PAUL SCHERRER INSTITUT

D. Rochman

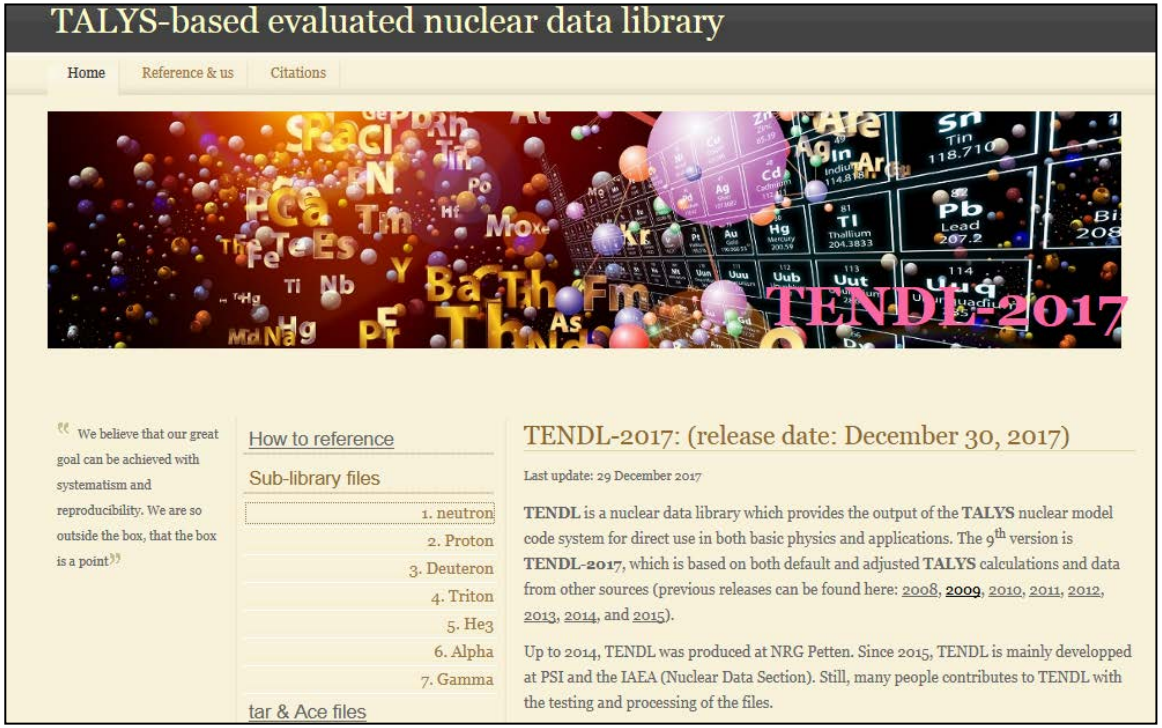
TENDL and Bayesian Monte Carlo: how far can we go ?

S. Chiba Laboratory, Laboratory for Advanced Nuclear Energy,
4 December 2018, Tokyo Inst. of Technology, Japan

Summary

- TENDL and T6: a short history and modern approach

- Examples for current research:
  - TMC
  - BFMC for thermal reactors
  - BMC for fission yields



- All slides are available here: https://tendl.web.psi.ch/bib_rochman/presentation.html

What is the TENDL project ?

- TENDL: TALYS evaluated nuclear data library,
- Goal: improve simulations for TENDL and/or other libraries, or solving

$$\boxed{0 \leq \chi^2 \leq 1}$$

$$\chi^2 = \frac{1}{n}\sum_{i=1}^{n}\left(\frac{C_i - E_i}{\Delta E_i}\right)^2$$

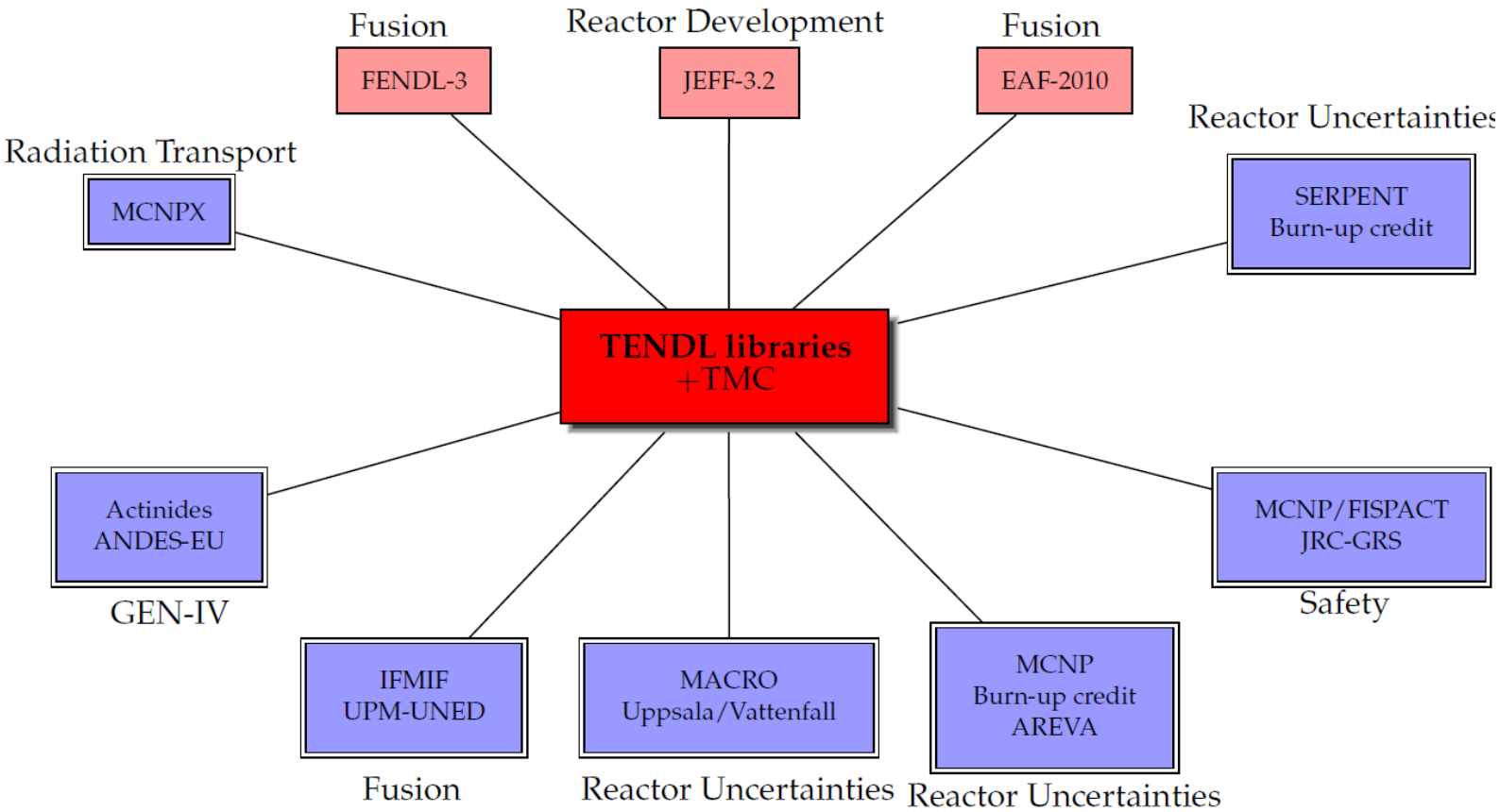
- Available at https://tendl.web.psi.ch/home.html
- Comes from T6 (software package)
- T6 leads to TENDL, TMC, BMC, HFR…
- See for instance NDS 113 (2012) 2841, ANE 51 (2013) 60, NDS 139 (2017) 1

What is the TENDL project ?

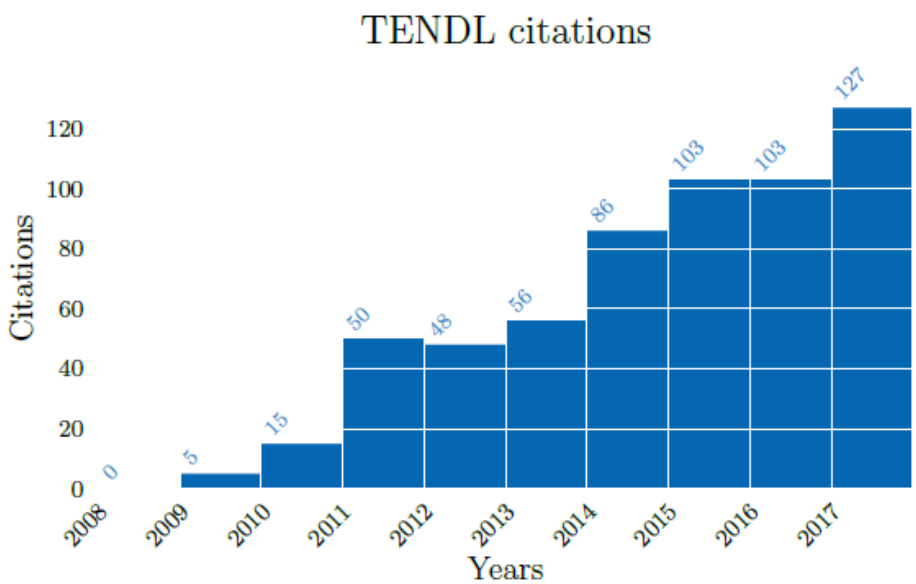
- TENDL is in fact a by-product of a series of codes,
- This is one fundamental difference with other libraries (no manual work),
- It allows to perform „TMC“ for Total Monte Carlo (uncertainty propagation)
- Methods: reproductibility & completeness, development of a portable system, and making use of the knowledge included in other libraries (JEFF, ENDF/B, JENDL),
- Background: theoretical calculations (TALYS) with experimental inputs, with original resonance evaluations,
- Impact:
  - TENDL-2008 to 2017 (2800 isotopes),
  - Neutrons, protons, deuterons, tritons, He3, alpha and gamma induced,
  - all isotopes, all cross sections with covariances, 0-200 MeV,
  - more than 300 isotopes in the NEA JEFF-3.3 library,
  - more than 50 isotopes in the US ENDF/B-VIII.0 library,
  - more than 450 publications using TENDL

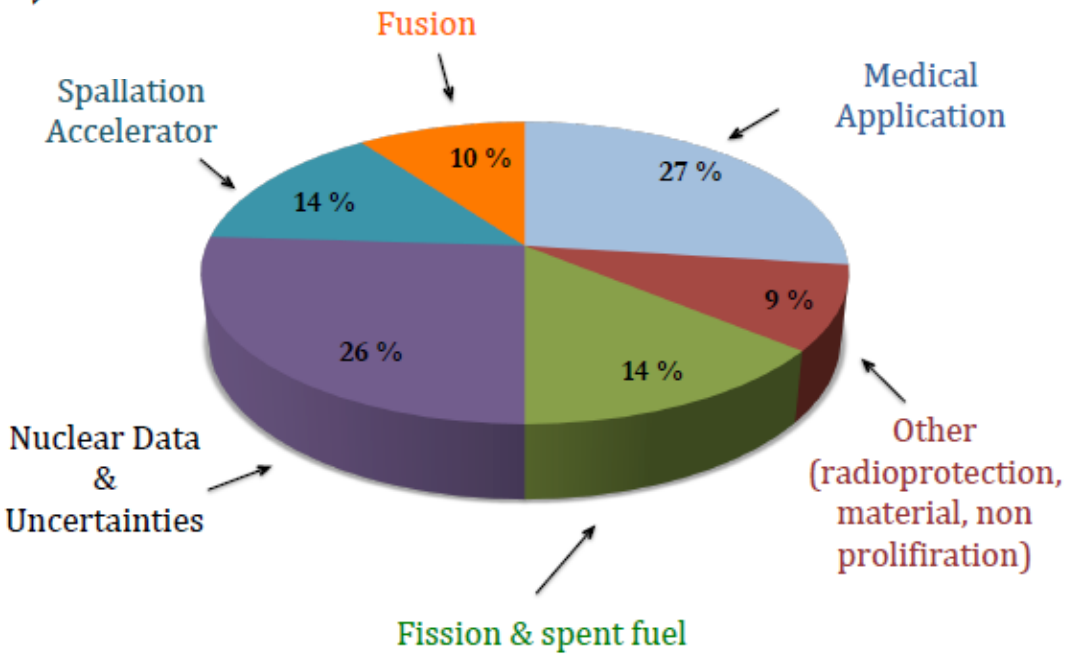
What is the TENDL project ?

