PAUL SCHERRER INSTITUT

PSI

D. Rochman

Nuclear data evaluation in TENDL and needs in reactor and fuel simulations: *a Technical Support Organization perspective*

JAEA, Nuclear Data Center, Tokay-mura, 5 December 2018, Japan

Zertifiziertes Managementsystem STARS ISO 9001

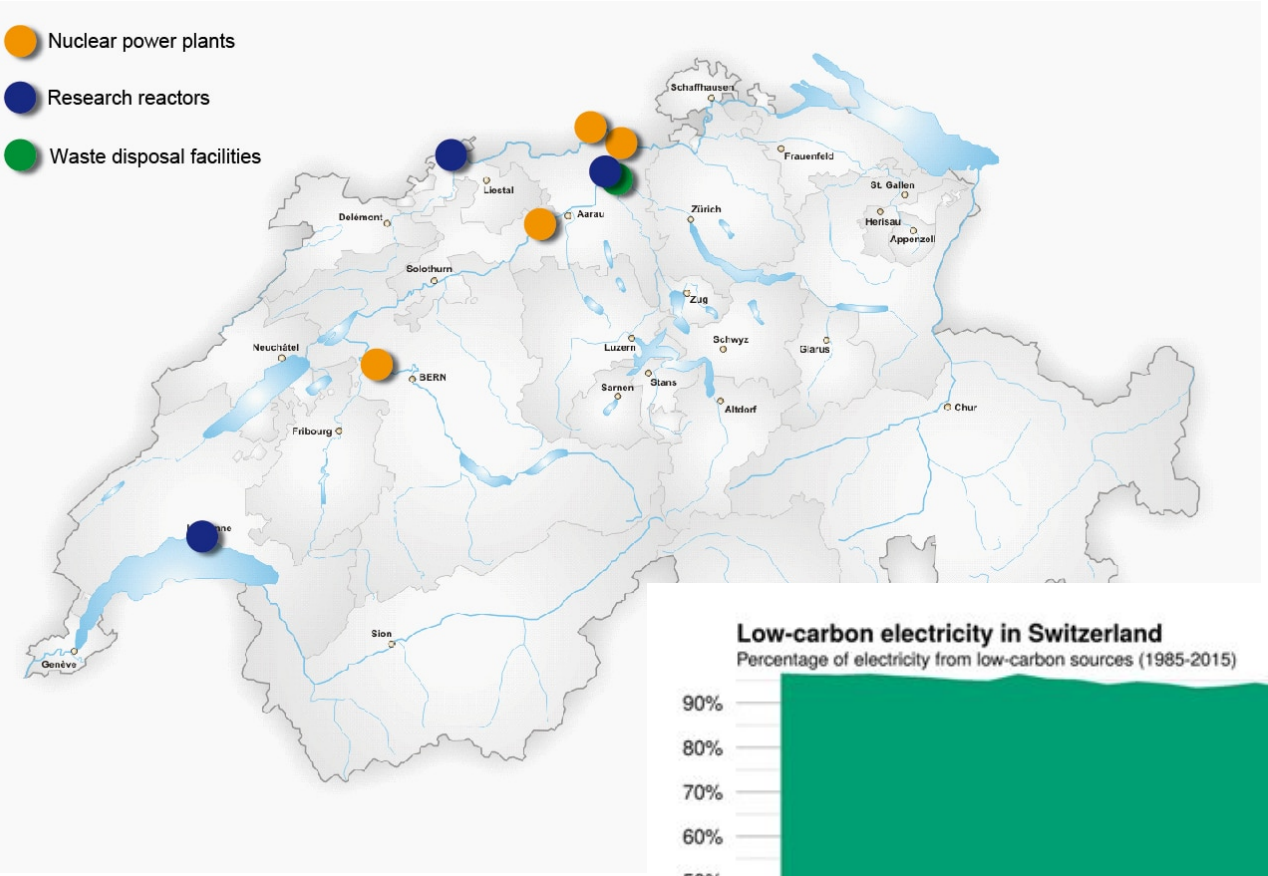
Summary

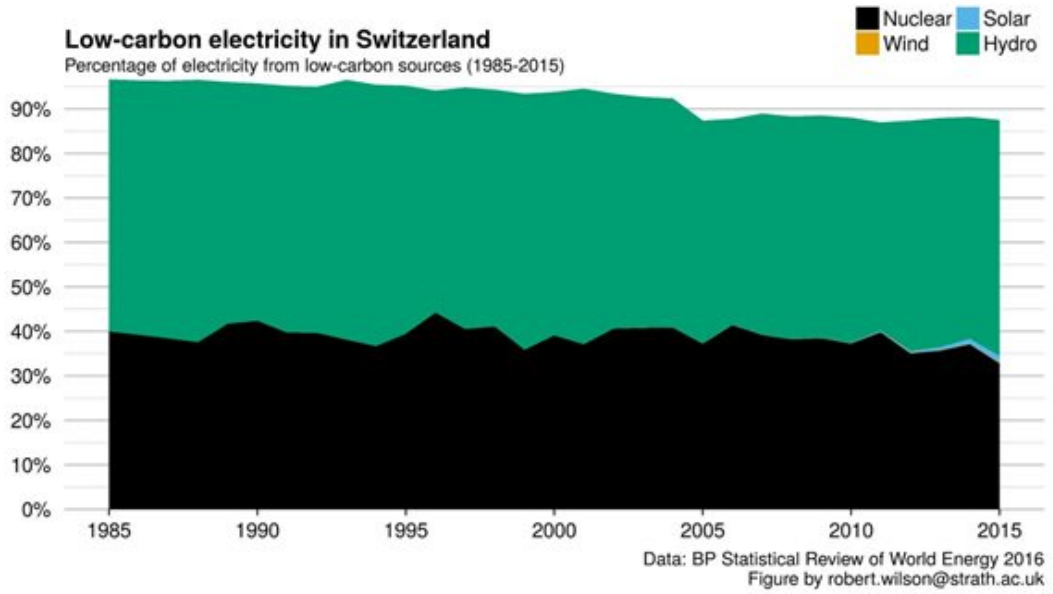
- TENDL and T6: a short history and modern approach
- Some remarks on nuclear data evaluation procedures
- Uncertainty propagation methods: TMC/BMC/BFMC
- Examples for uncertainty propagation to applied systems


photo courtesy of Gerry Hofstetter

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

Situation in Switzerland





PSI: a R&D institute and TSO

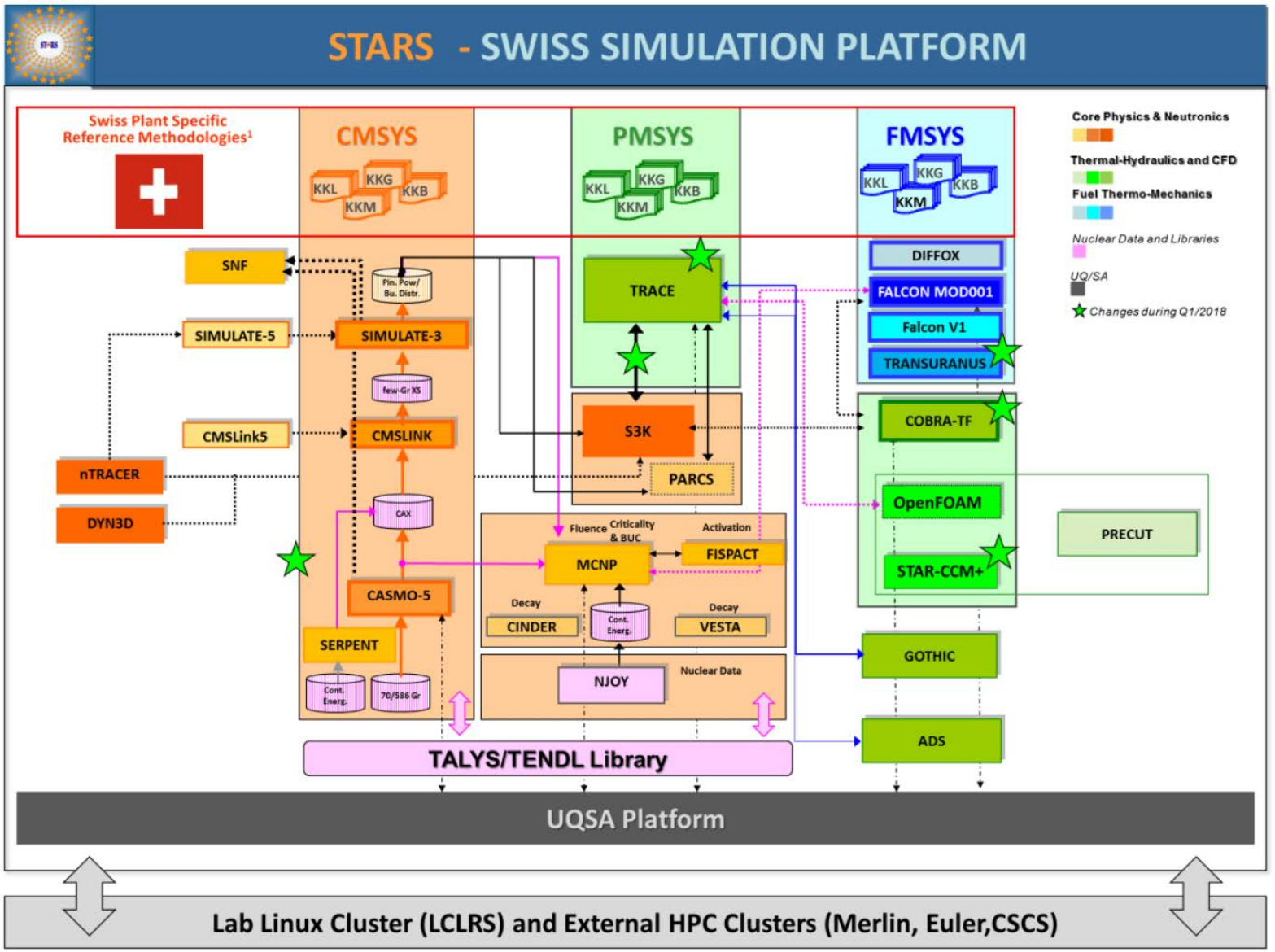
- At PSI, the Nuclear Energy and Safety Department is the Swiss competence center for nuclear energy

Vision

NES is the Swiss **national center of competence for nuclear energy**.
It addresses **nuclear R&D issues** of current and future national interest as active partner of the international nuclear research community.
It recognizes the **multi-disciplinary character of nuclear safety** by fostering corresponding intensive interactions across disciplinary boundaries within NES, PSI, and the ETH domain.
It achieves an adequate **balance between research and services** and the corresponding mix of financial resources.

