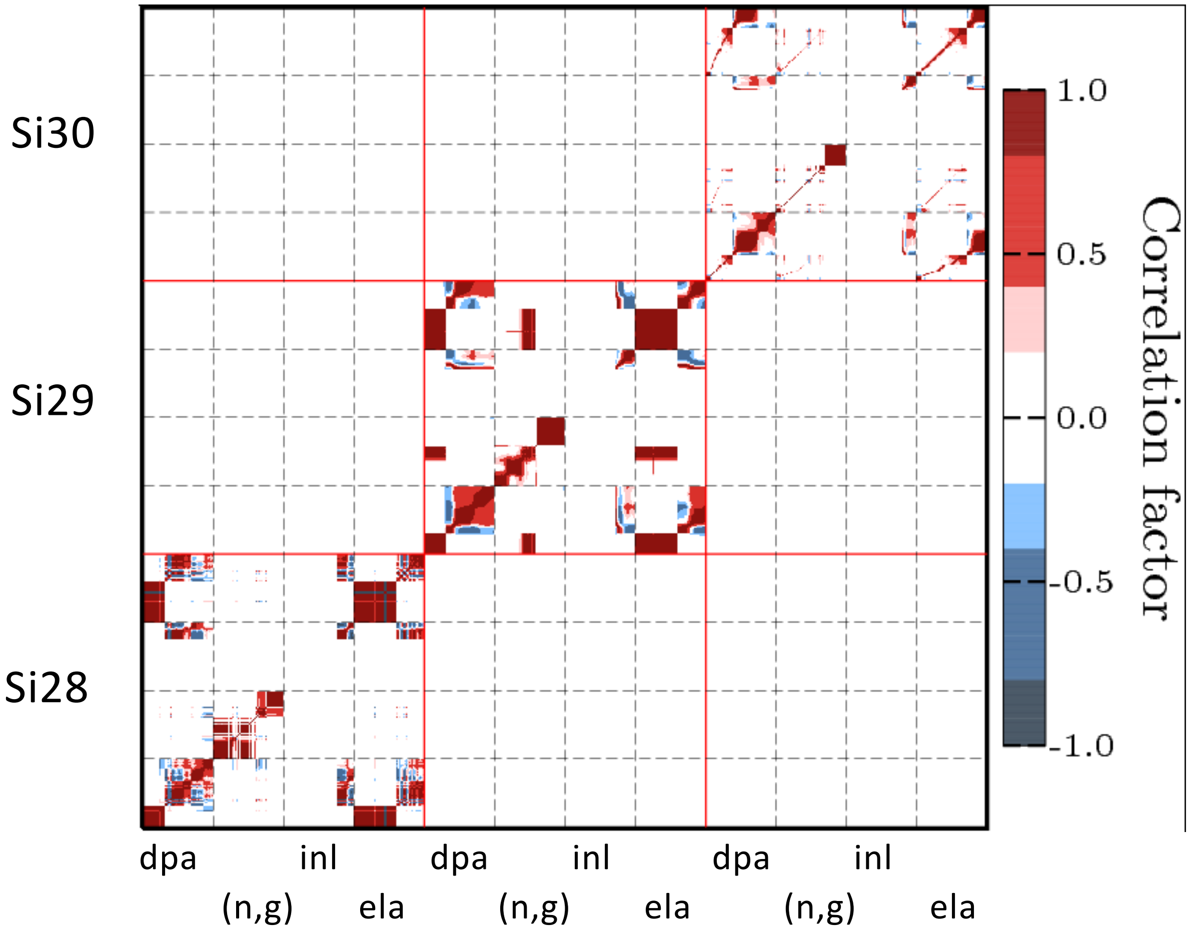






TENDL-2017: examples for Si, U, Pu

- As only isotopic data are considered, there are no correlations between Si isotopes.