- Fully implemented in FISPACT-II, part of GEANT, CASMO…,
- Used in fission, fusion applications, medical isotope productions



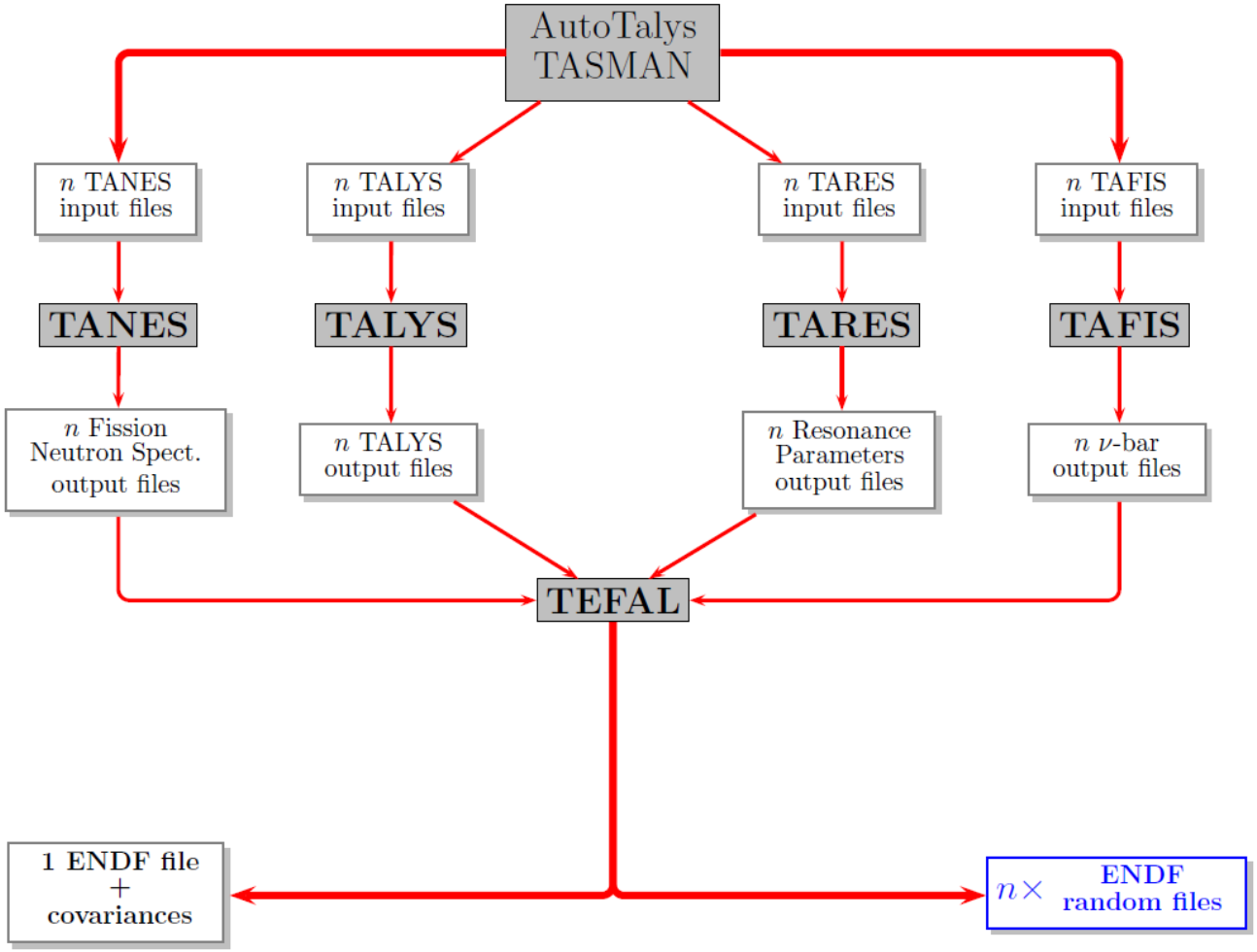
What is the TENDL project ?





T6: source of TENDL

- T6: at the origin of TENDL. Combination of 6 codes plus utilities,
- Available on demand, easy to install,
- Make your own TENDL !



TENDL: from MF-1 to MF-40, 200 MeV

- MF-1: Description + fission parameters
- MF-2: Resonance parameters (Reich-Moore or Multi-level Breit Wigner)
- MF-3: Cross sections (n,tot), (n,el), (n,non), (n,inl$_i$), ..., (n,γ), (n,p$_i$), (n,α_i)
- MF-4: Elastic angular distribution (Legendre Polynomials)
- MF-5: Fission neutron spectrum
- MF-6: Double differential distributions and spectra for (n,2n), ..., (n,α_i)
- MF- 8-10: Isomeric cross sections
- MF- 12-15: Gamma yields, angular distributions and spectra
- MF- 31-32-33-34-35, 40: nubar, Resonance parameter, cross section, angular distribution and fission neutron spectrum, radionuclide production.

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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

TENDL: Complete Nuclear Data Library for innovative Nuclear Science and Technology

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(Dated: November 7, 2018; Received xx July 2018; revised received xx September 2018; accepted xx October 2018)

TENDL: not only an ENDF-6 file

1. Tabular angular distributions
2. Tabular Gamma-ray intensities
3. Tabular partial cross sections to discrete levels
4. Tabular residual cross sections
5. Tabular cross sections
6. ENDF files including covariances
7. EAF cross section and variance files
8. Processed ACE files (with NJOY)
9. Processed covariances (tabular and plots)
10. Random ENDF files (to get uncertainties on anything with TMC)

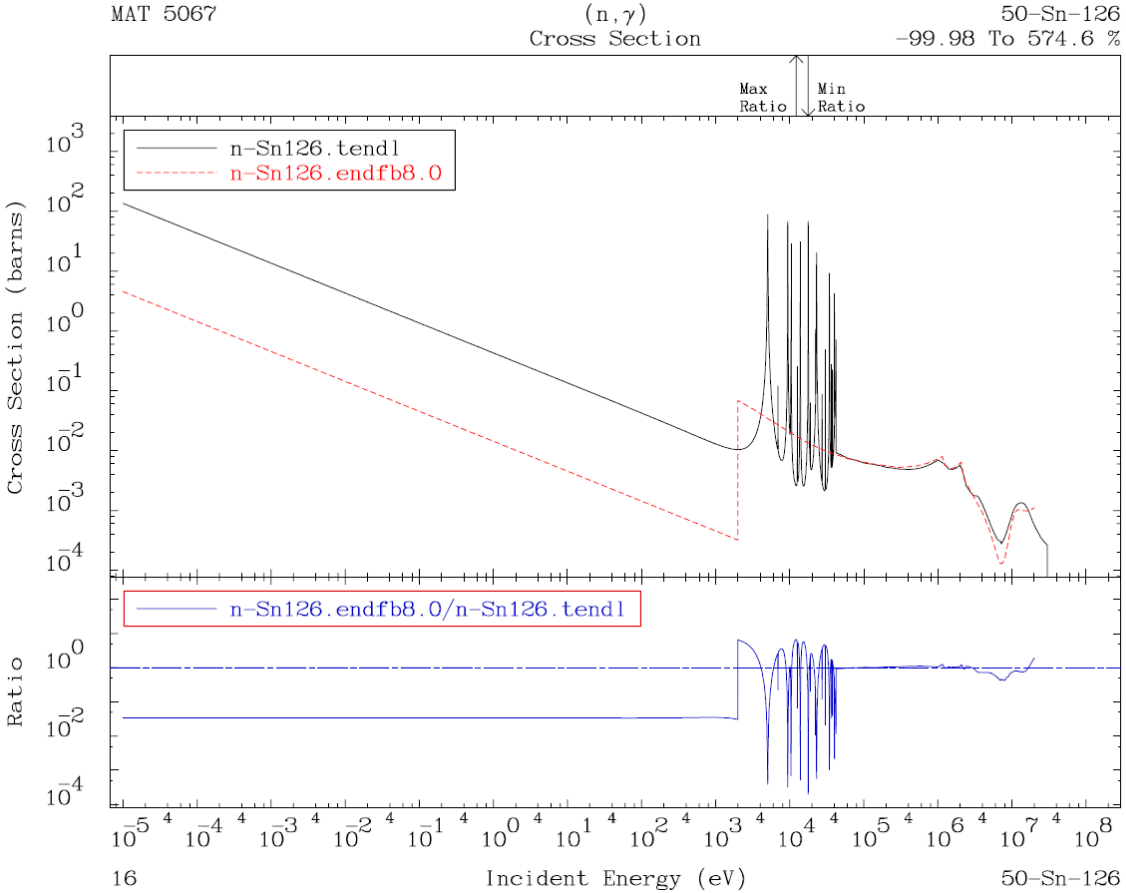
TENDL related projects

The TENDL way is strongly linked to other methods:

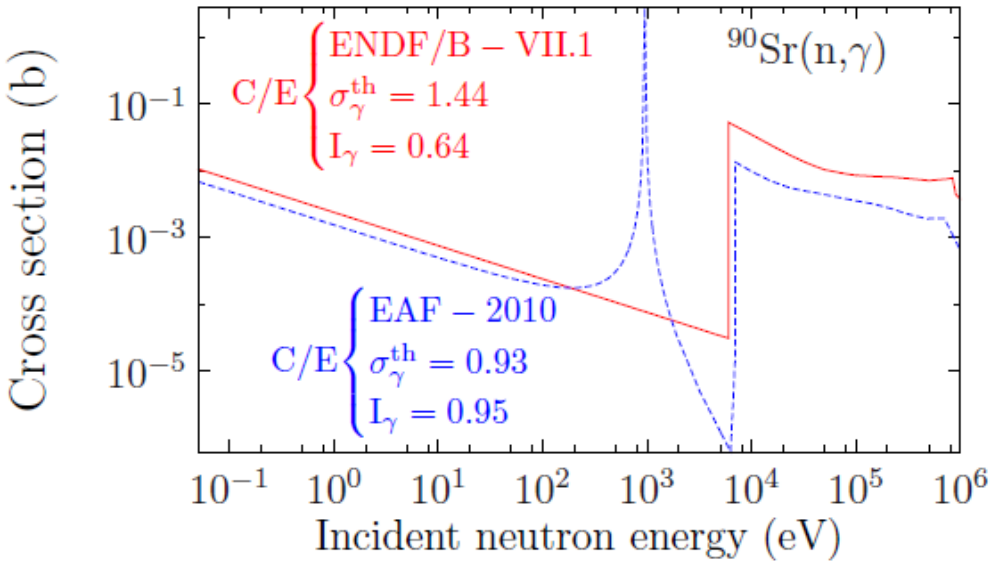
- (fast) TMC: Total Monte Carlo for uncertainty propagation,

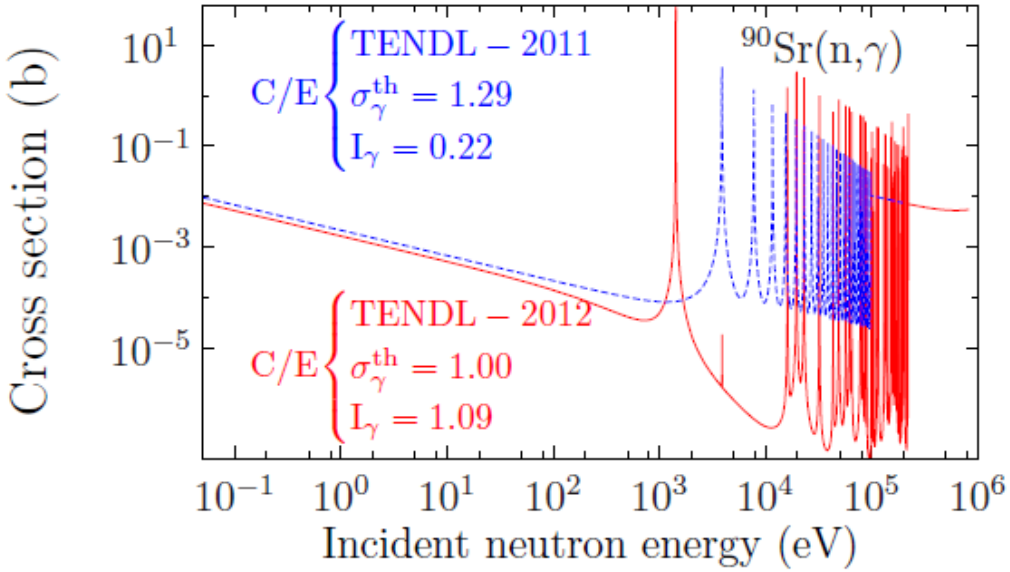
- BMC: Bayesian Monte Carlo for model parameter updates and sampling,

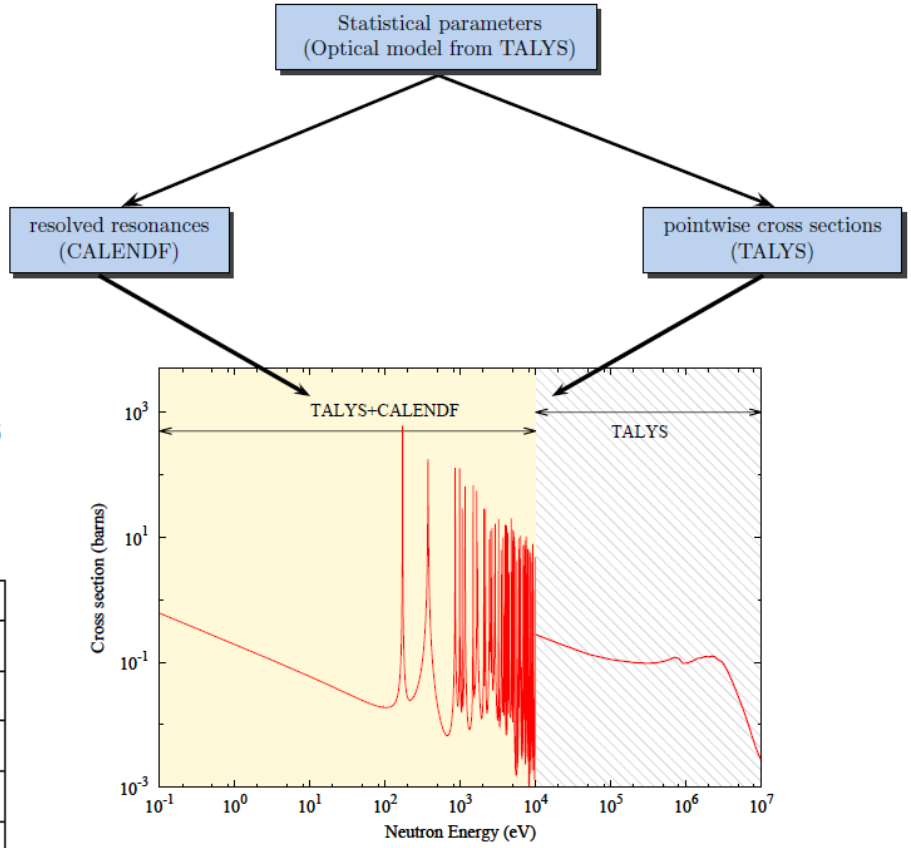
- HFR: Resonance parameters for all isotopes consistent with the fast neutron range.