Laboratory	Competencies
LRT	Multi-physics multiscale simulations for reactor systems Simulations and experiments for severe accidents and source term mitigation Experiments and instrumentation for thermal-hydraulic integral- and separate effect tests

Laboratory for Reactor Physics and Thermal-Hydraulics



Laboratory for Reactor Physics and Thermal-Hydraulics

- Our partners:
  - Regulator ENSI
  - Power plant consortium: SwissNuclear
  - Radioactive Waste Management Agency: NAGRA
  - EU projects, Swiss National Foundation
  - EUROfusion
  - And international partners

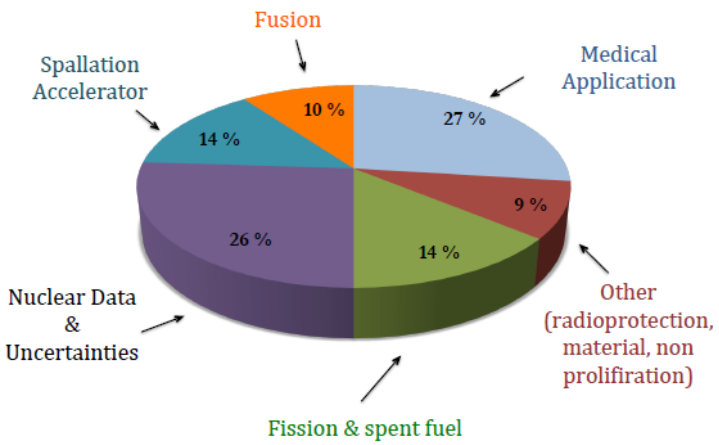
- My involvement:
  - Core licensing analyses for PWRs for new cycles
  - Spent Nuclear Fuel assessment (source term, radiations…)
  - Nuclear data (evaluation)
  - Uncertainty assessment

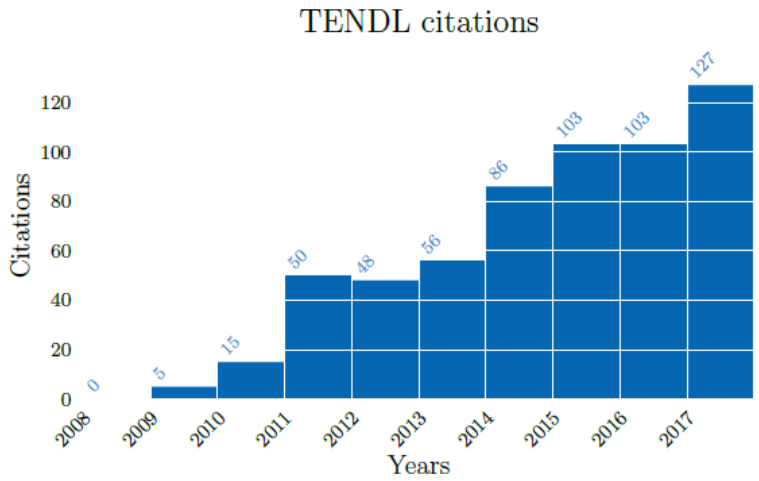
What is the TENDL project ?

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

$$0 \leq \chi^2 \leq 1$$

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





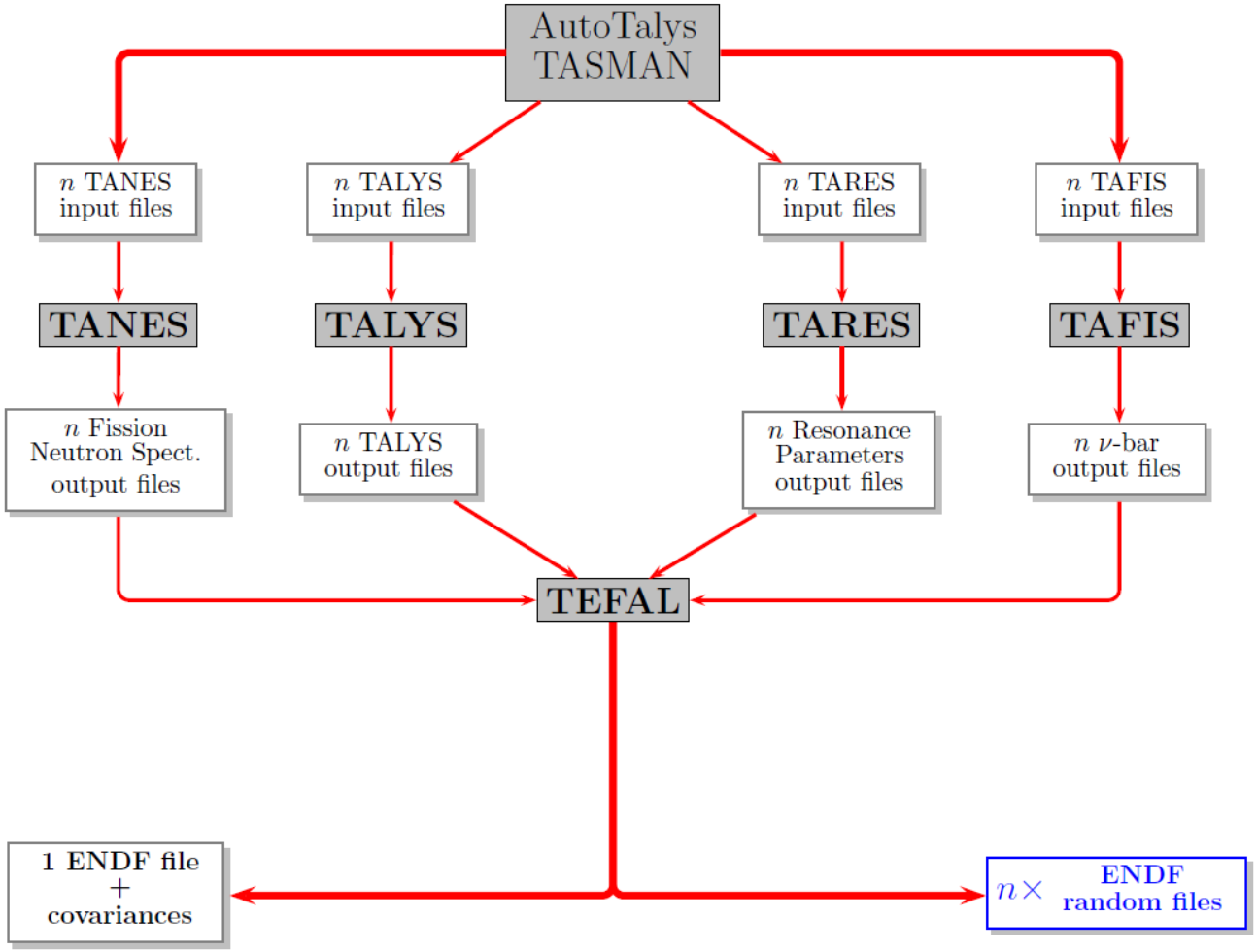
- See for instance NDS 113 (2012) 2841, ANE 51 (2013) 60, NDS 139 (2017) 1

What is the TENDL project ?

- TENDL is in fact a by-product of a series of codes (called T6),
- 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

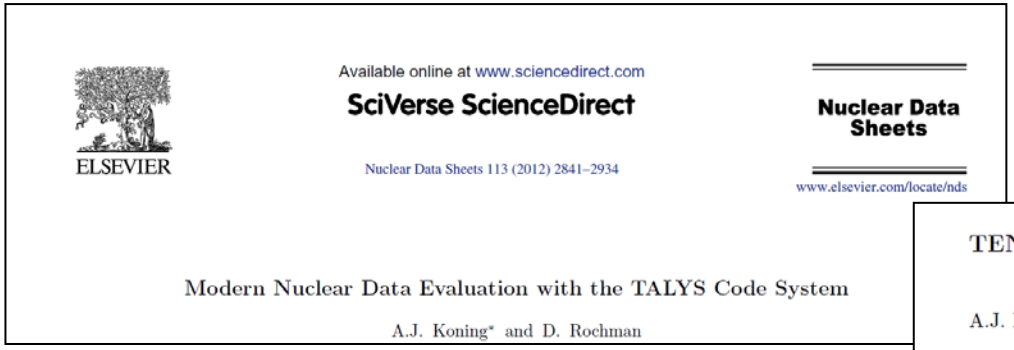
T6: source of TENDL

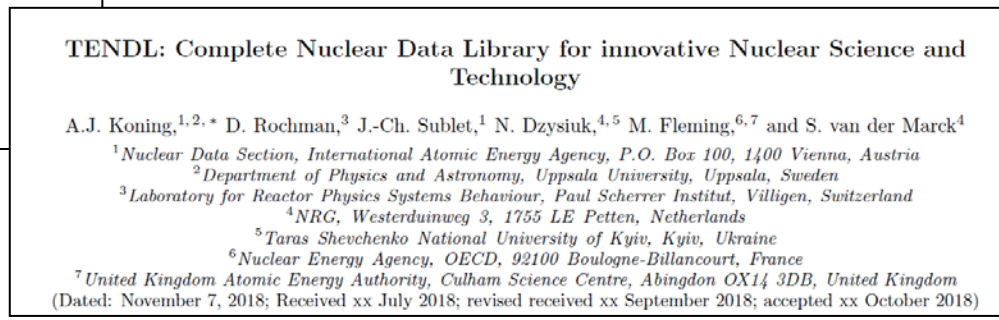
- T6: at the origin of TENDL. Combination of 6 codes plus utilities,
- Available on demand, easy to install,
- Make your own TENDL !