TENDL-2017: examples for Si, U, Pu

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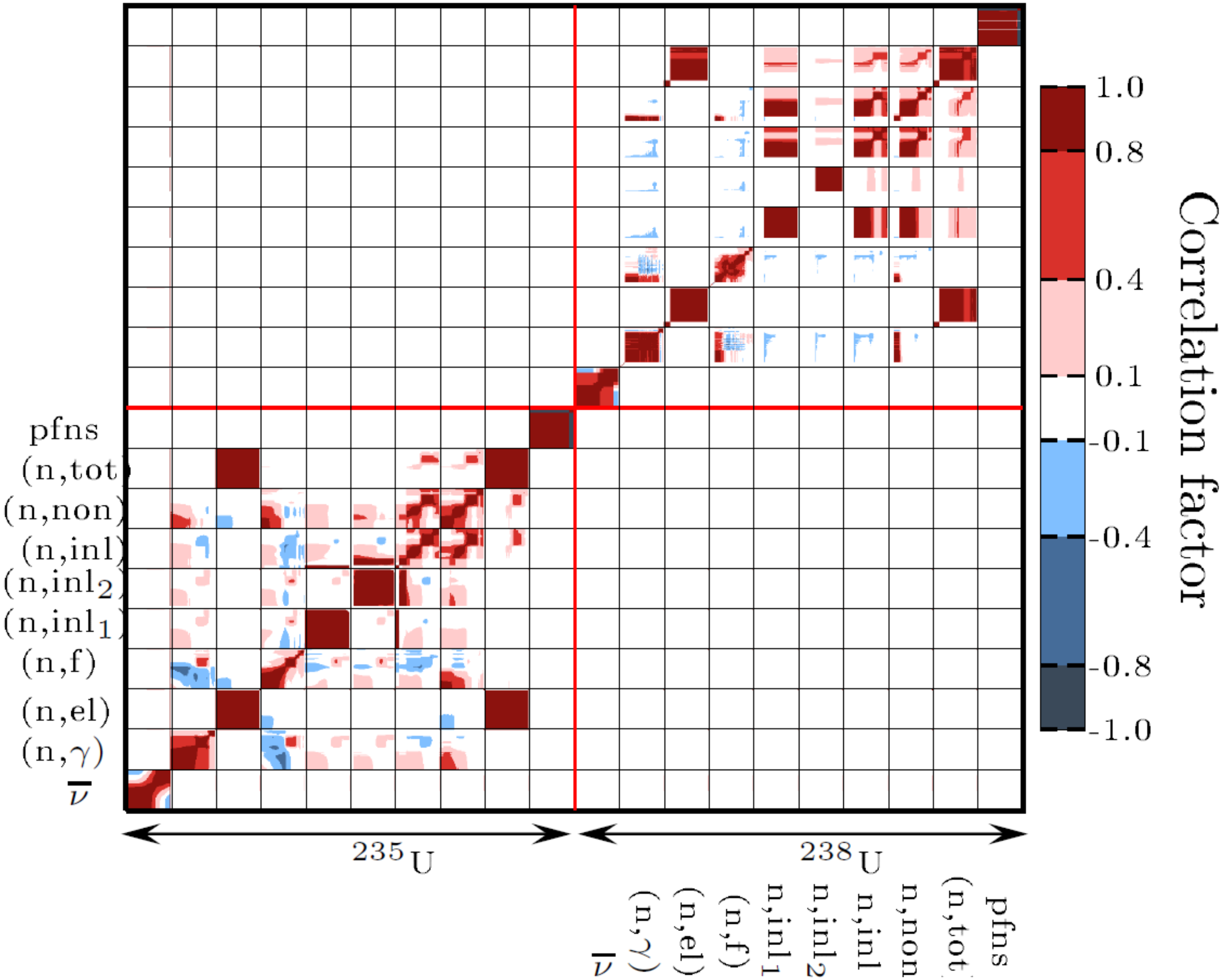
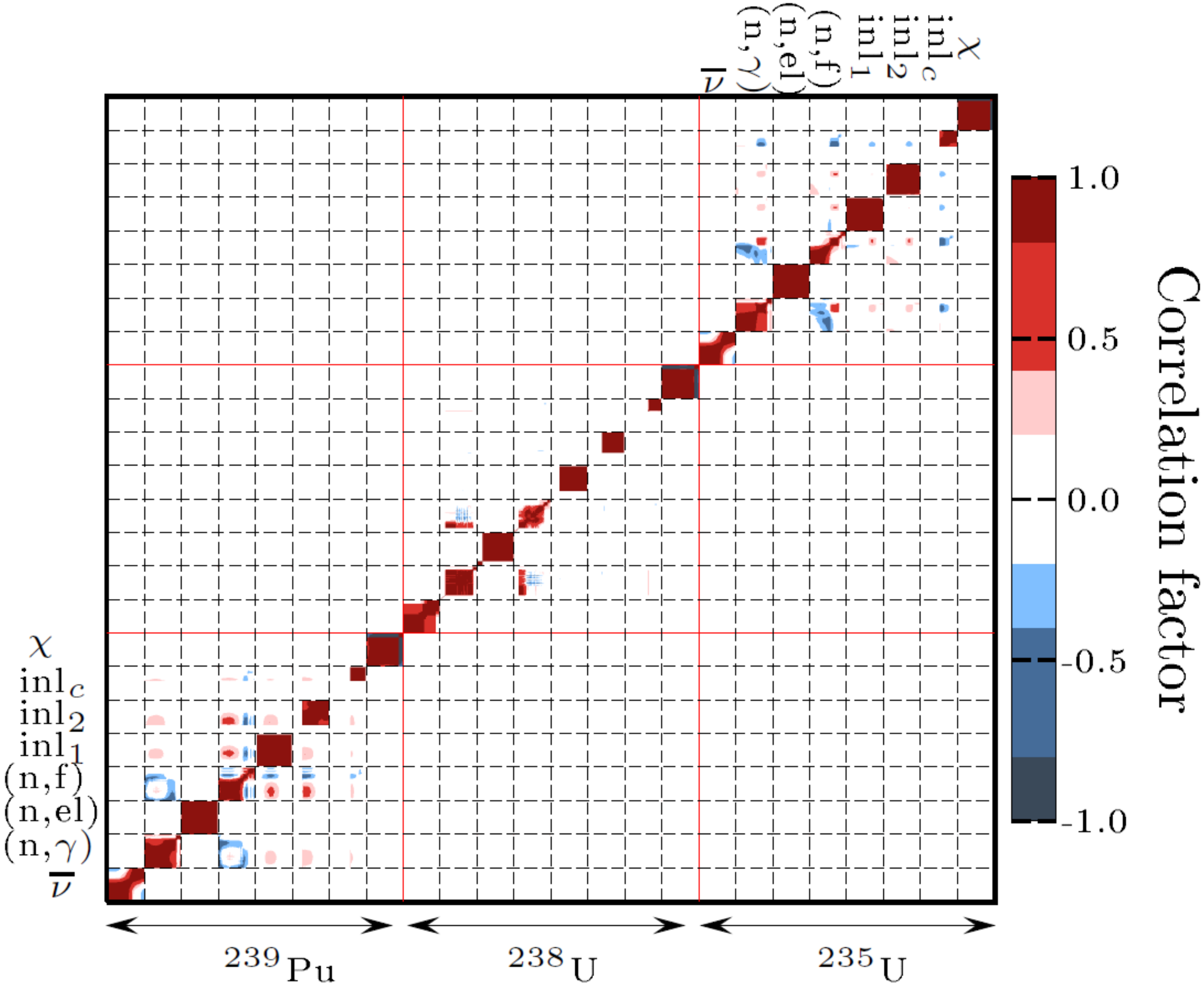


TENDL-2017: examples for Si, U, Pu

- As only isotopic data are considered, there are no correlations between U isotopes.