TENDL related project: the HFR







Making use of T6/TENDL: uncertainty propagation

Three methods exist today:

1. Based on nuclear data covariance data

- So-called “Sandwich rule” = sensitivity times covariances ,
- Provide uncertainties, sensitivities

2. Based on nuclear data parameter covariance data:

- So-called TMC (Total Monte Carlo)
- Sampling of model parameters,
- Provide uncertainties,
- Does not provide sensitivities, but importance factors.

3. In between: based on nuclear data covariance data:

- Sampling of cross section data, based on nuclear data covariances
- Provide uncertainties,
- Does not provide sensitivities, but importance factors,
- Many software: XSUSA, ACAB, NUDUNA, NUSS, SANDY, SAMPLER…

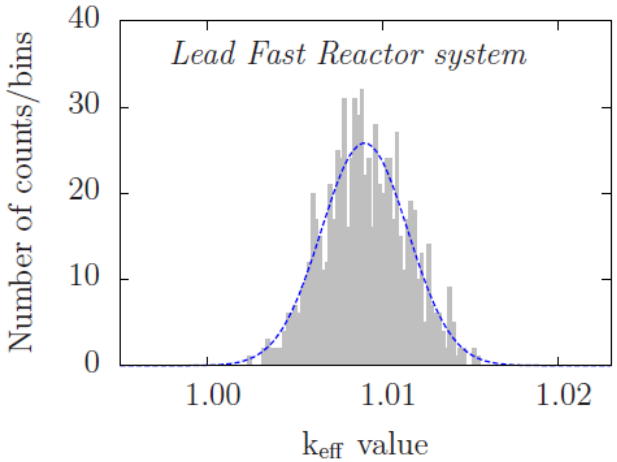
Making use of T6/TENDL: uncertainty propagation with TMC

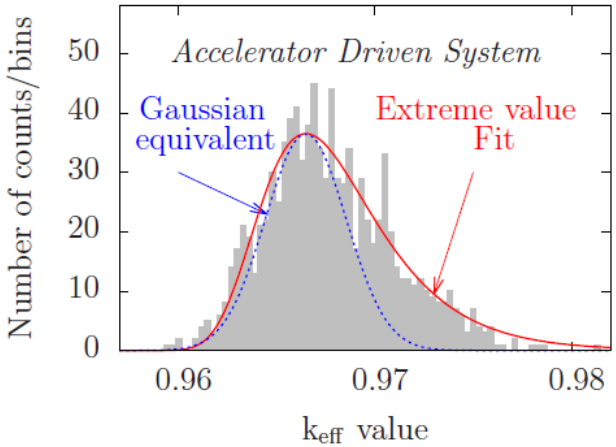
Control of nuclear data (TALYS system)
+ processing (NJOY)
+ system simulation (MCNP/ERANOS/CASMO...)

1000 times

For each random ENDF file, the benchmark calculation is performed with MCNP. At the end of the n calculations, n different k_{eff} values are obtained.

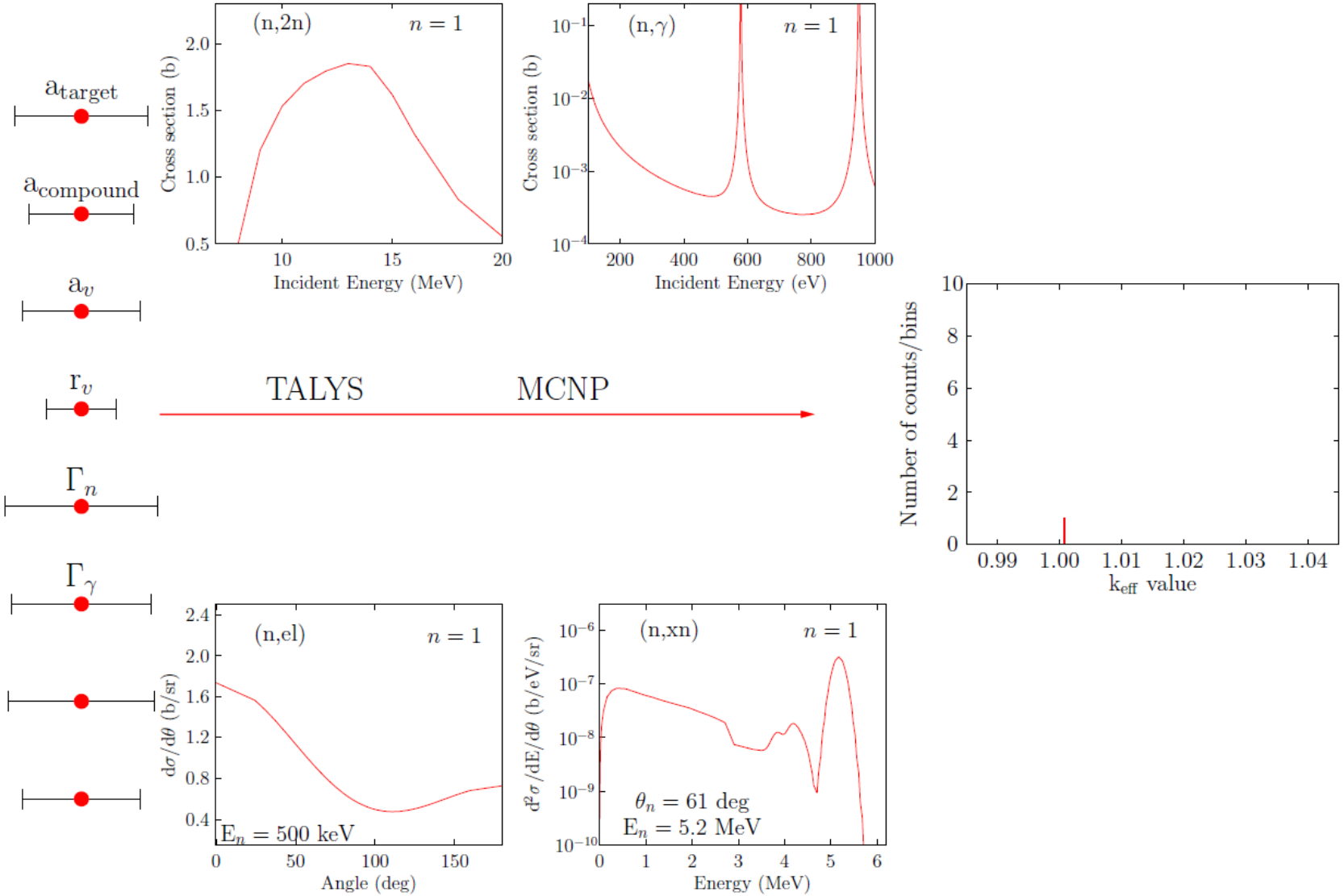
$$\sigma^2_{total} = \sigma^2_{statistics} + \sigma^2_{nuclear\ data}$$





"Towards sustainable nuclear energy: Putting nuclear physics to work",
A.J. Koning and D. Rochman, ANE 35 (2008) 2024.

Hands on “1000 ×(TALYS + ENDF + NJOY + MCNP) calculations”



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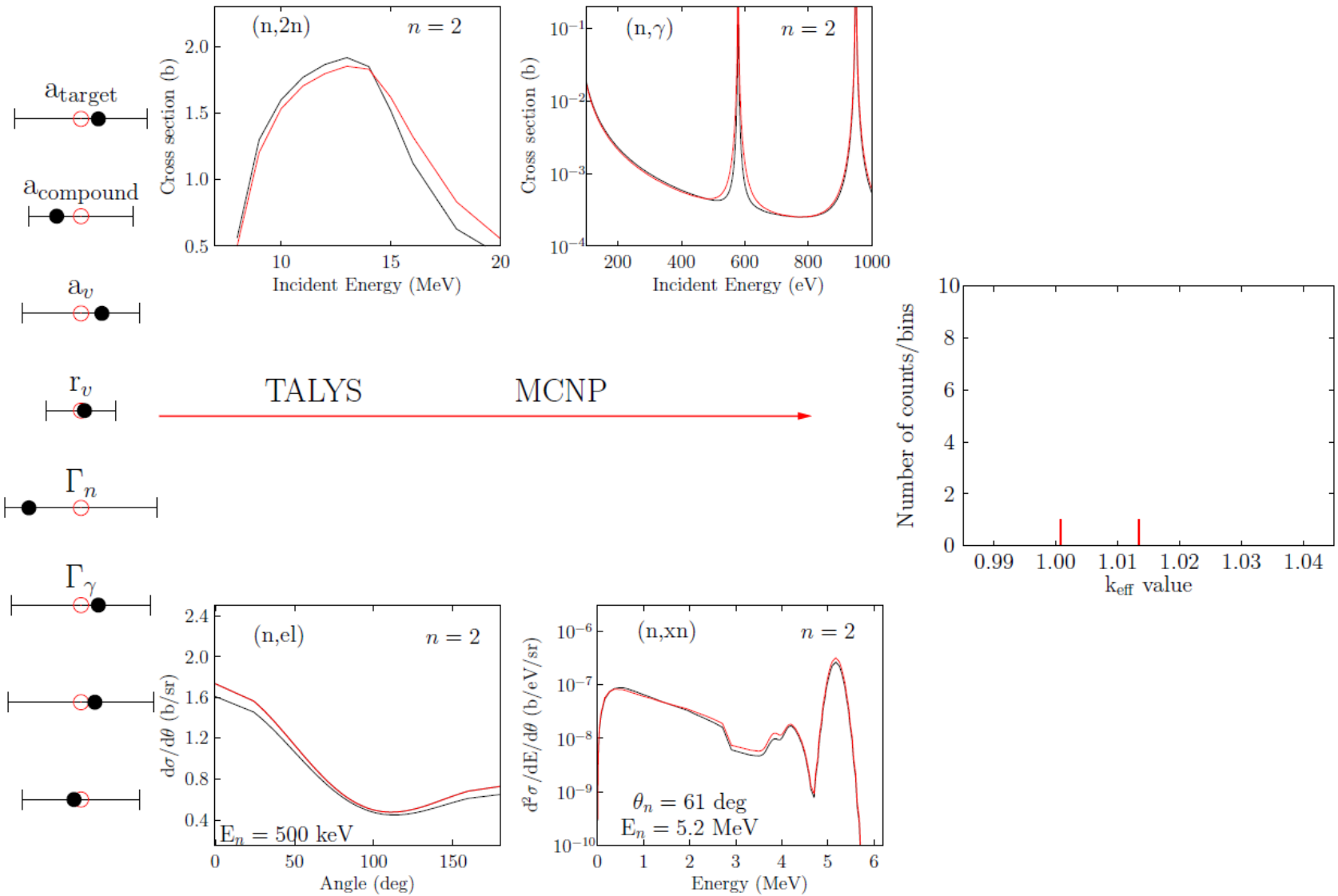