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.





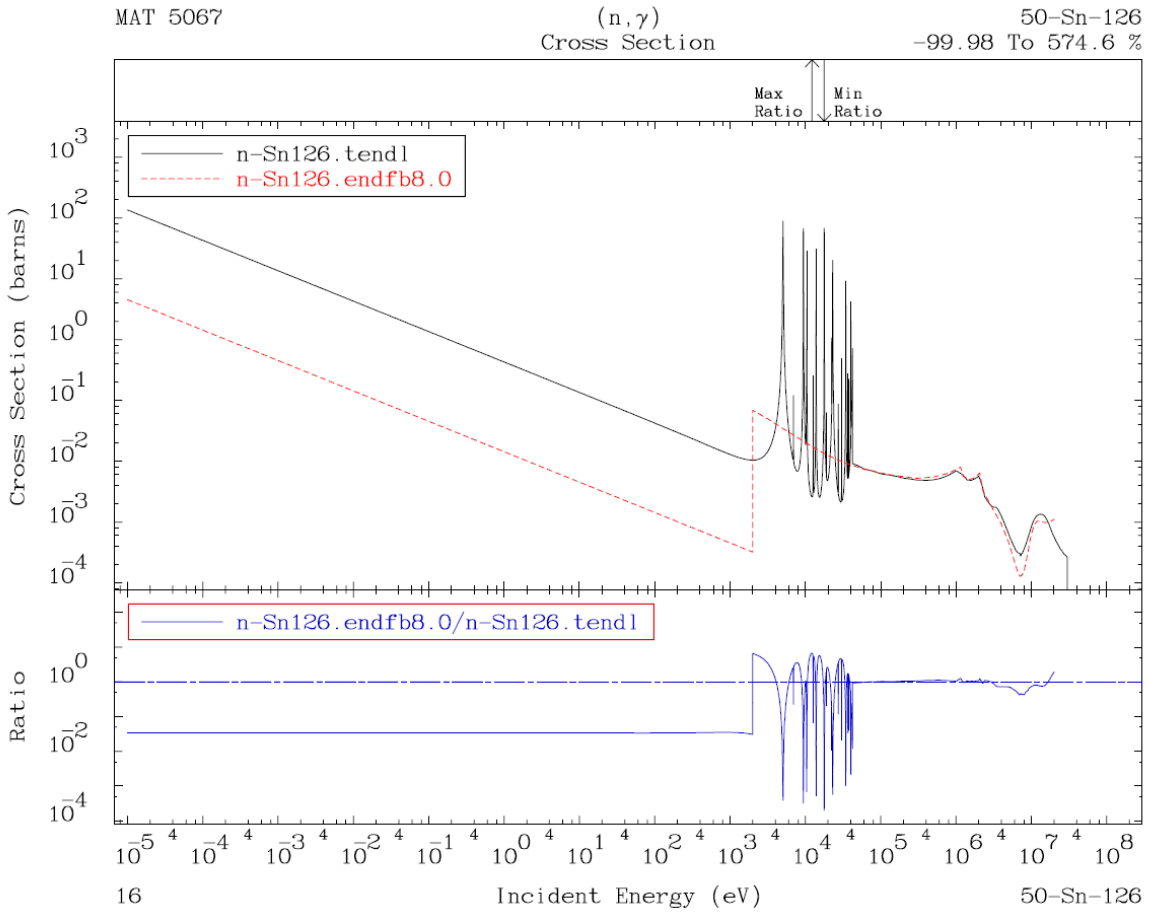
TENDL related projects

The TENDL way is strongly linked to other methods:

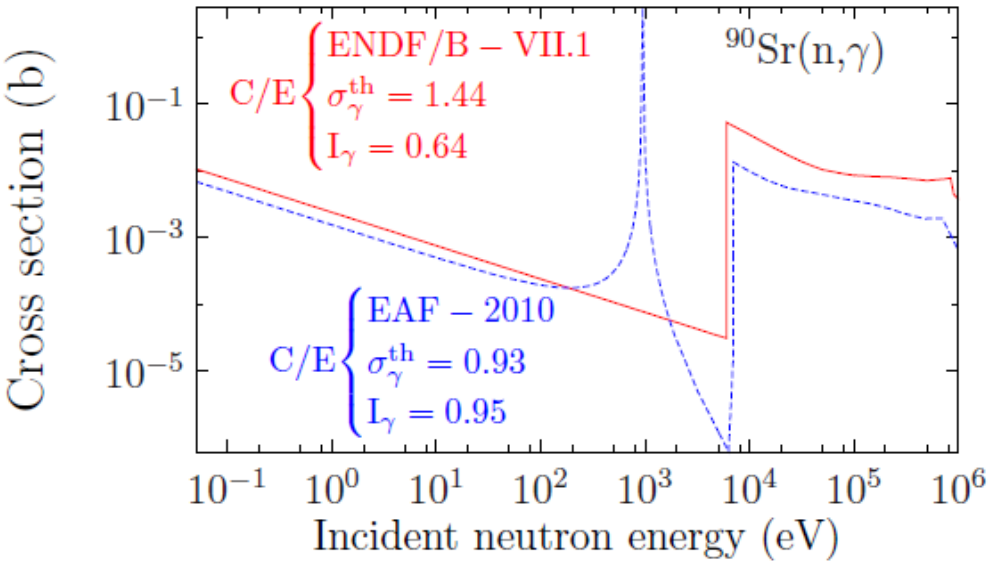
- (fast) TMC: Total Monte Carlo for uncertainty propagation,

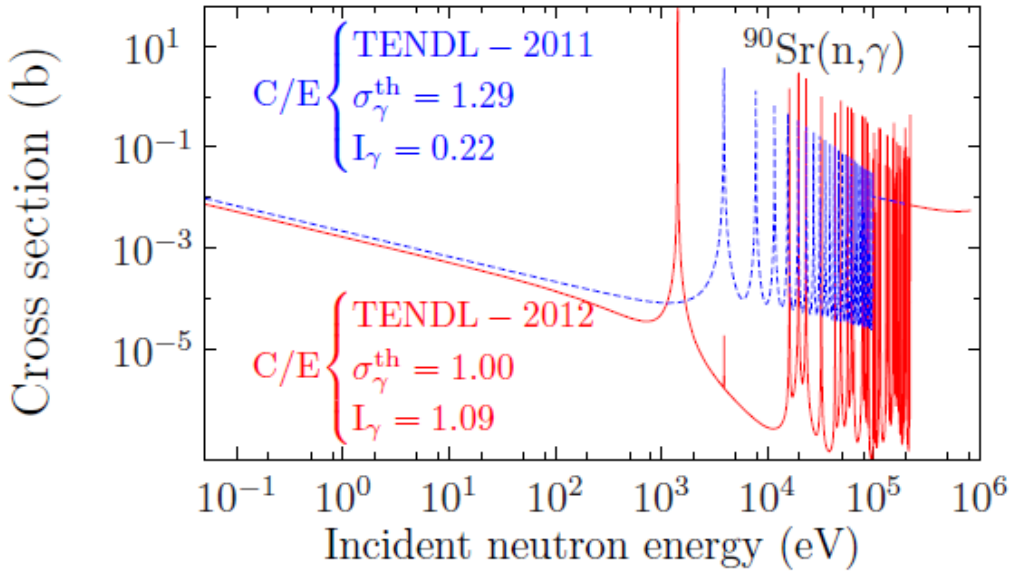
- BMC: Bayesian Monte Carlo for model parameter updates and sampling,

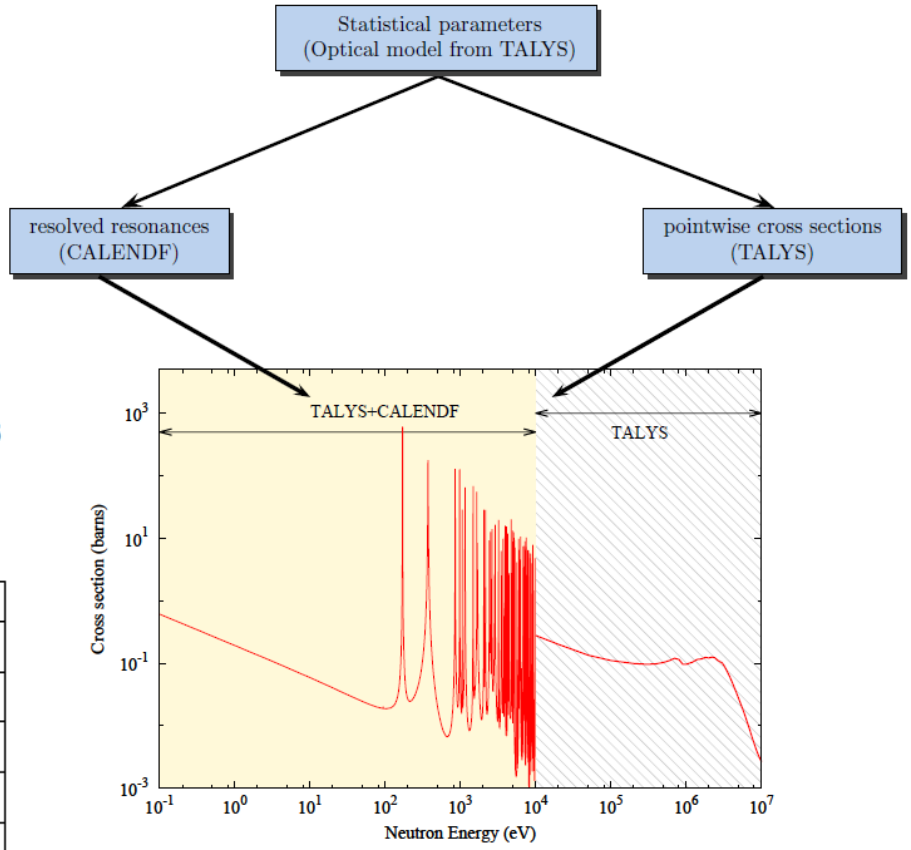
- HFR: Resonance parameters for all isotopes consistent with the fast neutron range.