Beyond TENDL-2017

- Some experimental data are not taken into account during the evaluation process:
  - integral data (k_{eff}, spectral indexes, shielding…)
  - cross sections for natural targets (e.g. ^{nat}Si)
  - cross sections for compound targets (e.g. SiO_2)

- These data can be included, but possibly not at the same level than isotopic cross sections
- One solution is to perform stepwise evaluations:
  - 1) "normal" evaluation process (e.g. BMC on isotopic data),
  - 2) based on these results, include other types of data (integral, natural…), still following the BMC approach

- This way, we still have a "general purpose library" and a "general purpose library with correlation".

Example on Si isotopes

- Goal: include the ^{nat}Si and SiO_2 EXFOR cross sections into the isotopic evaluations of $^{28,29,30}Si$,
- Method: using BMC based on the TENDL-2017 $^{28,29,30}Si$ files,

- Step 1: Produce 1000 random files for each isotope from TENDL-2017,
- Step 2: Select (n,tot) and (n,el) for ^{nat}Si and SiO_2 EXFOR cross sections
- Step 3: Use weights to update evaluated cross sections curves,

- Result: updated cross sections, uncertainties, and correlations between isotopes

- Side remark: this method is close to GLLS or Monte Carlo adjustment (see next slide), but with less approximations.

Remarks on TMC, BMC, GLLS and MOCABA

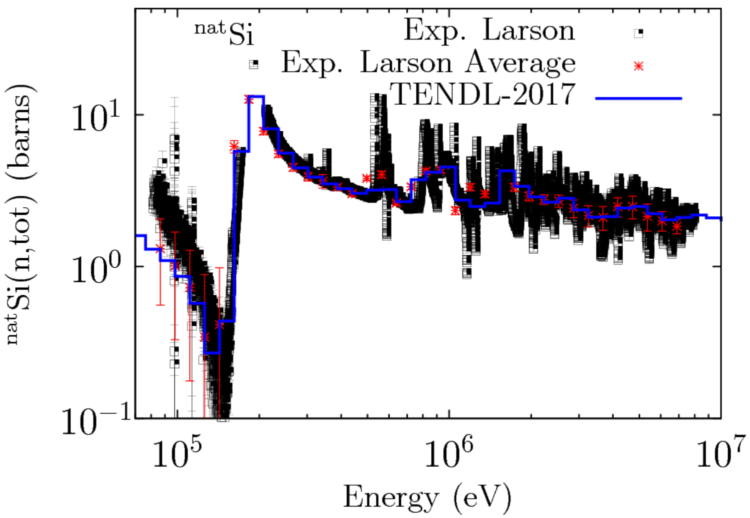
- TMC: Total Monte Carlo, see next presentation (creating random files),
- BMC: Bayesian Monte Carlo = TMC + weights on random files,
- GLLS: Generalized Linear Least Square
- MOCABA: Monte Carlo version of the GLLS

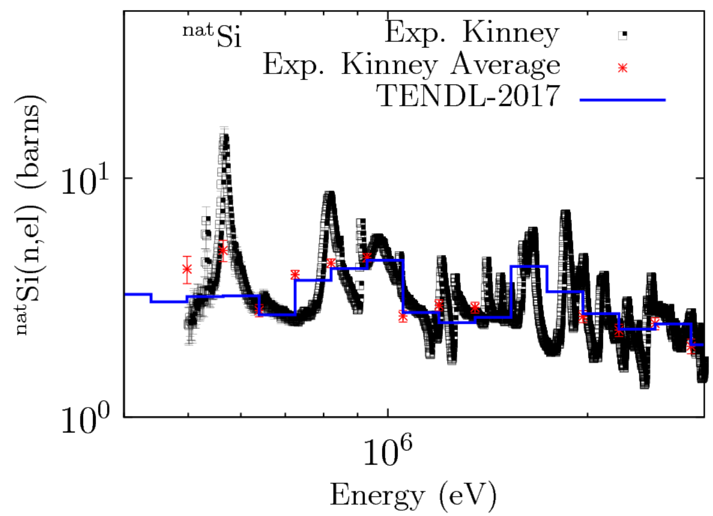
Method	GLLS	MOCABA	BMC
Assumption	Linear+Normal	Normal	None
Drawback/Advantages	Fast, ignore nonlinearity	Not so fast, ignore linearity	Even slower, accept non Normal inputs and nonlinear behavior

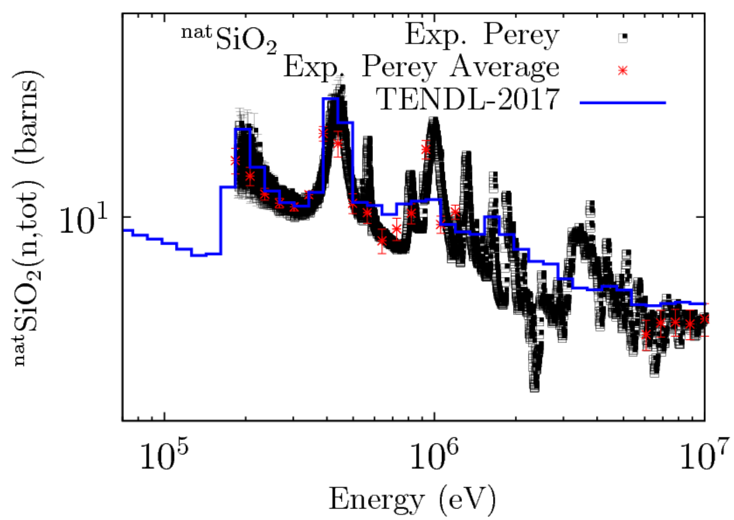
- All these methods are based on the “traditional” ones and can only be applied when time has been spent to select good experimental data, and adjust model parameters (no possibility to escape this).