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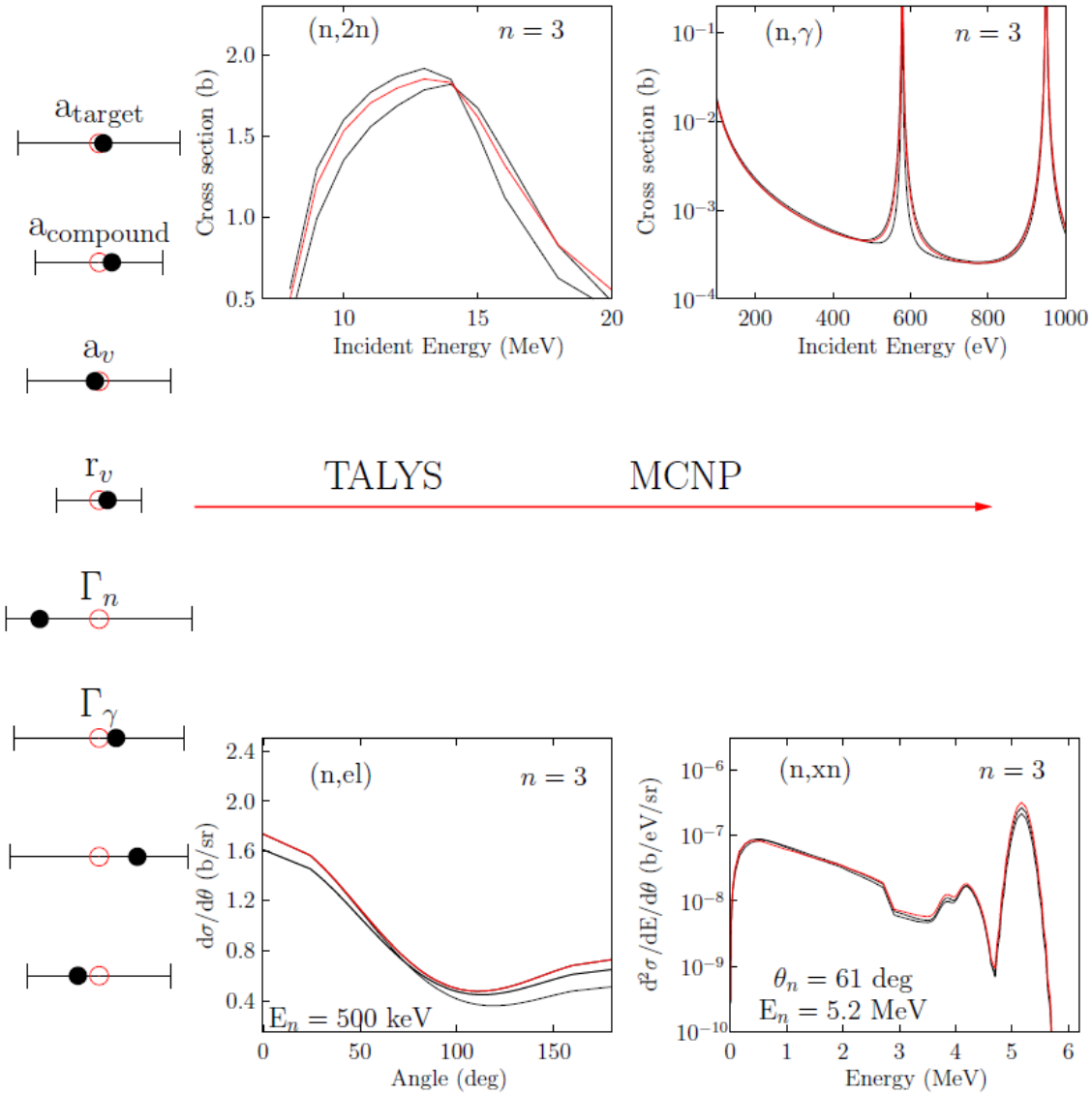

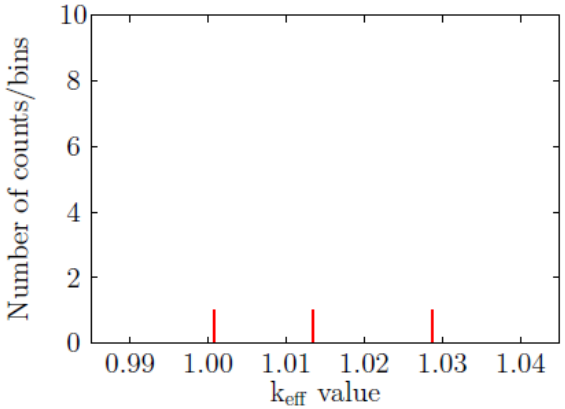

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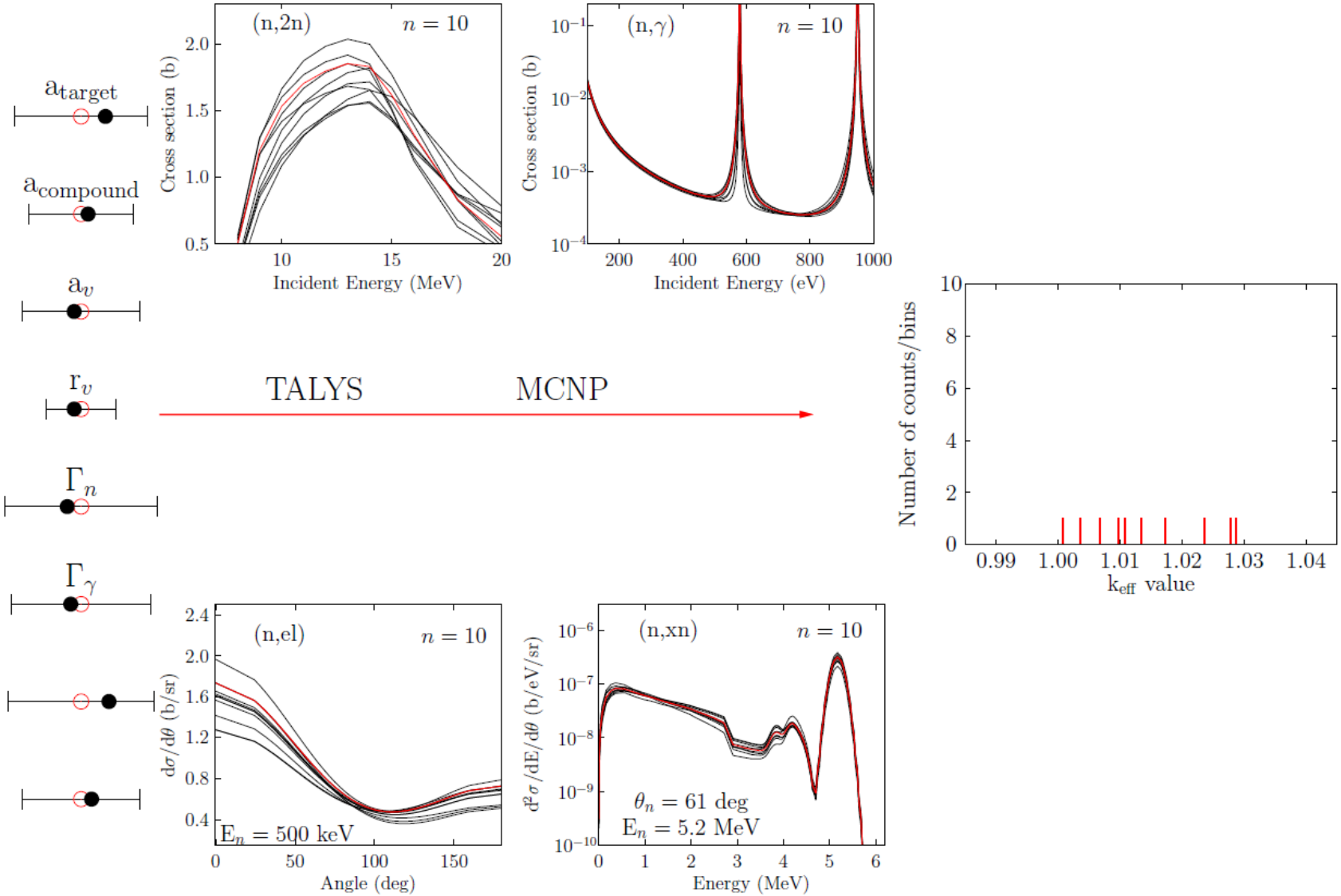

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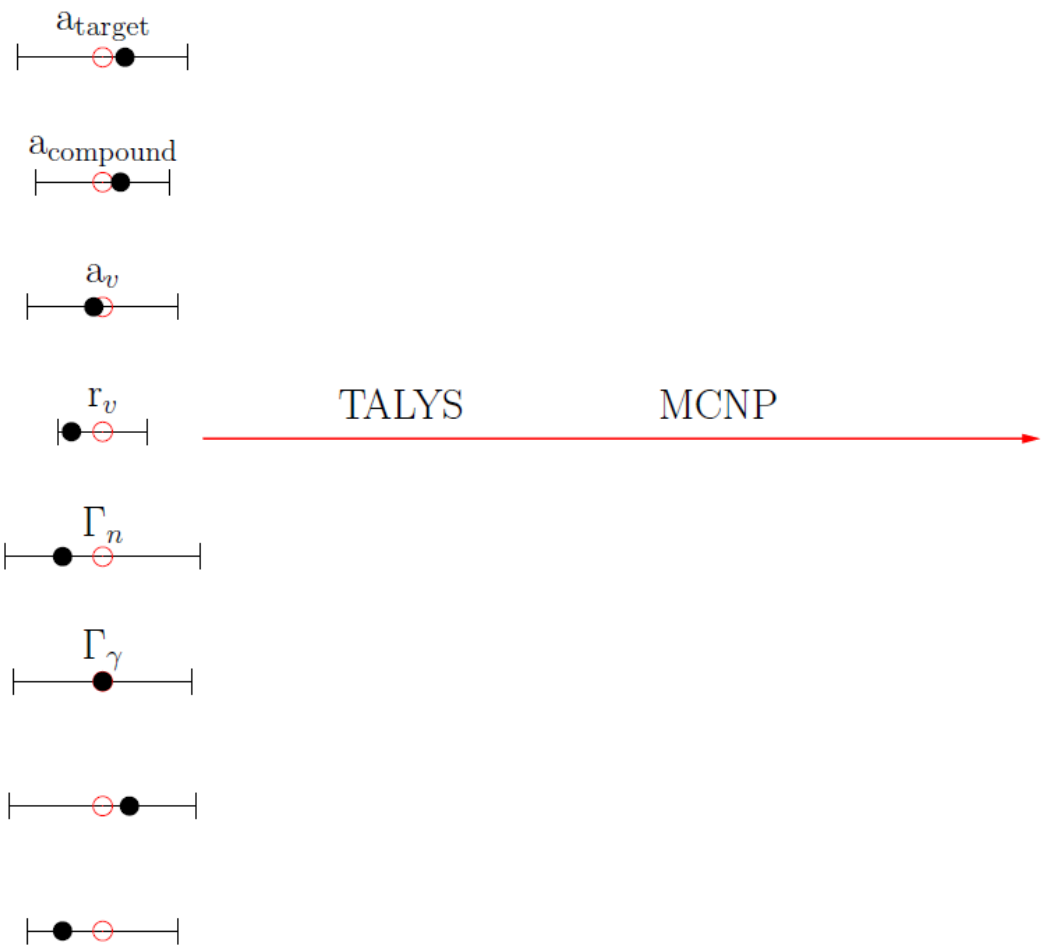

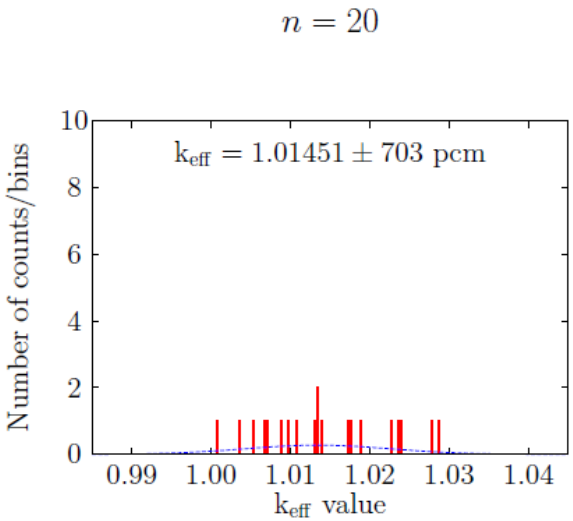

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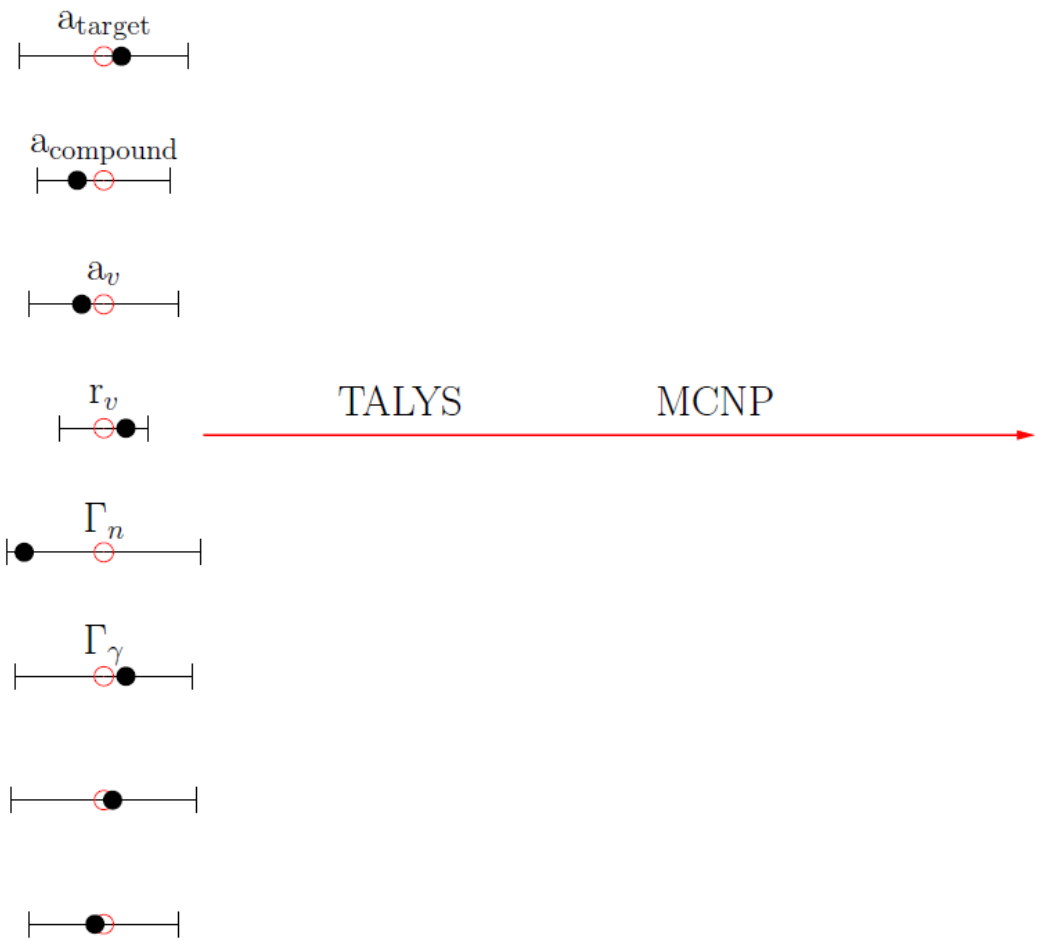