TENDL related project: the HFR







Are nuclear data important ?

In energy production, better nuclear data can help for:

- Fuel storage and processing,
- Life-time extension,
- Outside usual reactor operations,
- Dosimetry,
- Higher fuel burn-up,
- cost reduction in design of new systems,
- Isotope production,
- Shielding (people safety),
- Future systems,

Dry fuel storage, Zwilag, Switzerland

Better nuclear data have a limited effect on:

- Current reactor operation,
- Current reactor safety,
- Accident simulation,
- Proliferation,
- Accidents.

Relation between evaluation and needs

- Two main related dilemma:
  1. Preliminary question: “Does general-purpose library exist ?”
     - It certainly can, but today all libraries are adjusted (even JENDL ??)
     - There are correct/wrong covariances: only reflect the knowledge we put in
     - Same for cross sections

  2. From users, two typical questions/remarks are

“Why do you get 500 pcm uncertainty on k_{eff} ? We know it better, please do it again.”
“Are these correlations correct ?”

- Solution for the time being:
  - Produce two evaluated files: (1) without integral feedback
    (2) with integral feedback
  - The key point being: do it at the evaluation level !

Making use of T6/TENDL: uncertainty propagation

1st Example: TMC (Total Monte Carlo)

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…

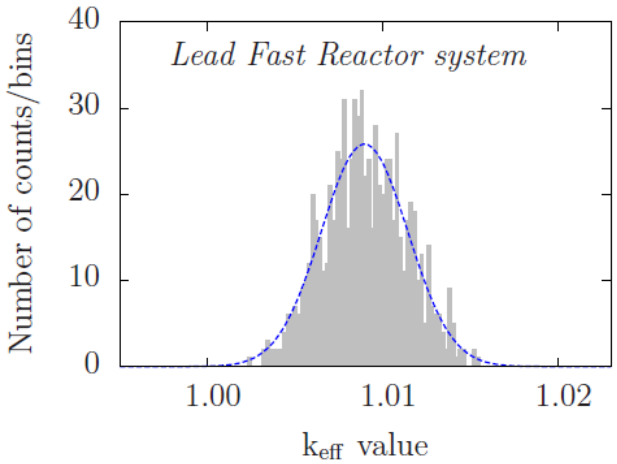
Making use of T6/TENDL: uncertainty propagation with TMC

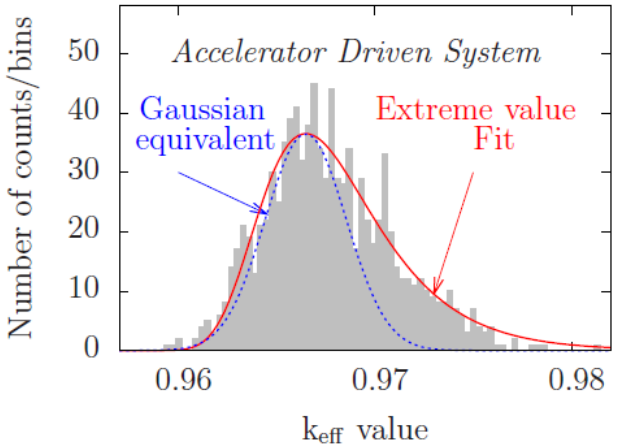
Control of nuclear data (TALYS system)
+ processing (NJOY)
+ system simulation (MCNP/ERANOS/CASMO...)

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.

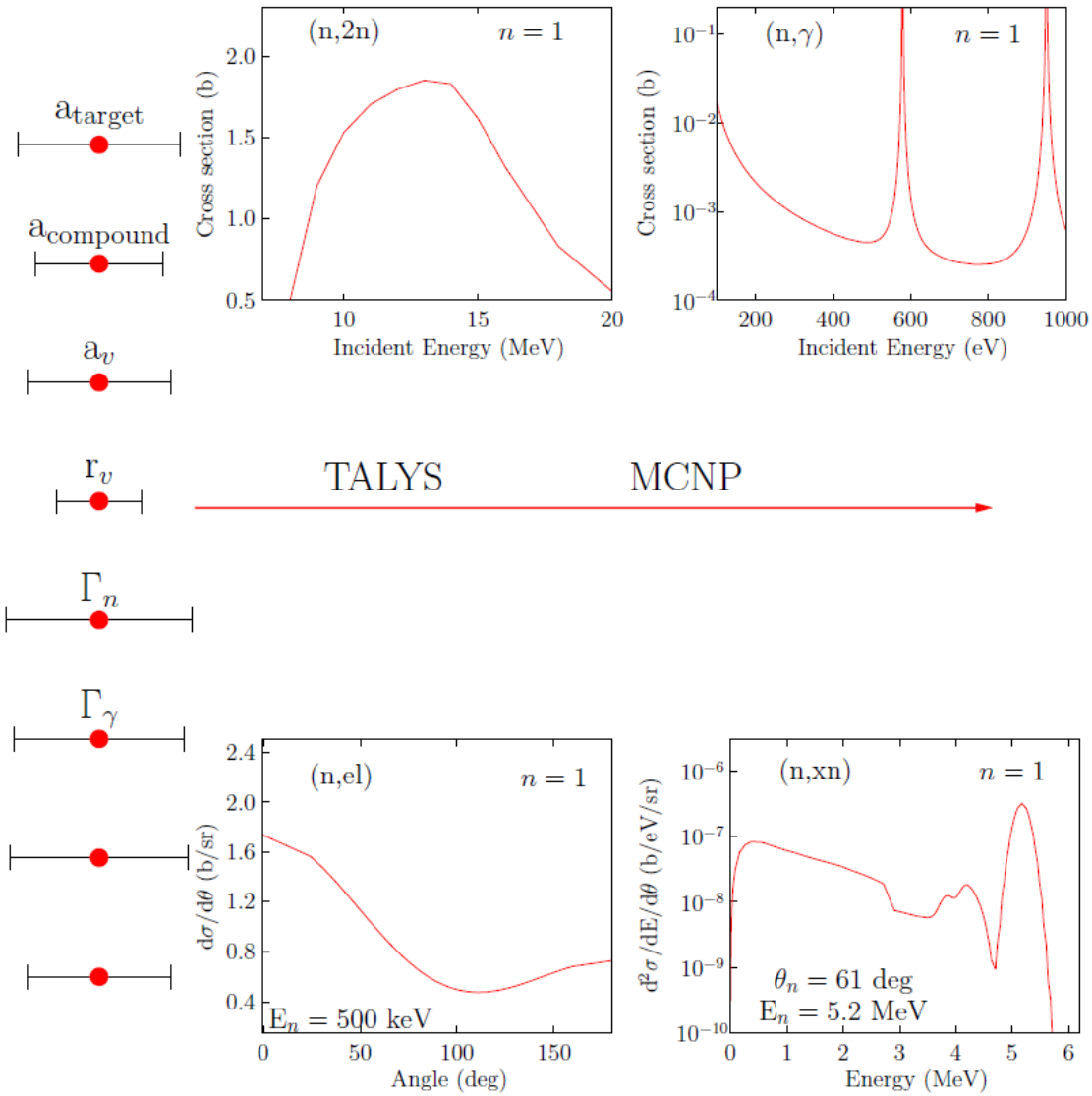
$$\sigma^2_{total} = \sigma^2_{statistics} + \sigma^2_{nuclear\ data}$$

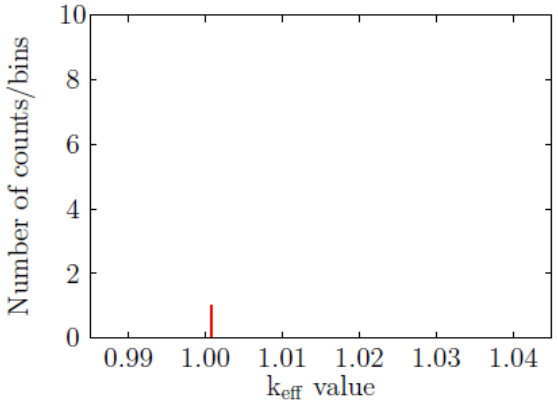




"Towards sustainable nuclear energy: Putting nuclear physics to work",
A.J. Koning and D. Rochman, ANE 35 (2008) 2024.