Example on Si isotopes

- Additional cross sections for the step 2:





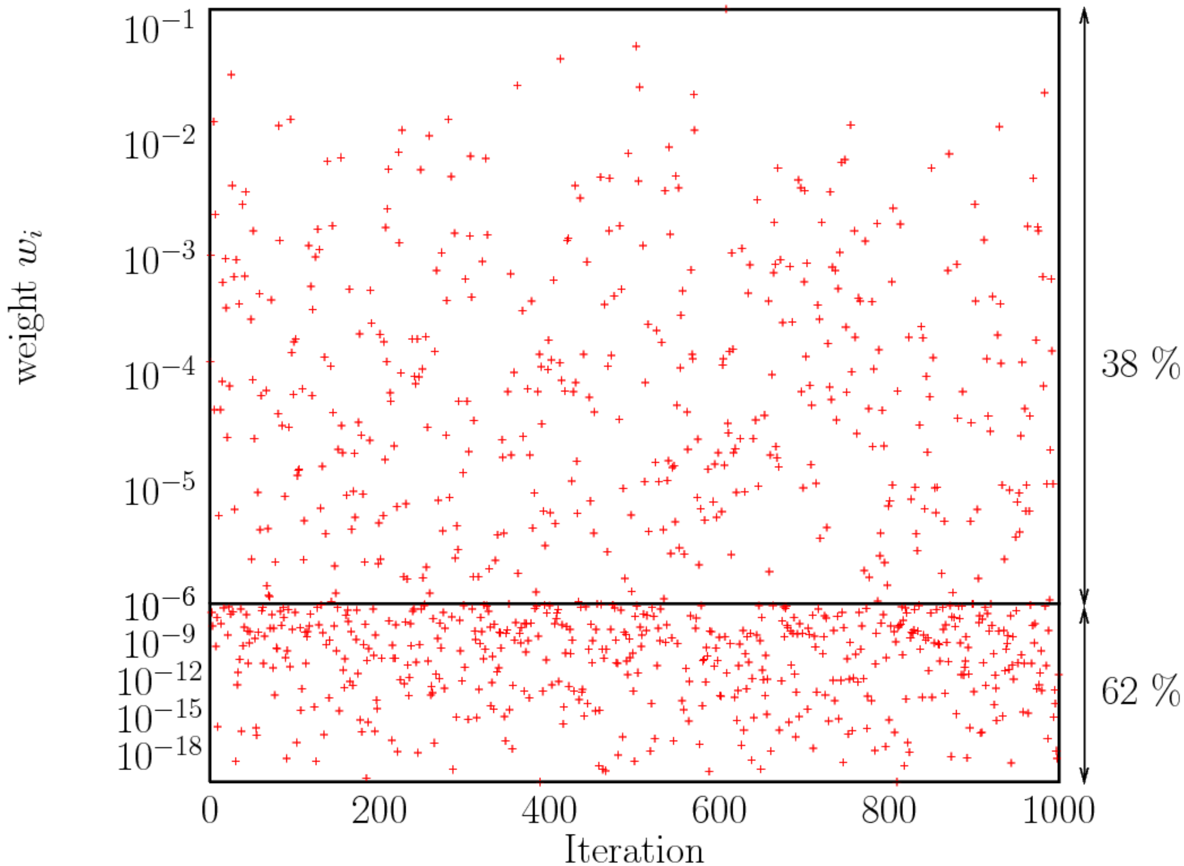


Example on Si isotopes: weights

- Weights on random files using ^{nat}Si and SiO_2 data:

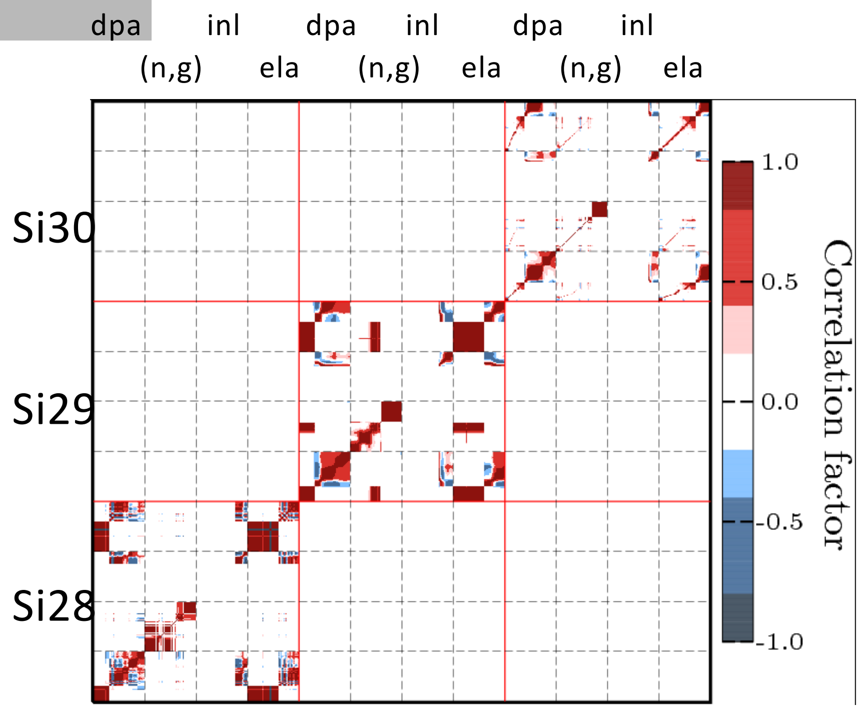
$$\chi_i^2 = \left(\frac{\sigma_i - \sigma_{exp}}{\Delta\sigma_{exp}}\right)^2$$