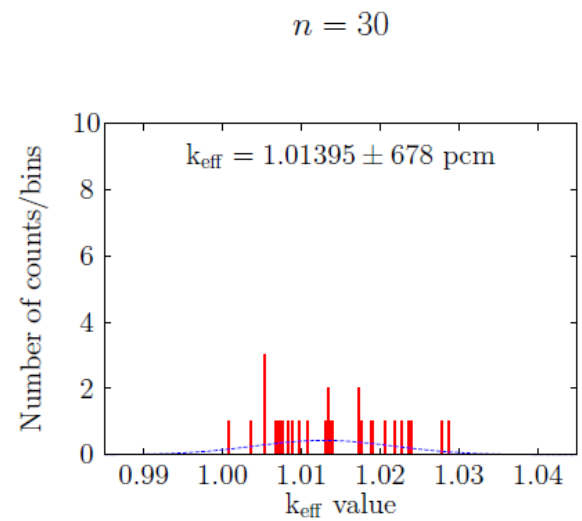

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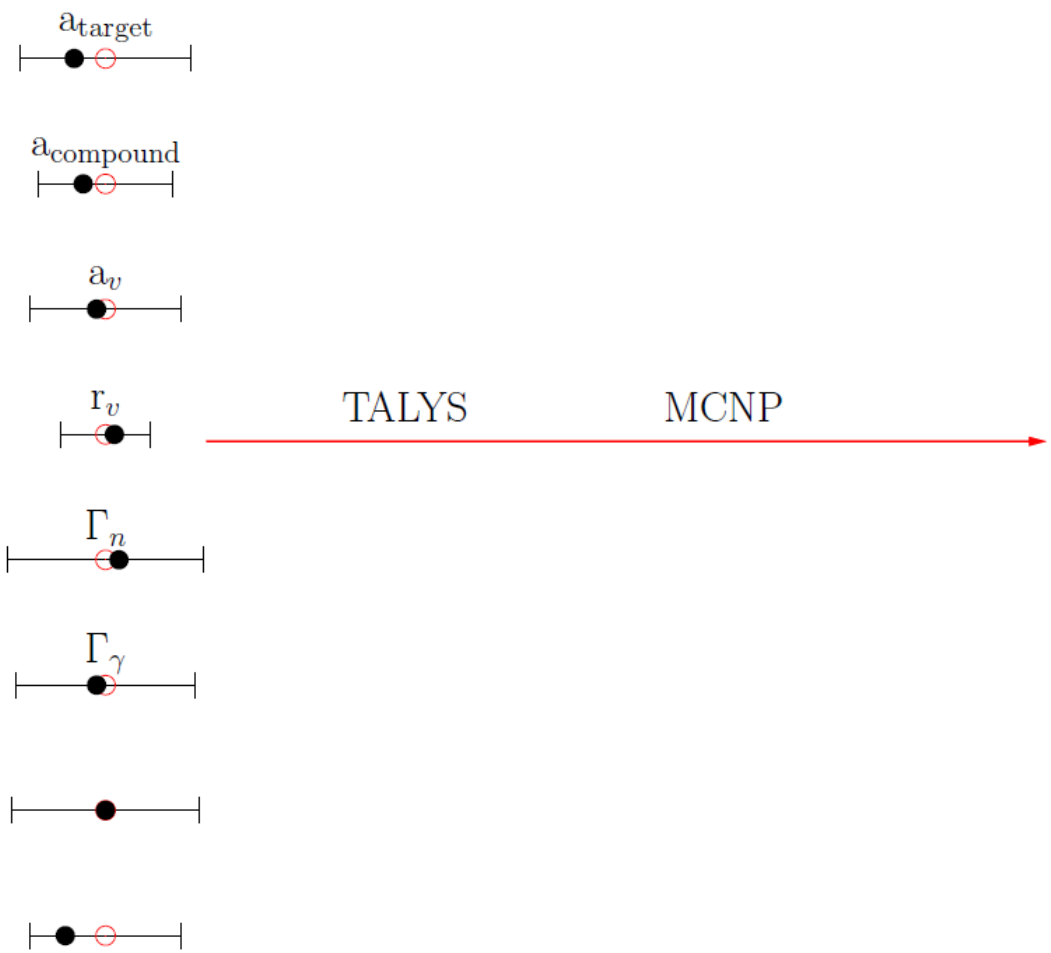

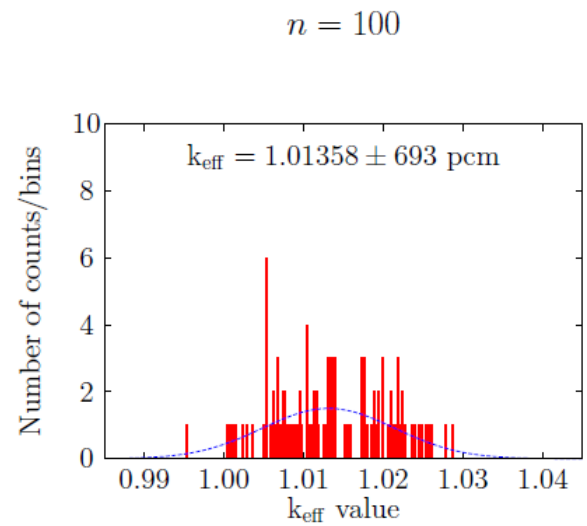

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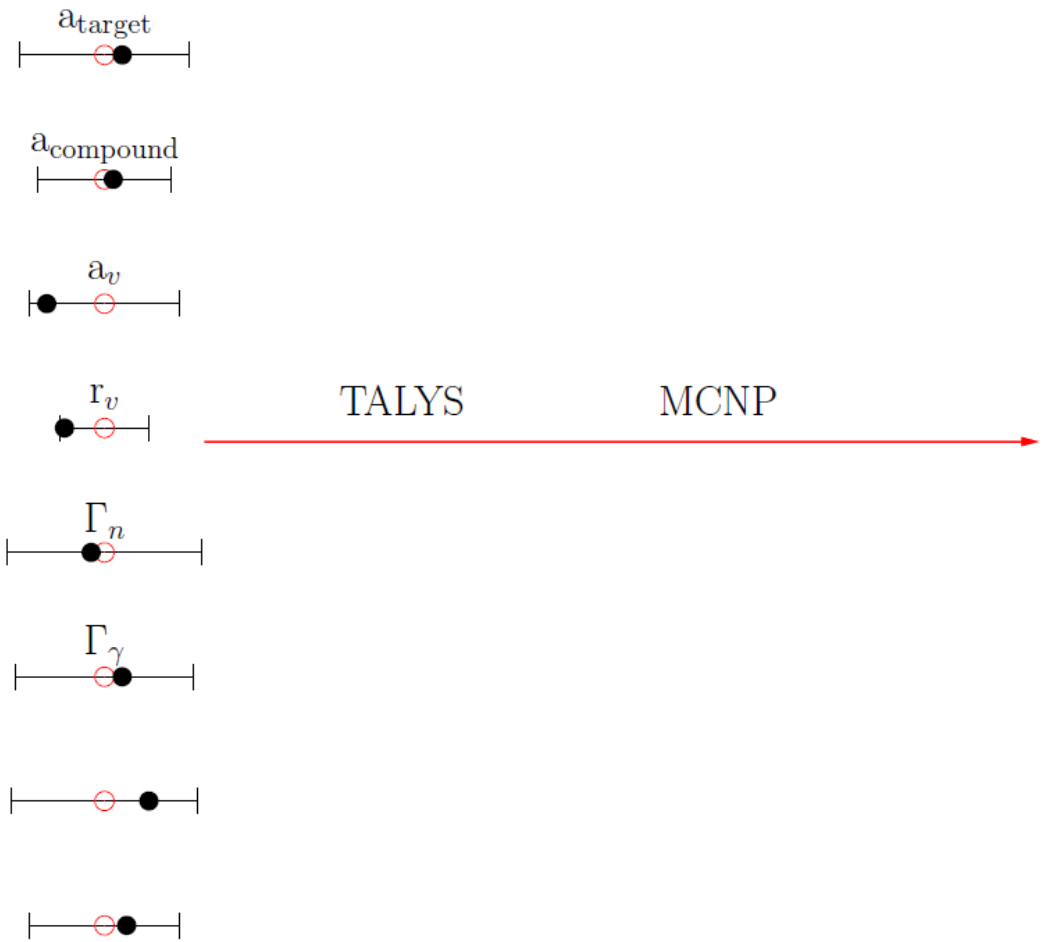

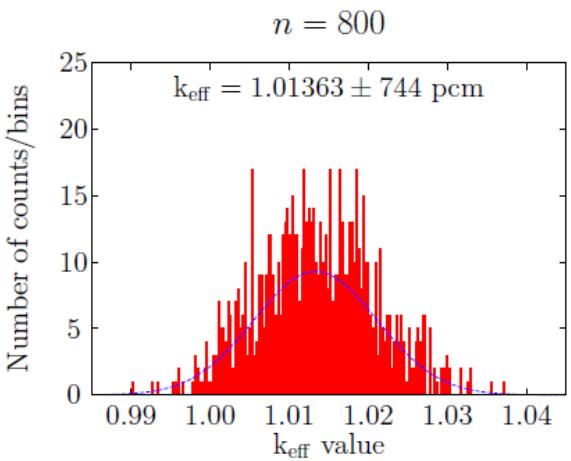

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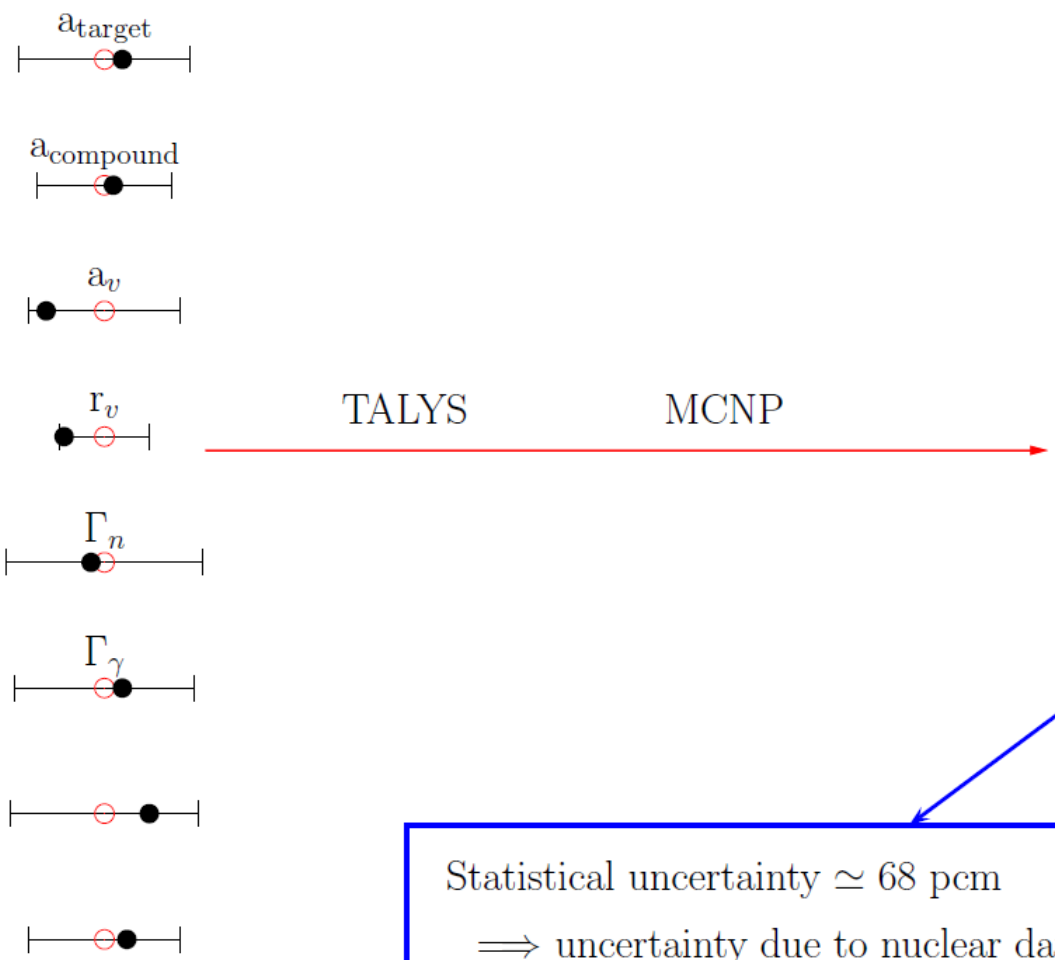
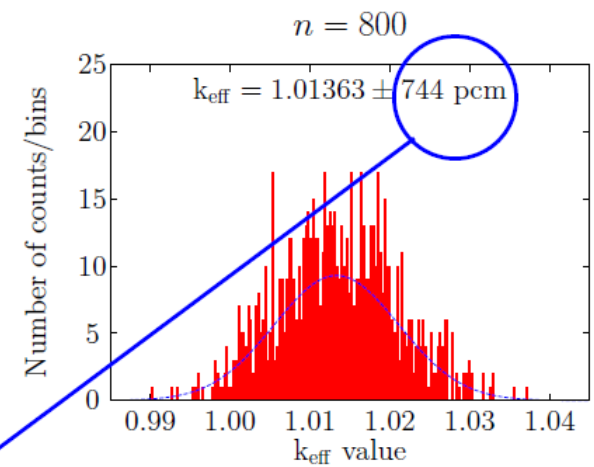