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





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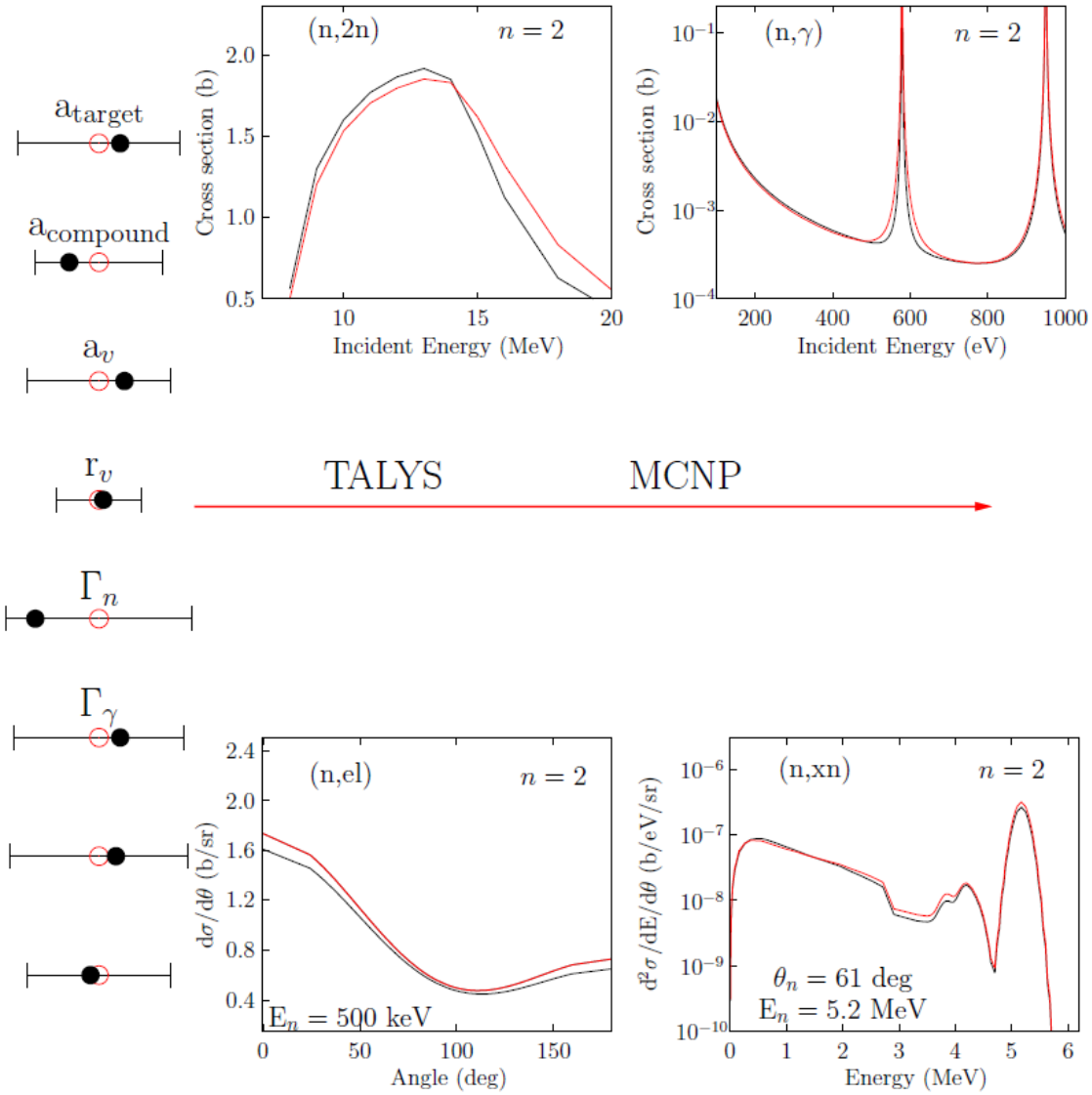

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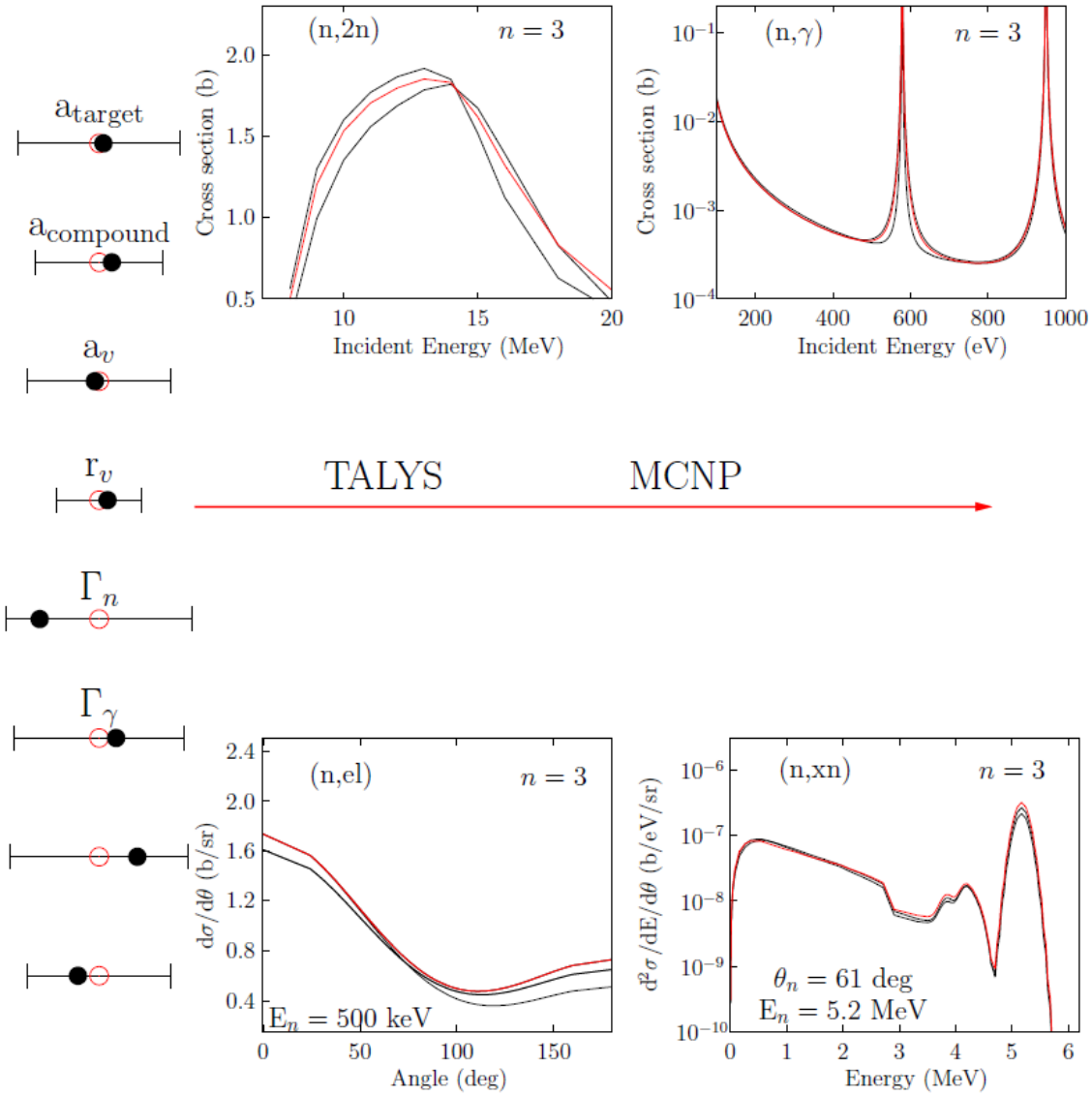

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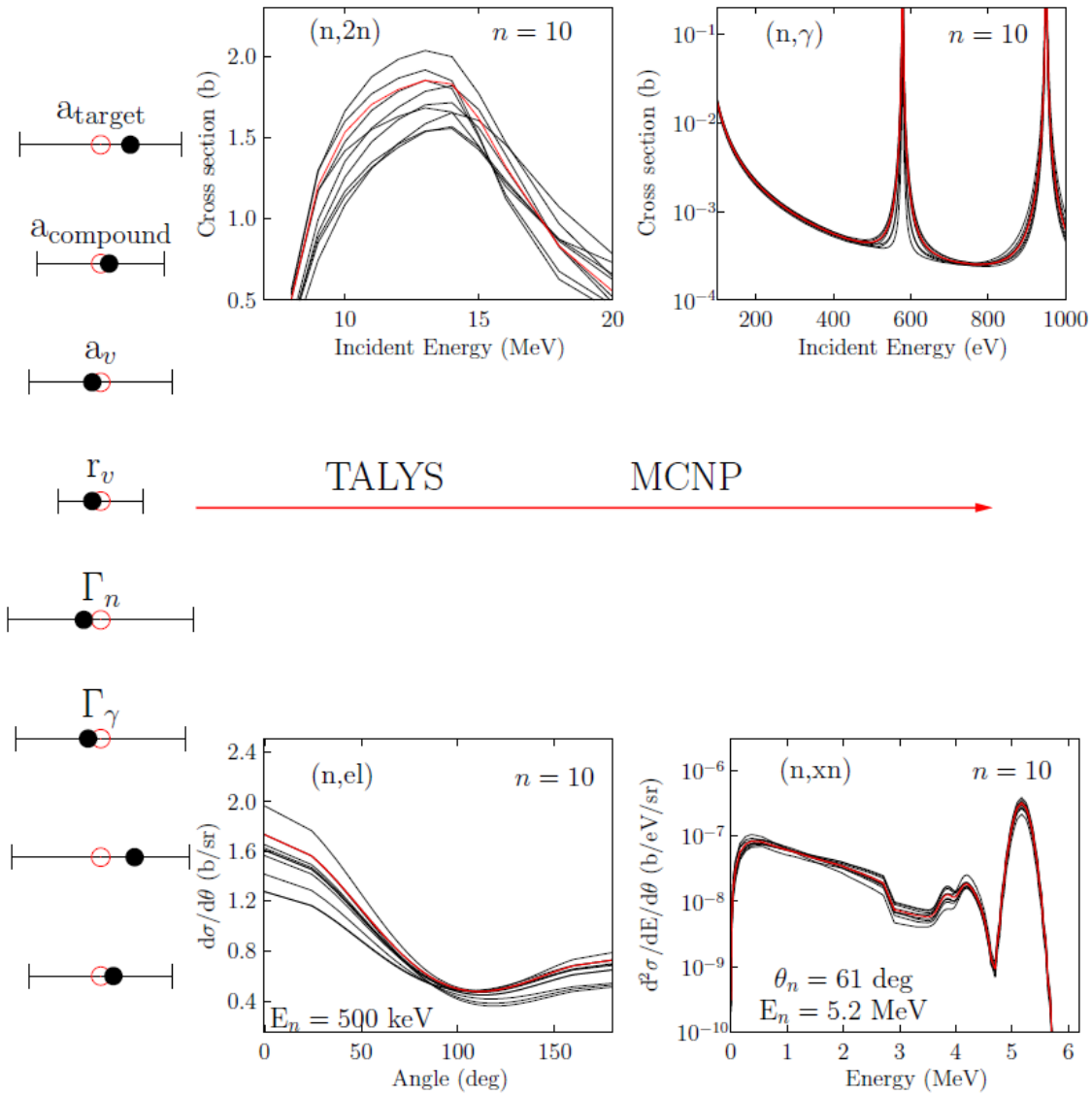