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

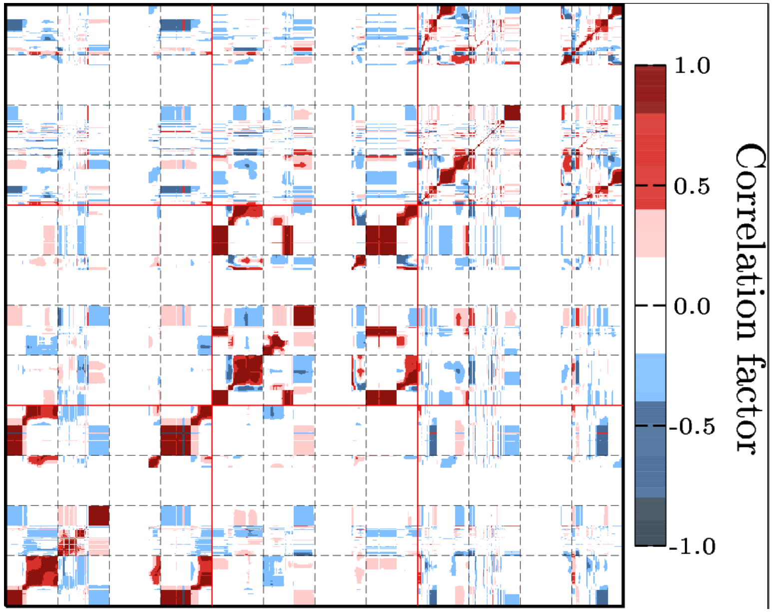


Example on Si isotopes: updated correlations

- The new EXFOR cross sections (^{nat}Si and SiO_2) create correlations between isotopes.
- Example on the dpa and cross section correlation matrices between Si isotopes:



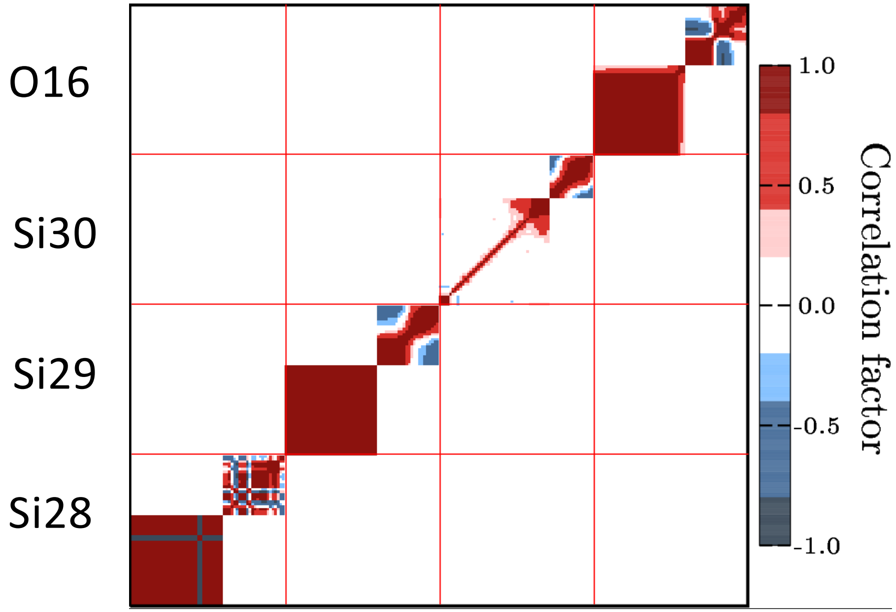
No ^{nat}Si and SiO_2



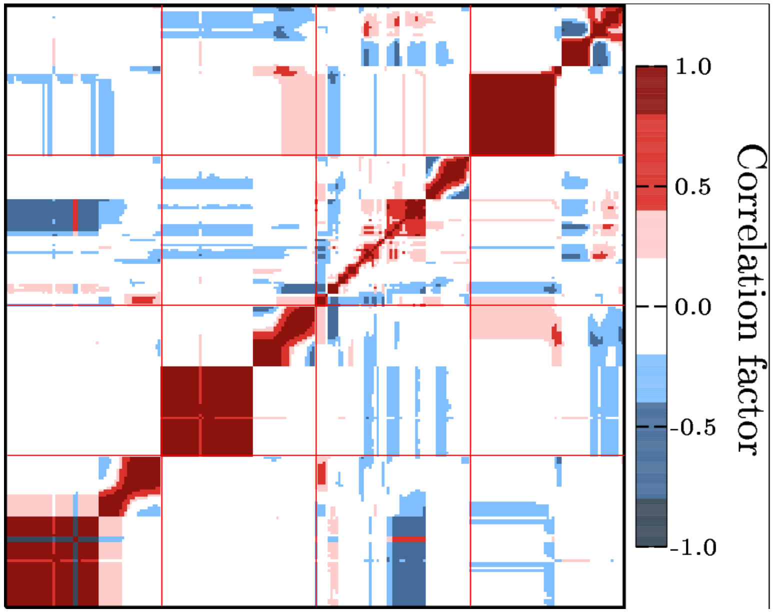
With ^{nat}Si and SiO_2

Example of correlation Si-O

- From the SiO_2(n,tot) cross section, correlations between the Si isotopes and ^{16}O can be obtained, example for the (n,tot) cross sections:



No ^{nat}Si and SiO_2



With ^{nat}Si and SiO_2

Example with criticality benchmarks

- Produce 10 000 random files for $^{235,238}U$, ^{239}Pu and ^{16}O
- Use BMC to include benchmark results and update cross sections, uncertainties and correlations
- Example with imf7 (BigTen):

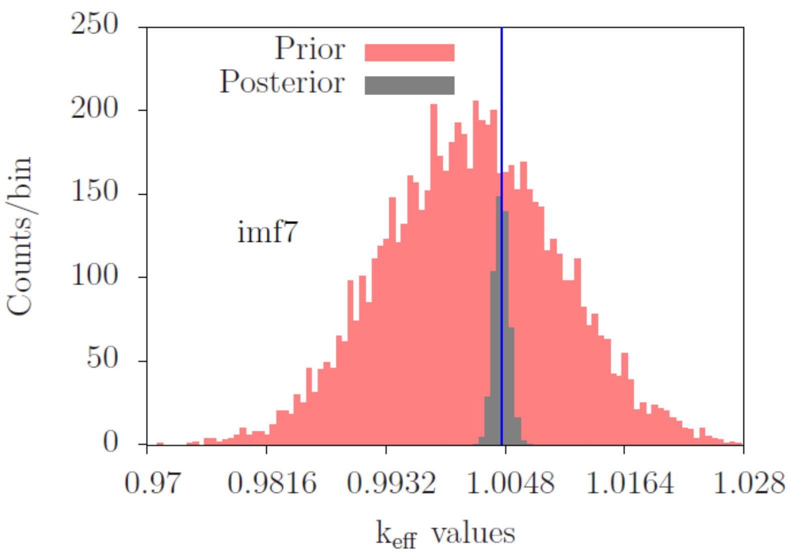


Fig. 12. Prior and posterior distributions of k_{eff} for imf7 benchmark. The blue line indicates the experimental value.

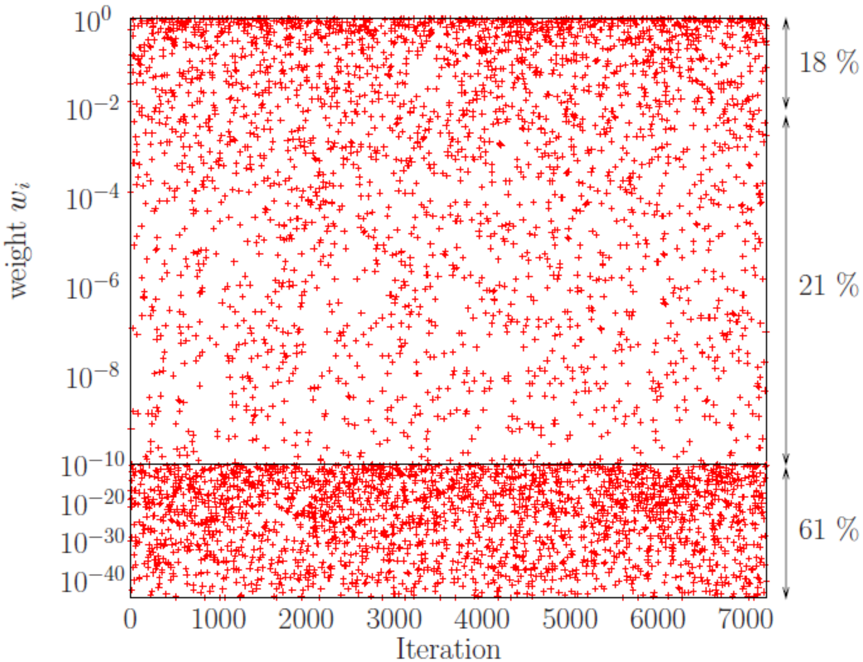


Fig. 1. Calculated weights w_i for the 7000 random cases considered in this work. The number on the right are the percent of weights within the space defined by the arrows.

Example with criticality benchmarks

- Correlation due to the BigTen benchmark:

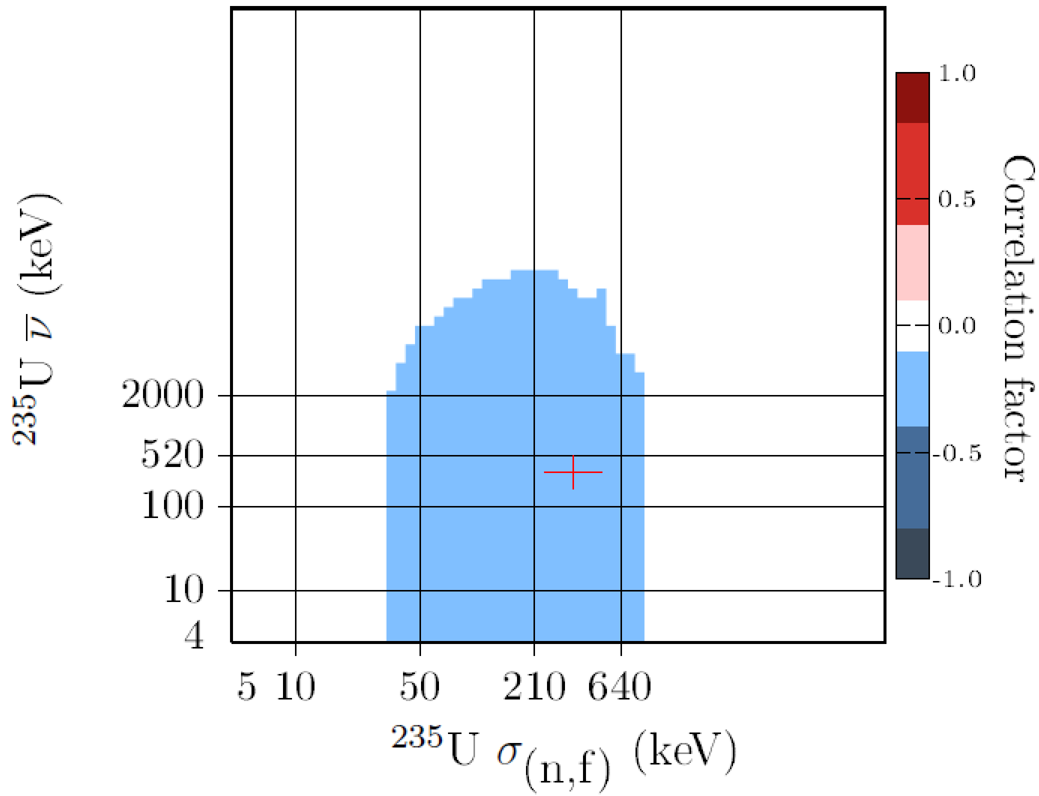
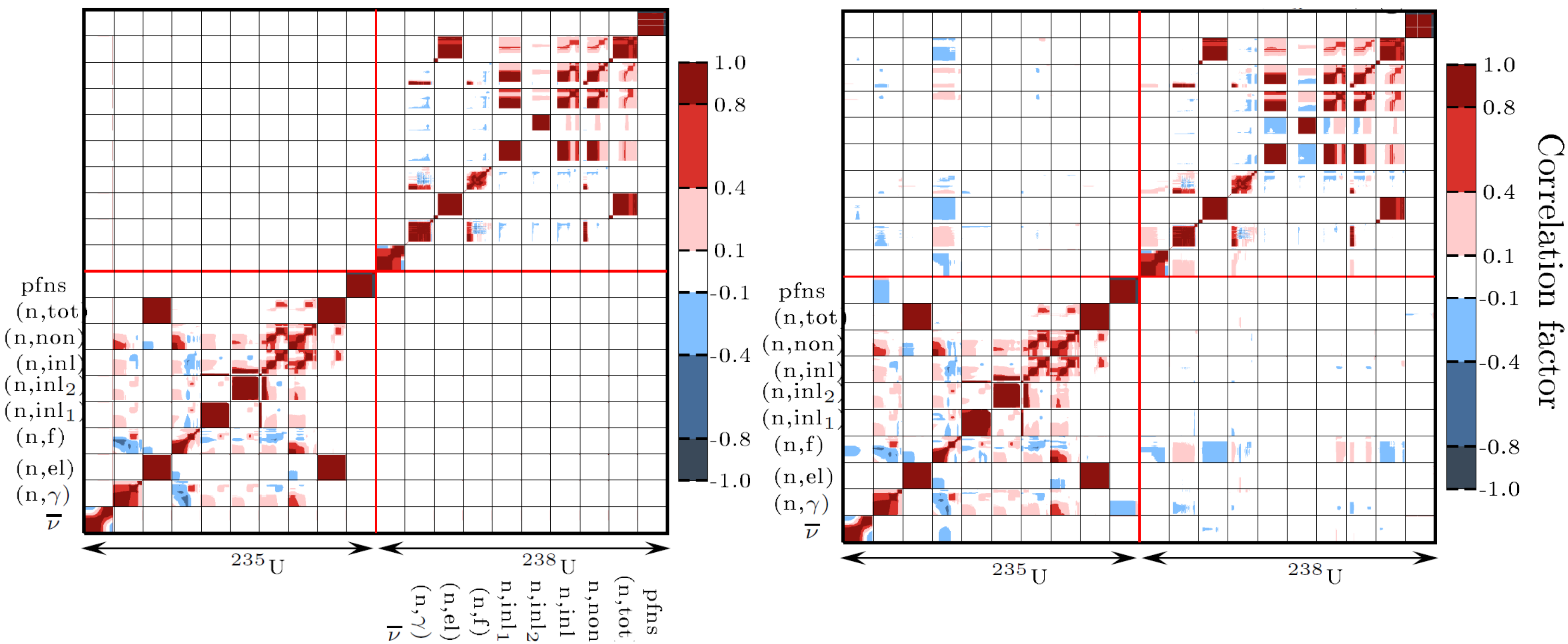


Fig. 5. Correlation sub-matrix between the $\overline{\nu}$ of ^{235}U and the fission cross section of ^{235}U. The red cross indicates the average energy of the neutron causing fission events (Table 1).

Example with criticality benchmarks

- Correlation due to the BigTen benchmark:



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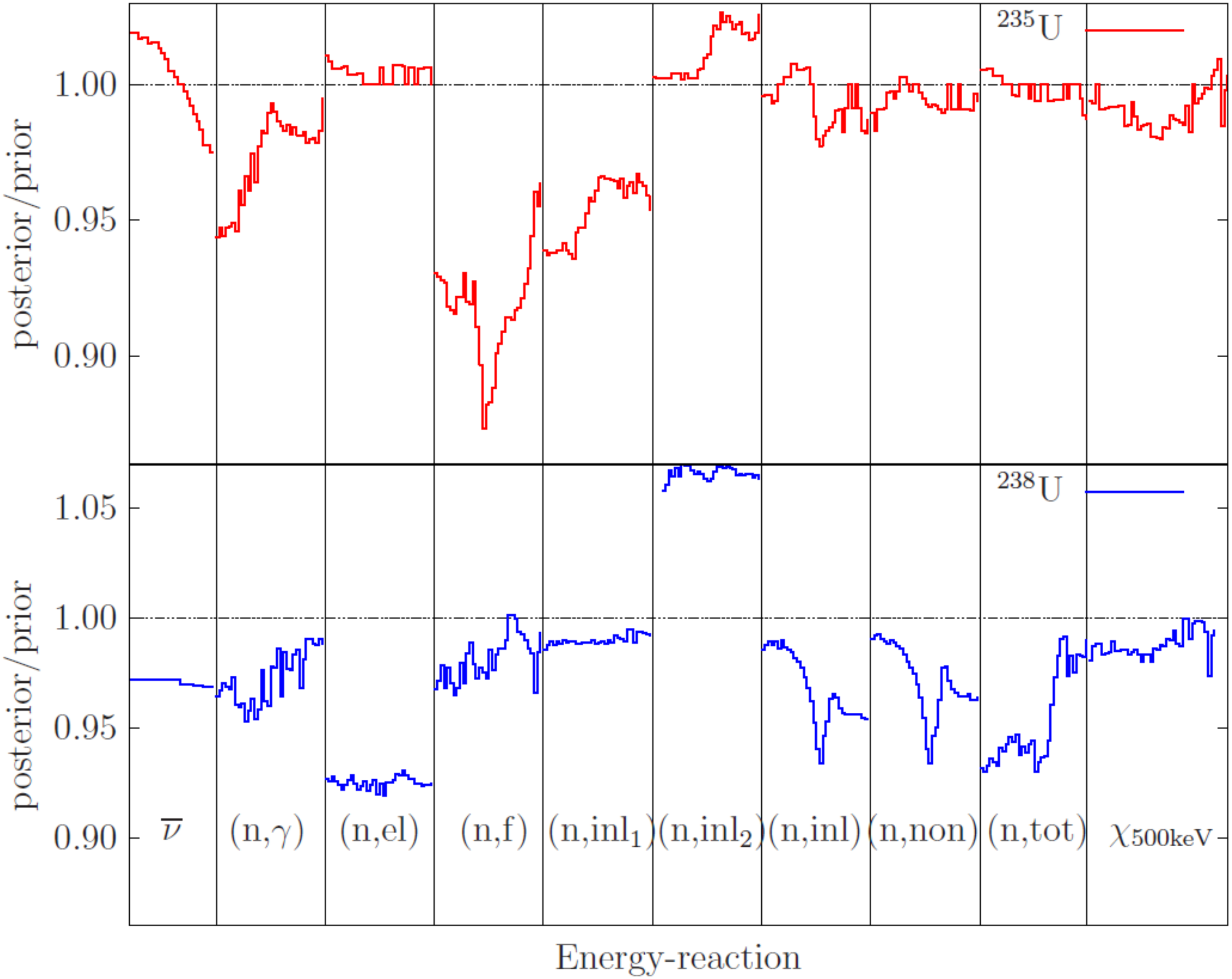
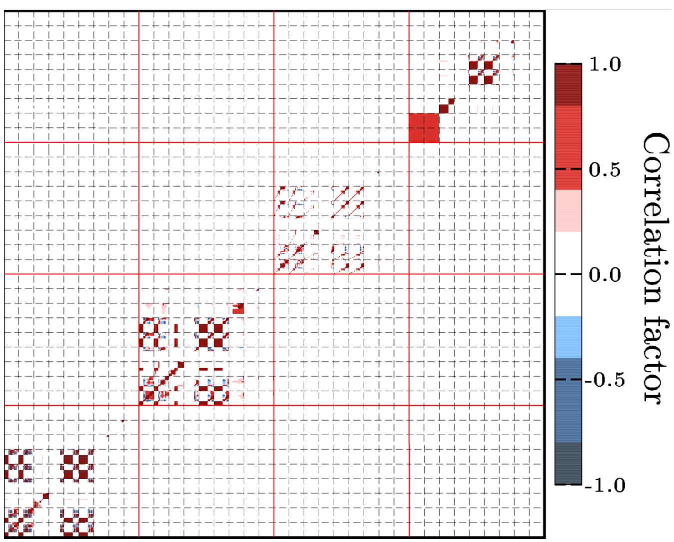
Example with criticality benchmarks

- Reduced cross section uncertainties due to the BigTen benchmark:

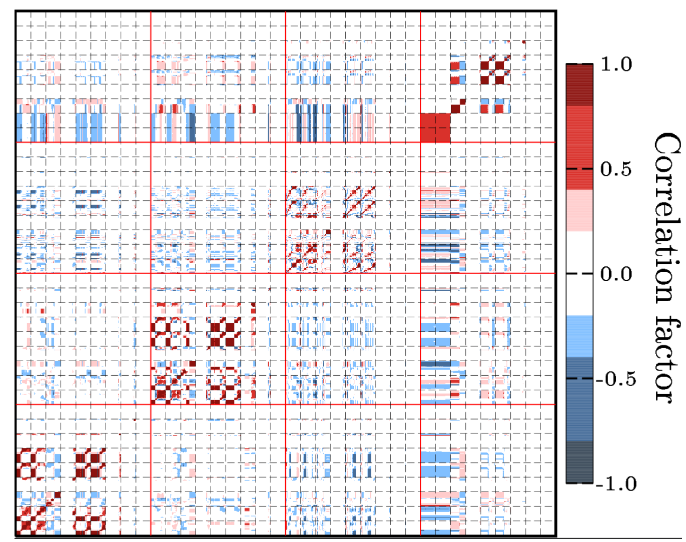


Conclusion

- TENDL-2017: great again, to be released end of 2017,
- Based on the BMC method with EXFOR isotopic data,
- Future: include integral and natural data with the BMC approach,
- Advantage: able to provide a new general-purpose library, with cross-isotope correlations and updated uncertainties (as for dpa or any derived quantity).



Today



Tomorrow

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Wir schaffen Wissen – heute für morgen