Statistical uncertainty $\simeq$ 68 pcm

$\Longrightarrow$ uncertainty due to nuclear data $\simeq$ 740 pcm

Making use of T6/TENDL: BMC or BFMC

- BMC: Bayesian Monte Carlo
- Each random file from TMC is weighted according to his “distance” to a measured value:

$$Q_i = \left(\frac{k_{\mathrm{eff},i} - k_{exp}}{\Delta k} \right)^2,$$

$$w_i = \exp\left(-\frac{Q_i}{2} \right).$$

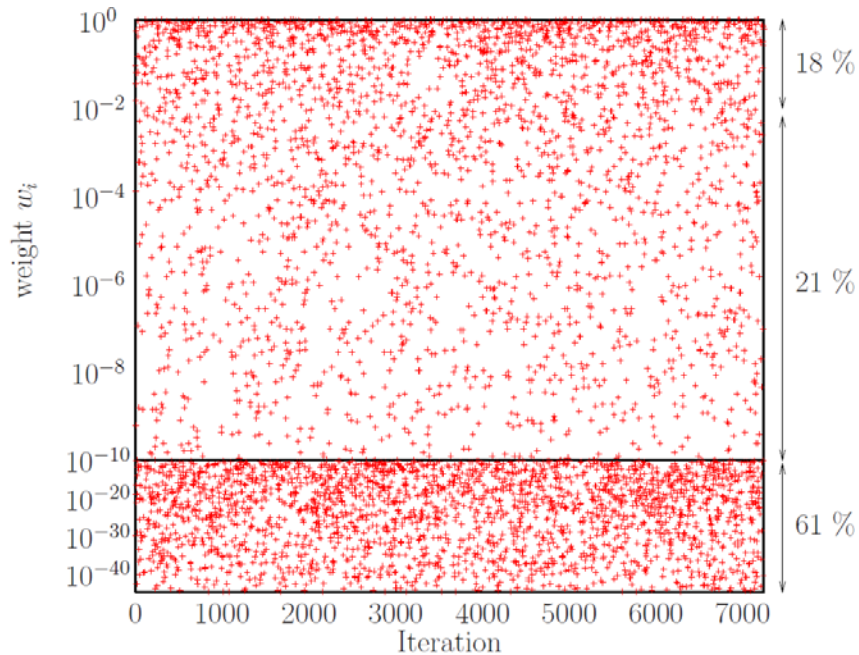


Fig. 1. Calculated weights w_i for the 7000 random cases considered in this work. The number on the right are the percent of weights within the space defined by the arrows.

- The best solutions have large weights, leading to updated values.

Making use of T6/TENDL: BMC or BFMC

- BFMC: Backward-Forward Monte Carlo (=BMC + “model defect”-like)
- Each random file from TMC is weighted according to his “distance” to a measured value:

$$\chi_i^2 = \sum_{j=1}^{J} \left(\frac{B_{\mathrm{calc},j}^{(i)} - B_{\mathrm{exp},j}}{\Delta B_{\mathrm{exp},j}} \right)^2$$

$$w_i = exp\left[- \left(\frac{\chi_i^2}{\chi_{\min}^2} \right)^2 \right].$$

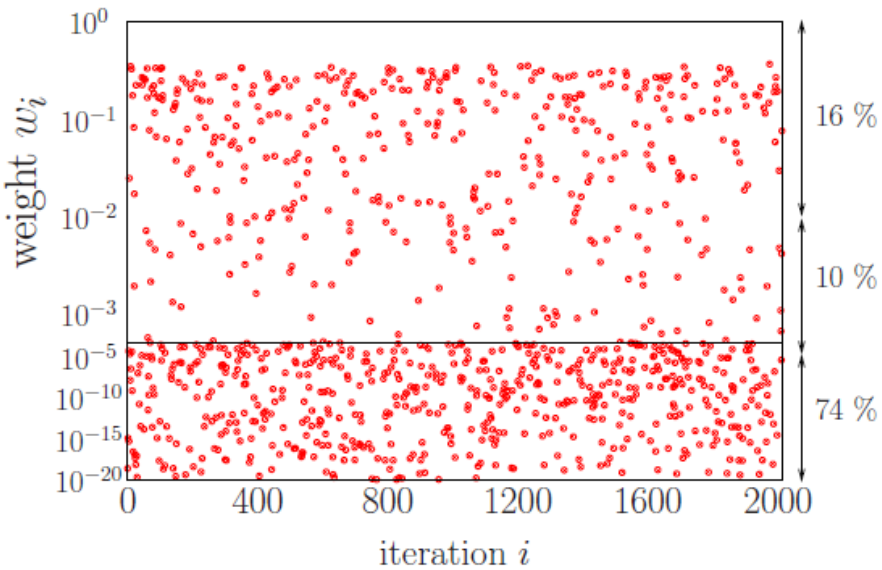
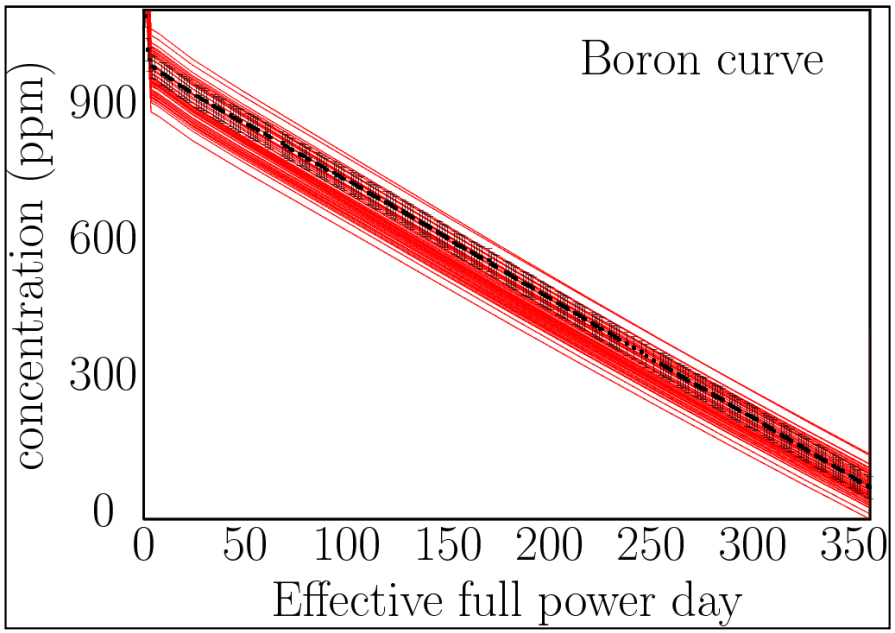


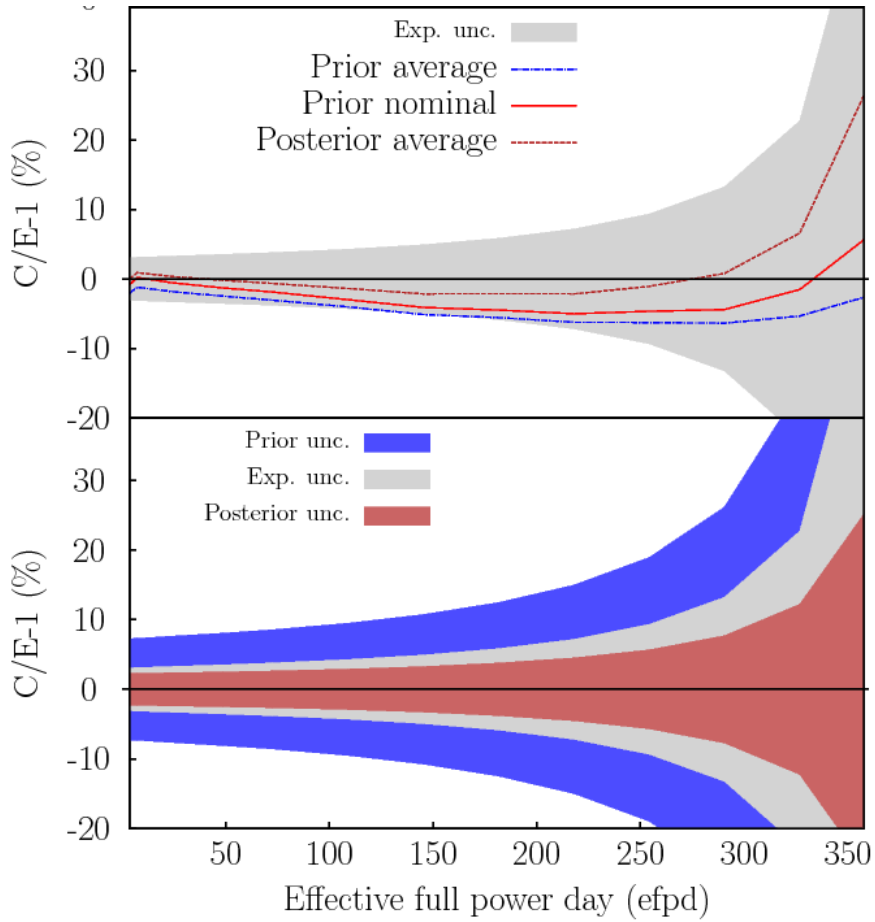
Fig. 1. Example of weights w_i calculated with Eq. (2) in the present case. The varied nuclear data are ^{235}U(n,f), ^{235}U-$\overline{\nu}_p$, ^{238}U(n,γ), ^{239}Pu-$\overline{\nu}_p$ and ^{239}Pu(n,f). The experimental data are presented in section 3.1. The horizontal solid line indicates a break in the Y-axis with a zoom above $w_i > 10^{-5}$.

- The best solutions have large weights, leading to updated values.

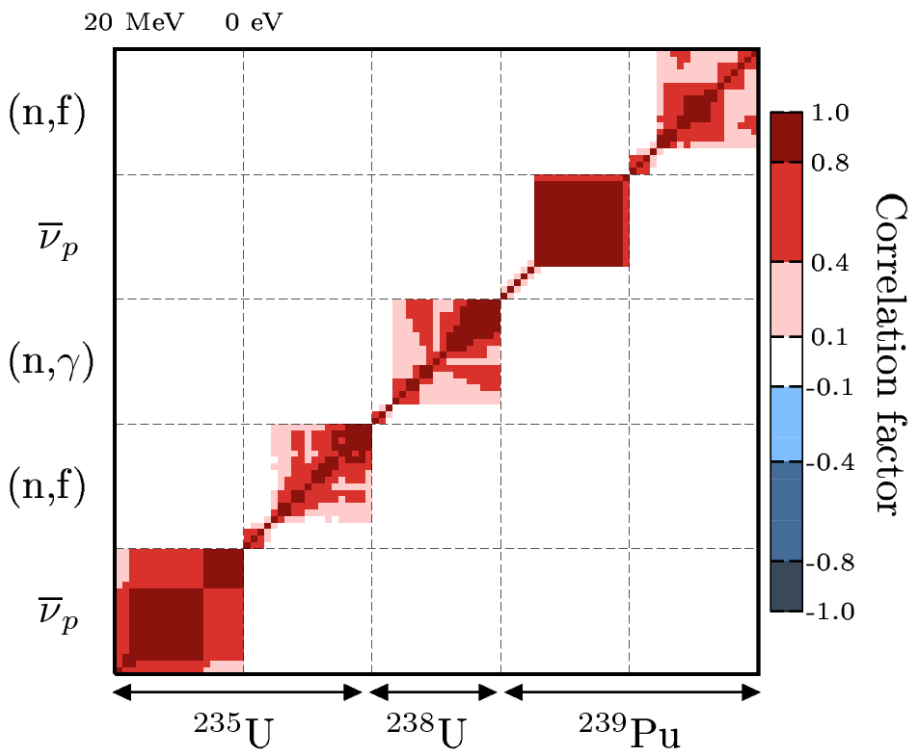
Making use of T6/TENDL: BFMC

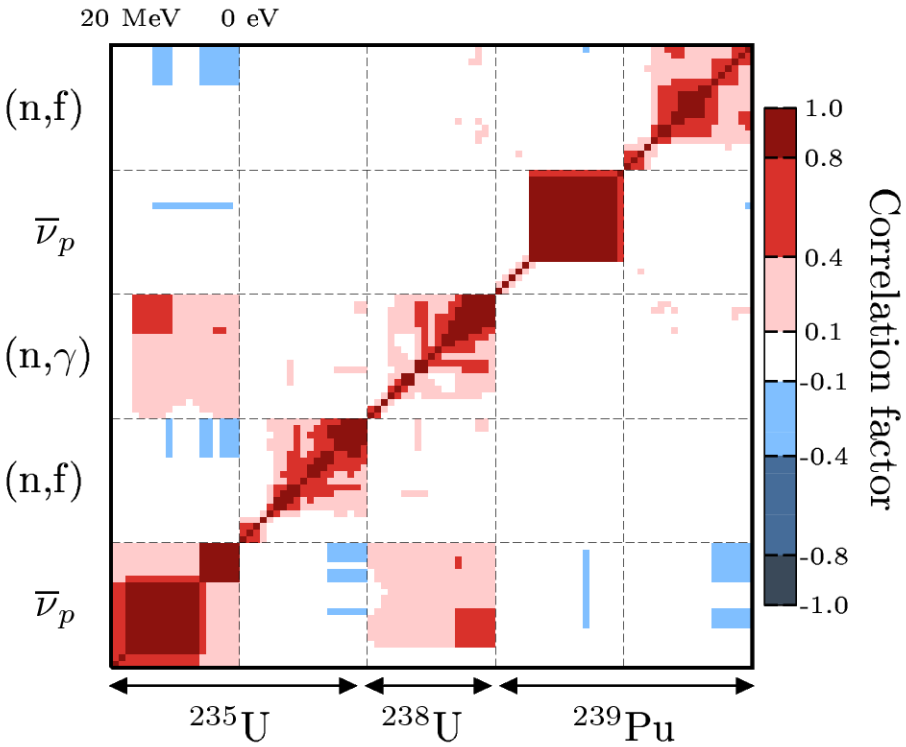
- BFMC: Application to "Boron letdown curve measurements" from an existing PWR
- System: realistic PWR cycle with measured boron concentration
- Random nuclear data: generated based on the ENDF/B-VII.1 library for all isotopes
- Simulation tool: (CASMO5 + SIMULATE5) x (a few thousands of random files)





Making use of T6/TENDL: BFMC





Background/Need of covariances for fission yields

- In libraries, fission yields (FY) are provided with uncertainties only,
- No correlation between FY,
- For the next library release, FY covariances are needed.