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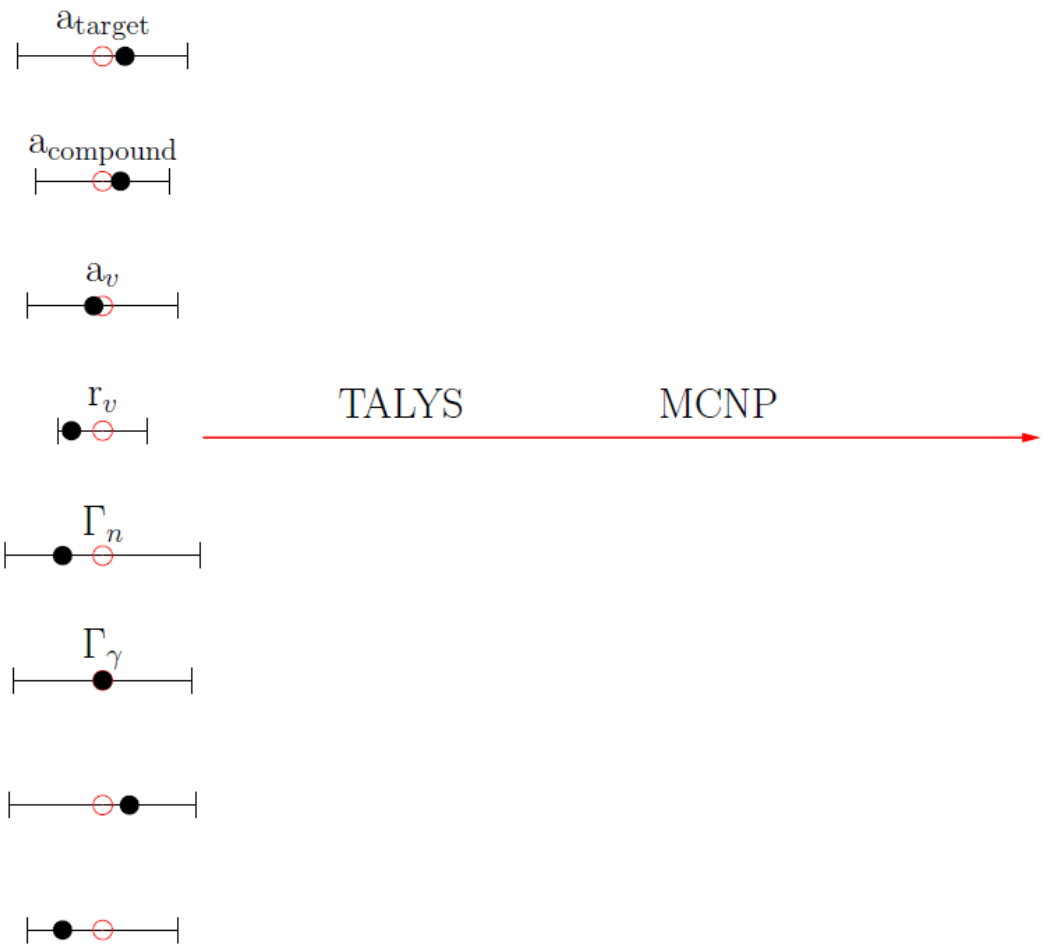

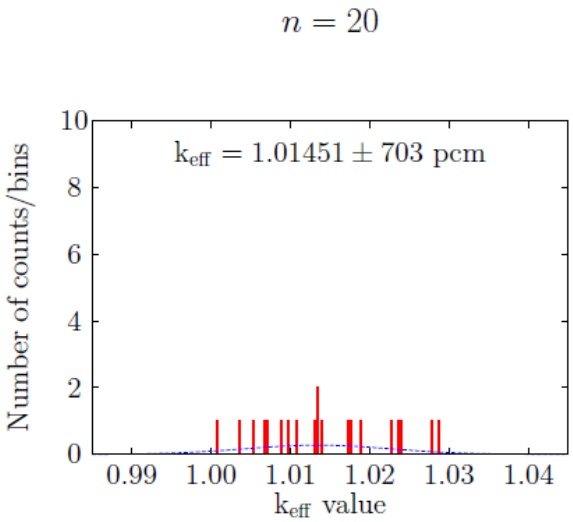

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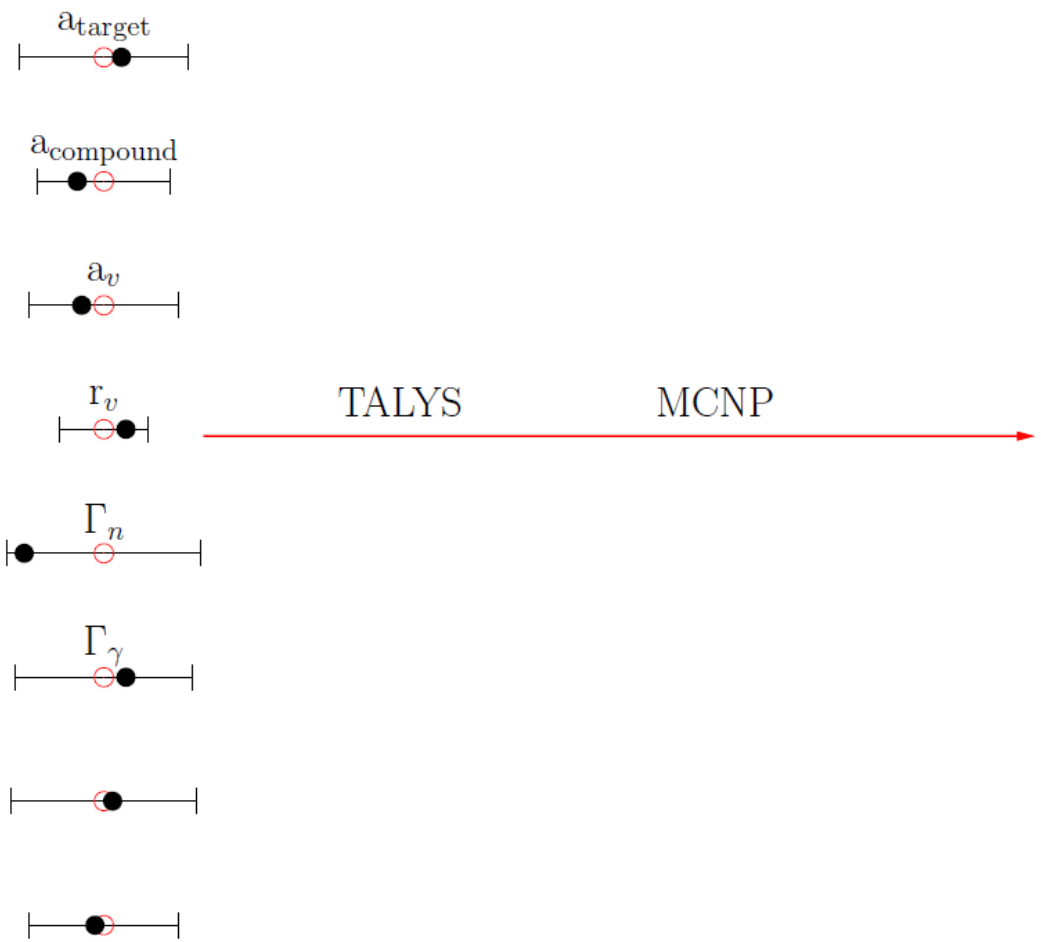

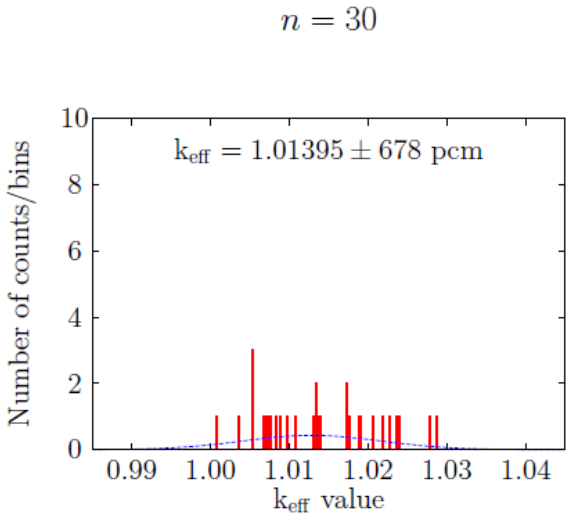

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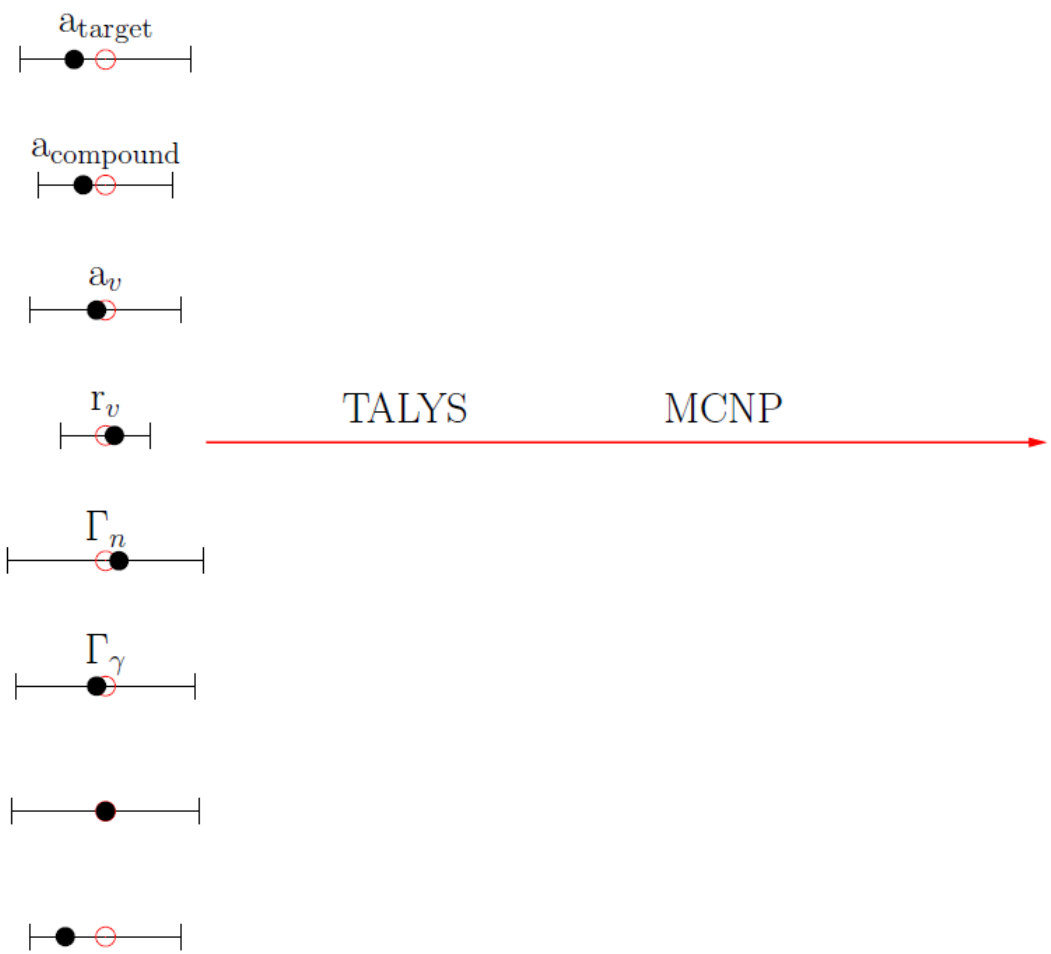