- A few methodologies exist (CEA Cadarache, SCK/UPM, ORNL, PSI…),
- No consensus is yet achieved,
- For the time being, we can develop methods and assess their impacts,

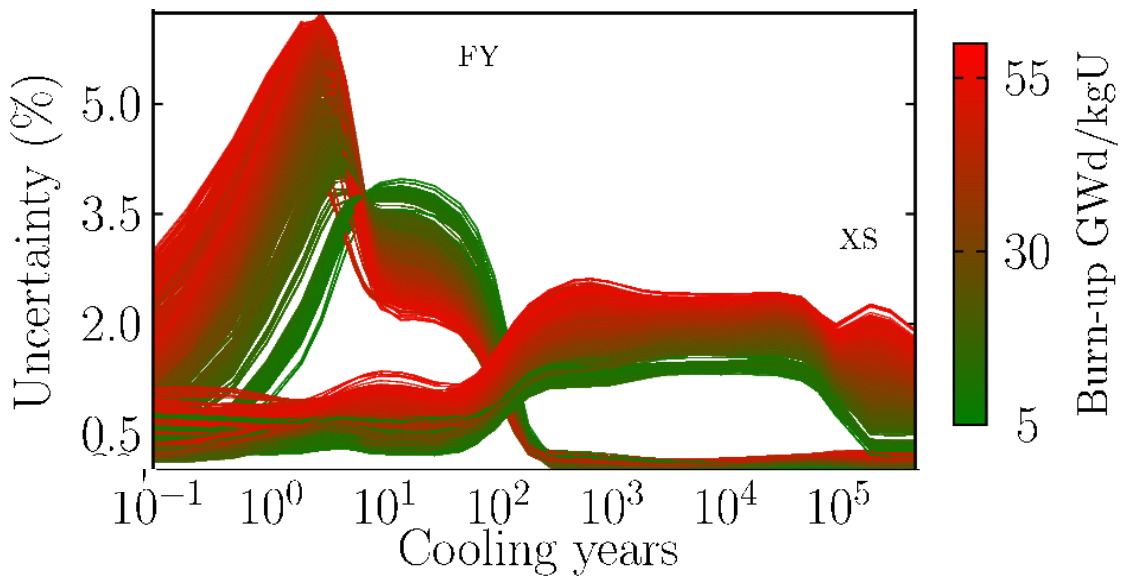
- These methods should “only” replace future evaluations based on both measurements and theory.

- In the following, a Bayesian Monte Carlo method is proposed,

Background/Need of covariances for fission yields

From the application point of view, FY covariances are important for

- Fuel inventory (PIE)
- Burn-up calculations (based on burn-up indicators)
- Decay heat & Dose calculations with uncertainties
- Fuel storage and transport, cask design (Criticality-safety with burn-up credit)
- Dose calculations with uncertainties
- Full core analysis with uncertainties



Example of decay heat uncertainties for BWR assemblies

Bayesian Monte Carlo with GEF

- GEF can produce good quality fission yields, based on physical models and a limited set of parameters,
- It is well suited for a Bayesian Monte Carlo (BMC) defined as

BMC= TMC + feedback to parameter distributions

- The method works as follows:
  1. Select parameter distributions,
  2. Produce random FY by sampling parameters,
  3. Compare to JEFF or ENDF/B-VII.1 FY: calculate a χ^2
  4. use weights to update the parameter distributions
  5. Sample again and calculate new χ^2
  6. Repeat 3 to 5 until convergence

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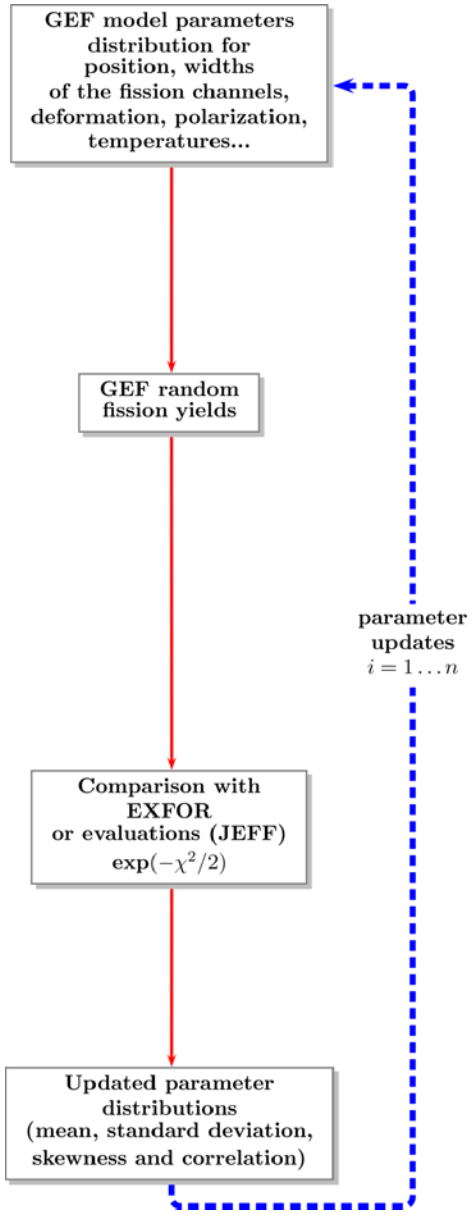
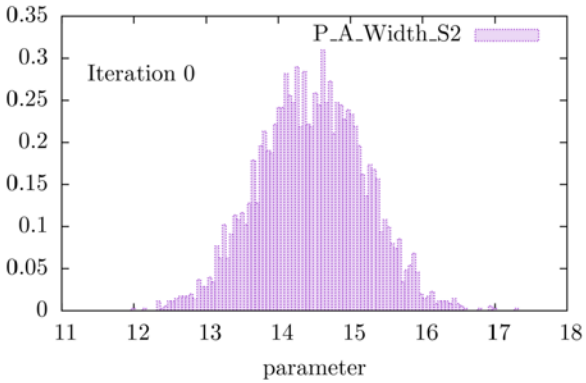
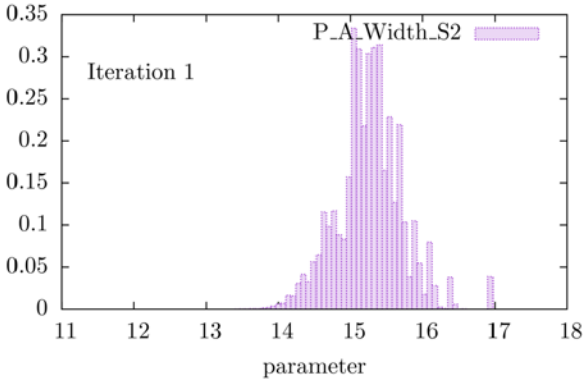
Bayesian Monte Carlo with GEF







BMC with GEF

- 21 GEF parameters are used (Table 7 in the JEFF-Report 24)
- Normal and independent distributions, X^2 defined as

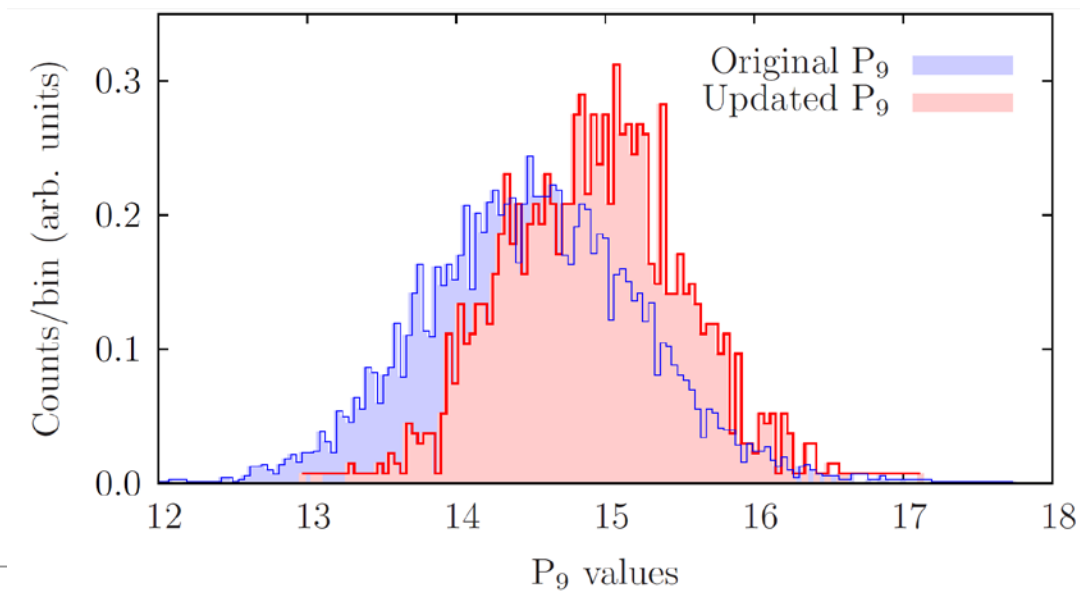
$$\chi_i^2 = \sum_{j=1}^{\mathrm{FY}} \left(\frac{C_j^{(i)} - E_j}{\Delta E_j} \right)^2$$

i random calculation

- Weights defined as

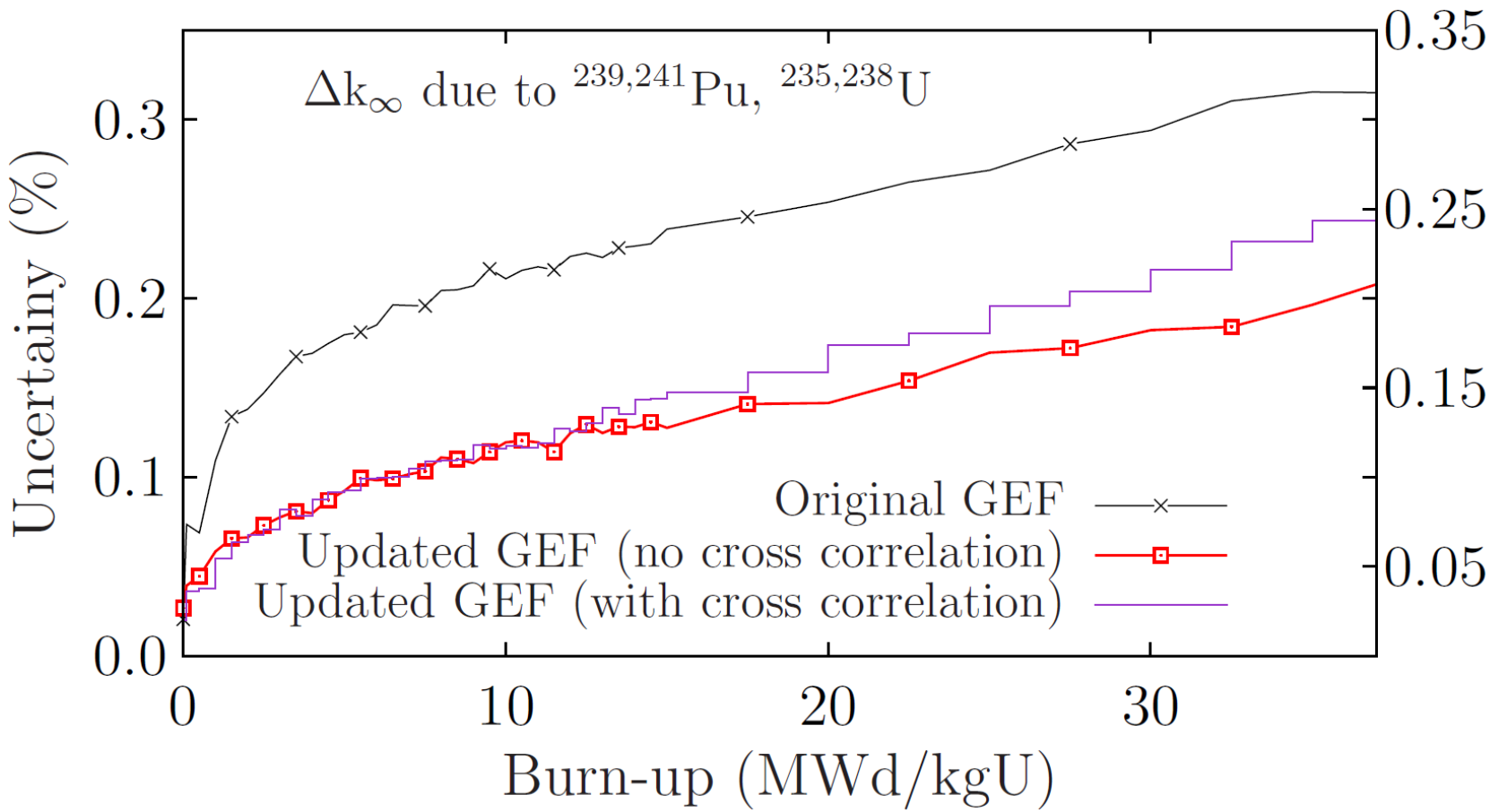
$$\omega_i = \frac{\mathrm{e}^{-\chi_\mathrm{i}^2/2}}{\mathrm{e}^{-\chi_\mathrm{min}^2/2}}$$