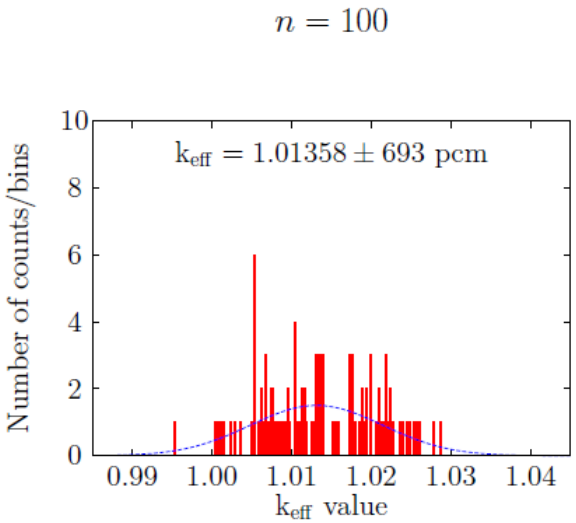

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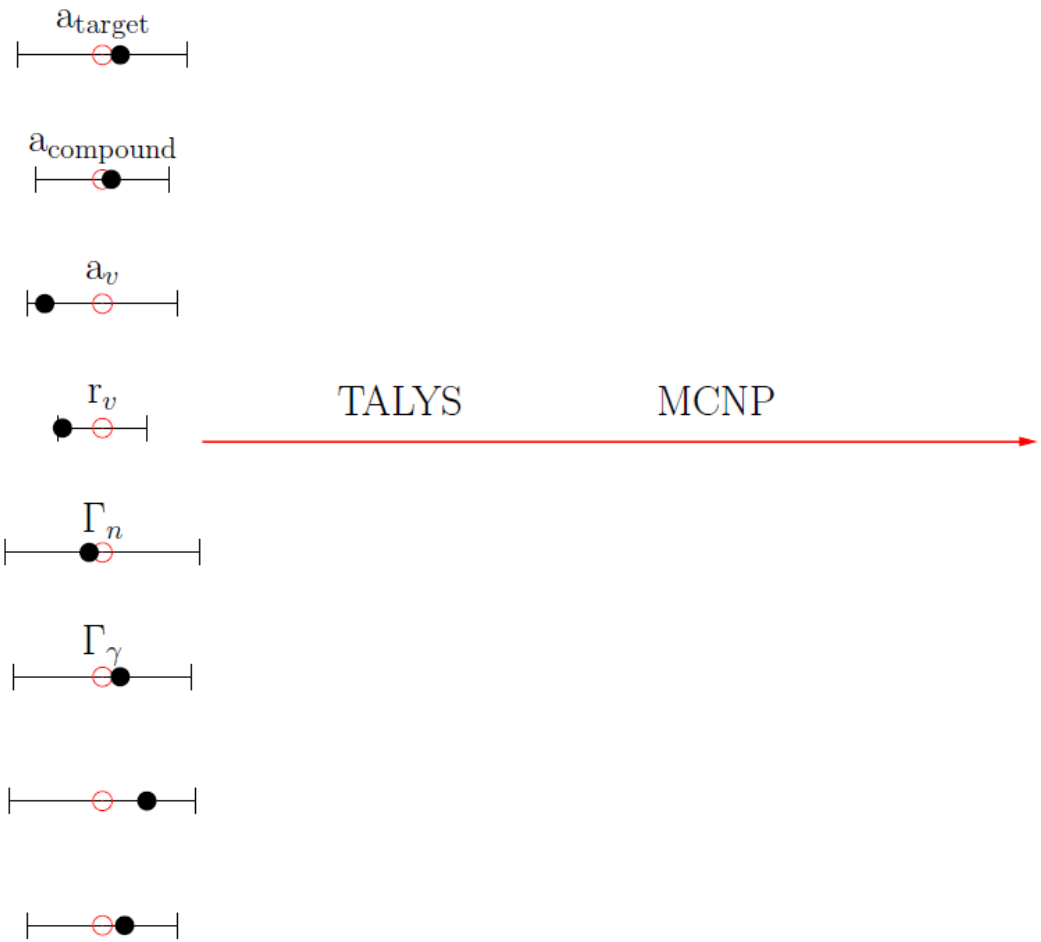

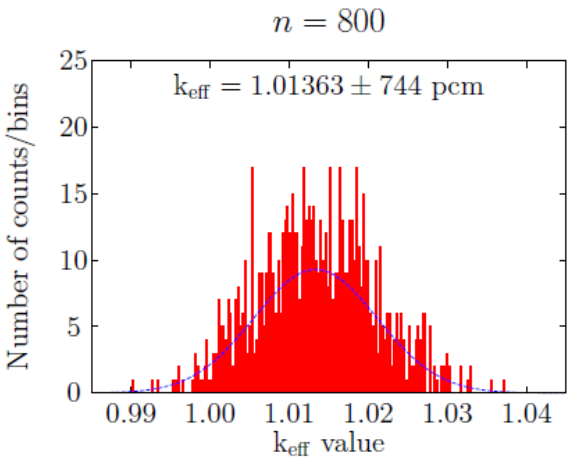

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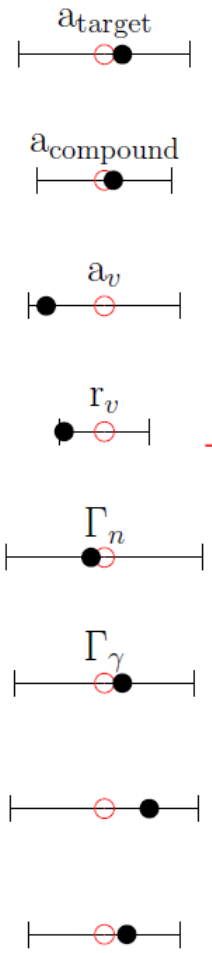
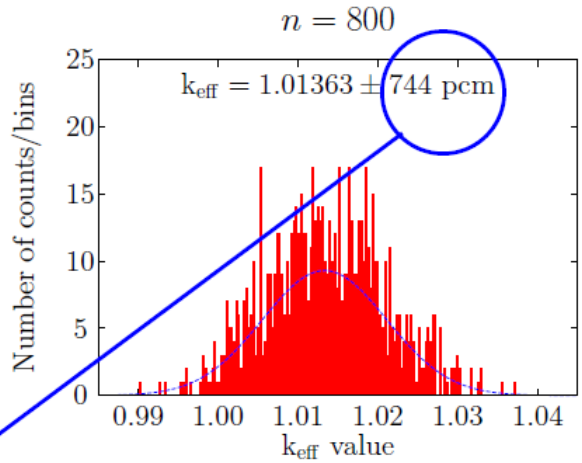


TALYS MCNP



Statistical uncertainty $\simeq$ 68 pcm

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

Making use of T6/TENDL: uncertainty propagation

2nd Example: Methods for Uncertainty reduction (at the evaluation level)

Uncertainty reduction

- Solution: include selected integral information in the evaluation process

- 3 methods:
  - BMC: Bayesian Monte Carlo = TMC + weights on random files,
  - GLLS: Generalized Linear Least Square (not detailed here),
  - GNLS: Generalized Nonlinear Least Square = MOCABA + feedback to nuclear data (Monte Carlo version of the GLLS)

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

Uncertainty reduction with BMC

- 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:

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

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

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

  - 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)

Example with imf7 (bigten) - BMC

- Based on 10 000 random files for $^{235,238}U$

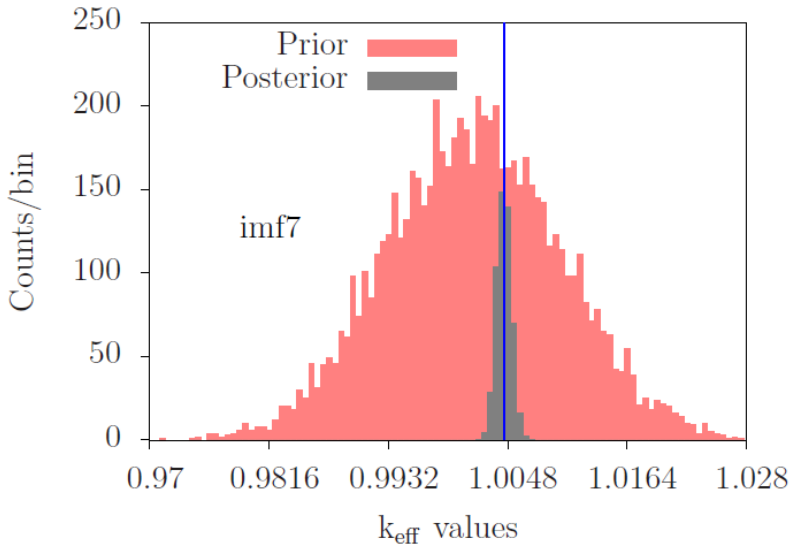


Fig. 12. Prior and posterior distributions of k_{eff} for imf7 benchmark. The blue line indicates the experimental value.