- Example for a specific parameter (P_9=P_AWidth for $^{235}U + n_{th}$)



Example for burn-up calculations

- Simple pincell calculation up to 40 MWd/kgU with SERPENT, varying the FY (3.6% UO_2)



Example for burn-up calculations

- Correlations between fission products arise from any type of Monte Carlo uncertainty propagation,

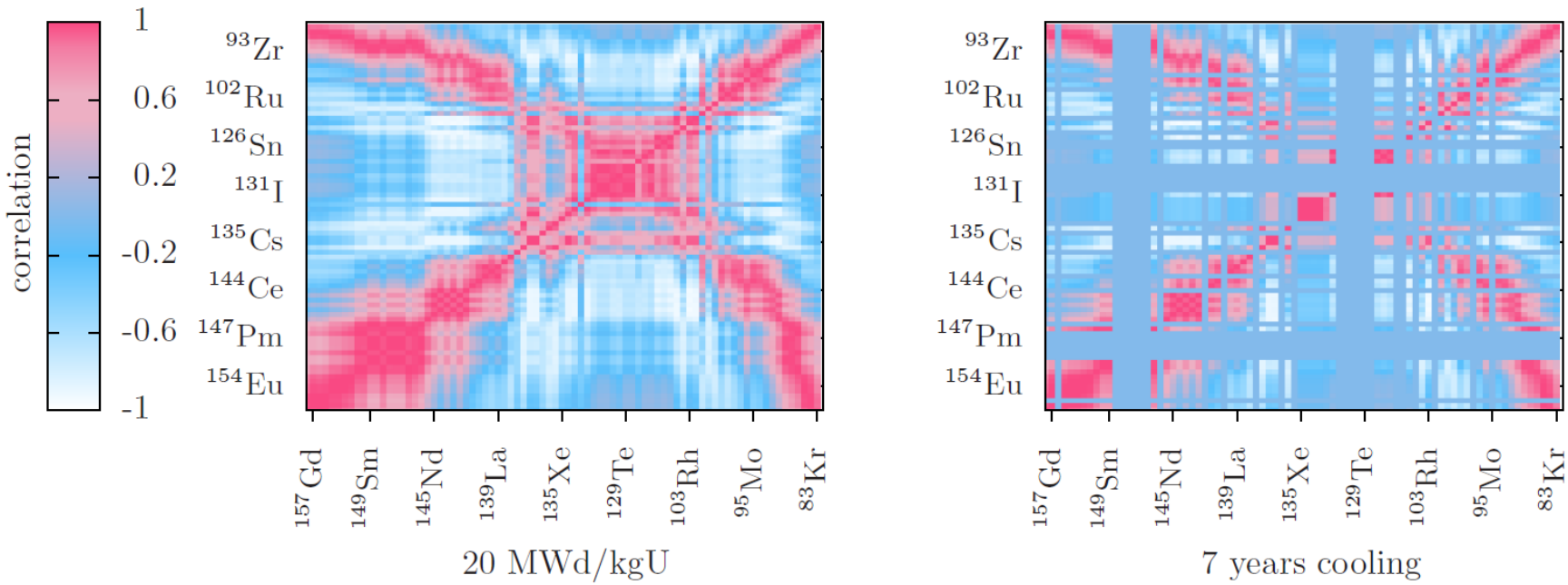
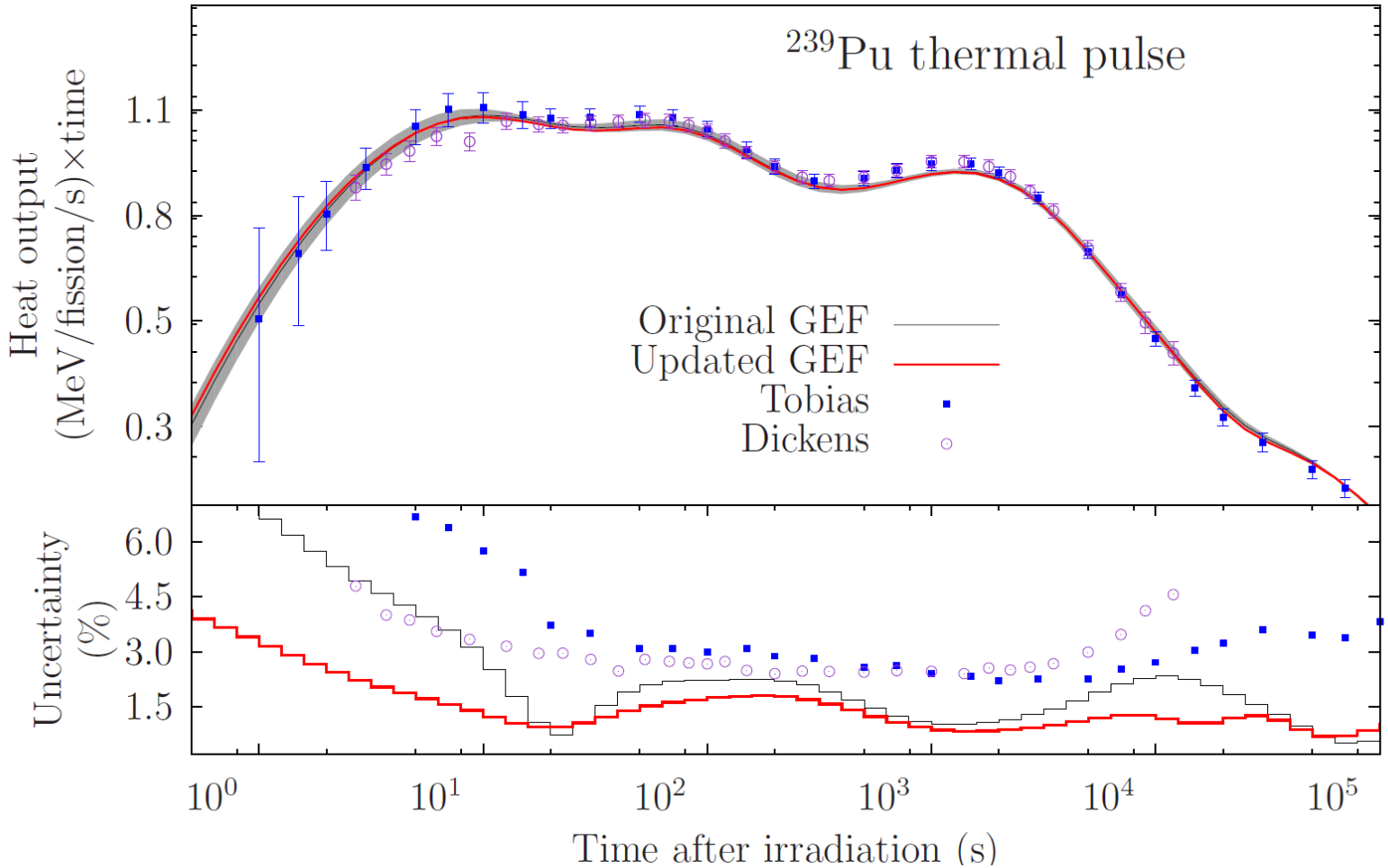


FIG. 43. Correlation matrix between fission products in the BWR MOX assembly due to the variations of fission yields. Left: at 20 MWd/kgU, Right: at 7 years after shutdown.

- These correlations are important for propagations to the "*next step*" (core simulator)

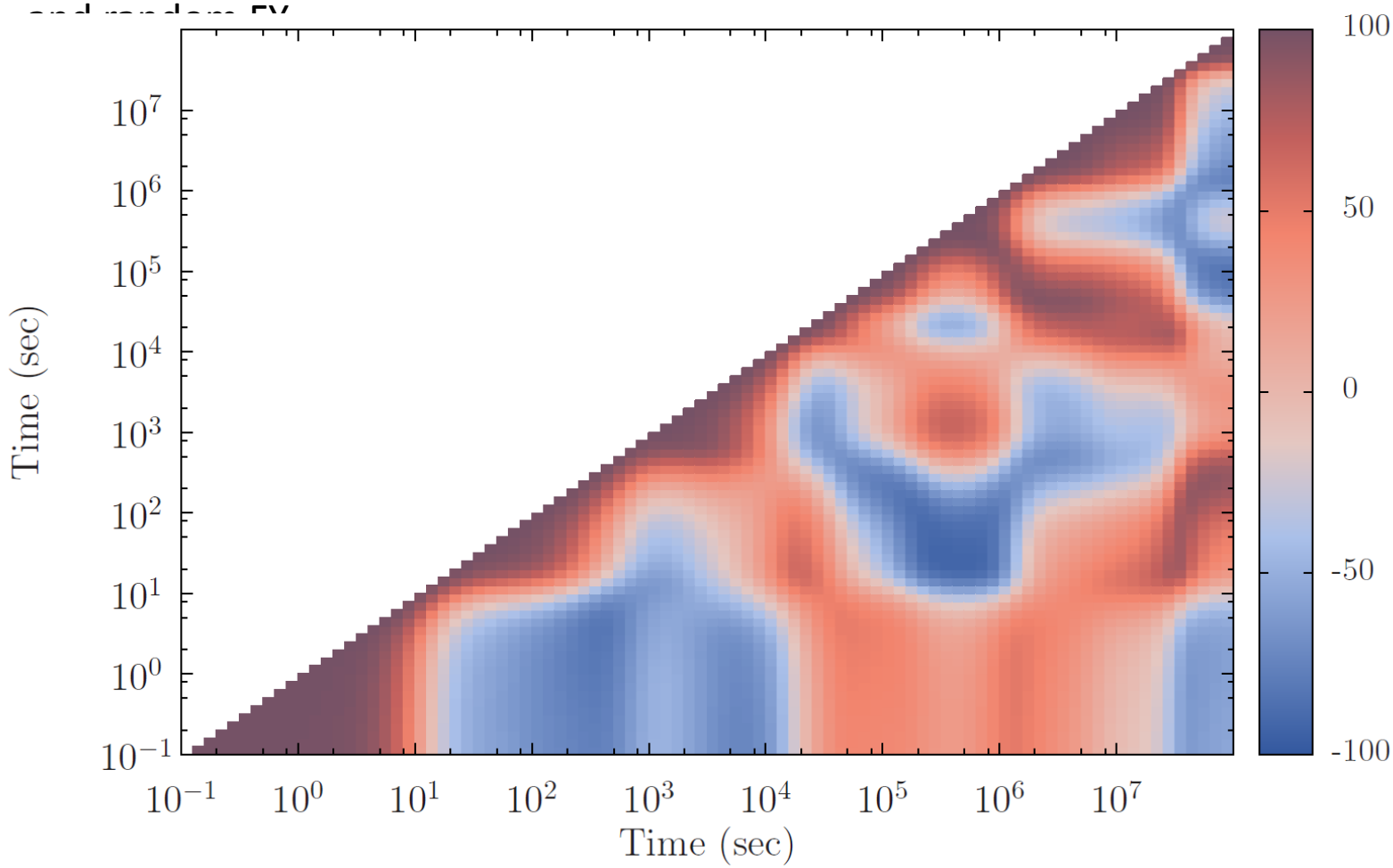
Example for decay-heat calculations

- Decay heat uncertainty from a thermal pulse on ^{239}Pu calculated with FISPACT-II and random FY



Example for decay-heat calculations

- Decay heat correlation from a thermal pulse on ^{235}U calculated with FISPACT-II and random FY



Conclusion

- The TENDL library is improving year after year,
- The T6 code package allows to produce TENDL, random files and to go further,
- We believe that we are slowly changing the evaluation process,
- Still, as proven by distributing T6, many improvements are necessary


photo courtesy of Gerry Hofstetter

PAUL SCHERRER INSTITUT

Wir schaffen Wissen – heute für morgen