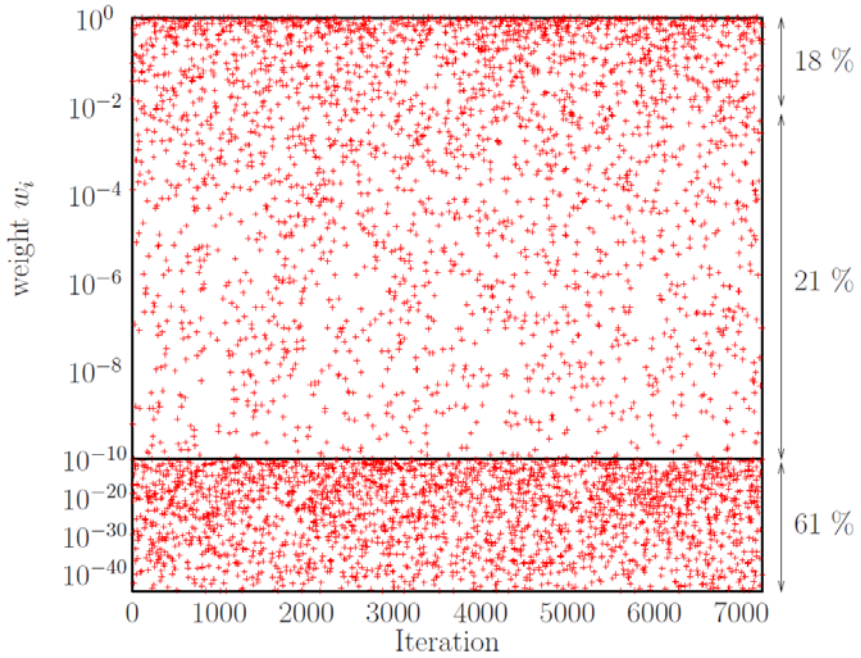


Fig. 1. Calculated weights w_i for the 7000 random cases considered in this work. The number on the right are the percent of weights within the space defined by the arrows.

Example with imf7 (bigten) - BMC

- Updated cross sections

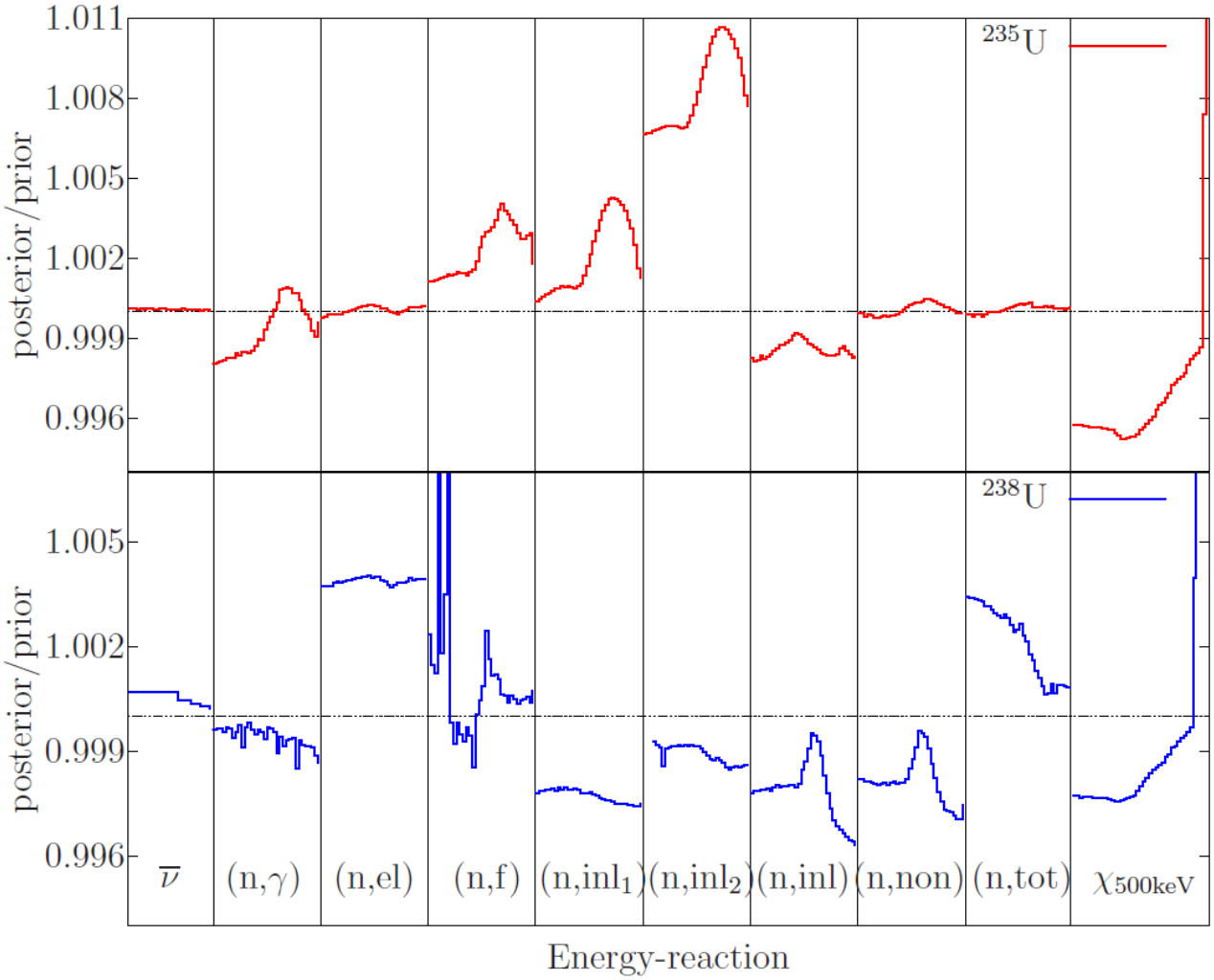
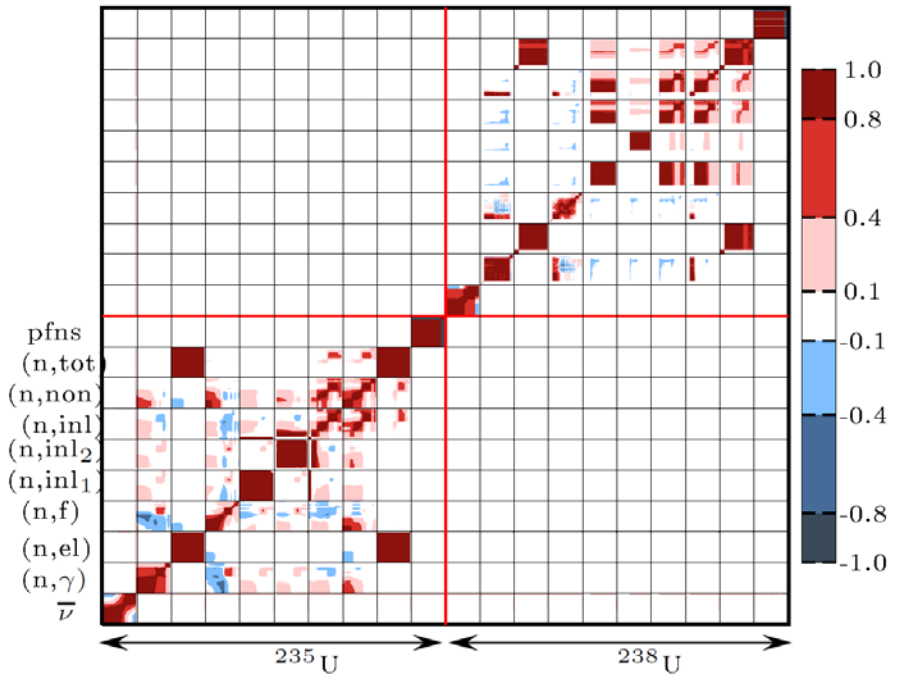


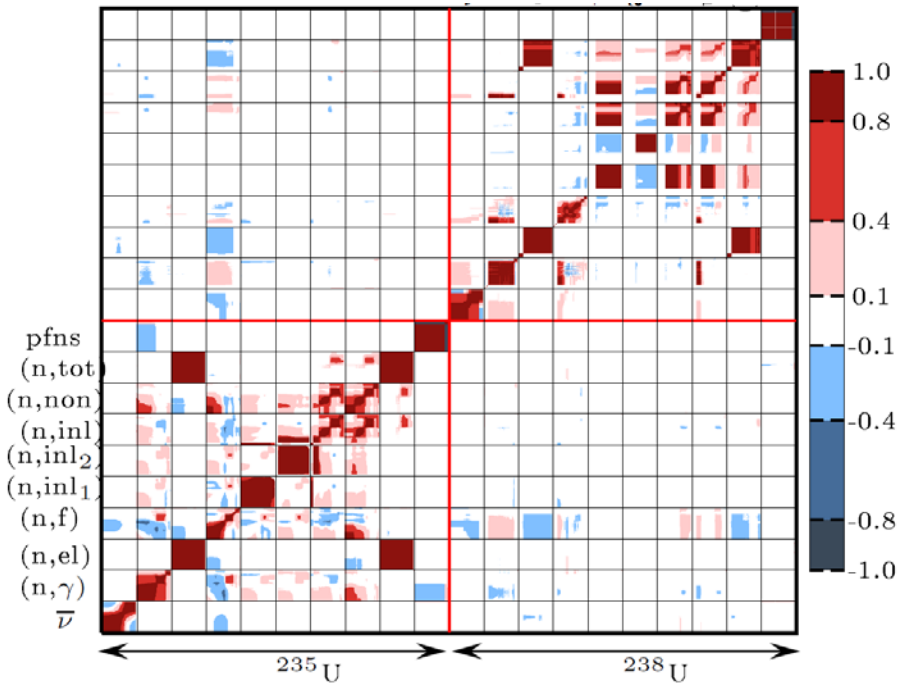
Fig. 9. Ratio of cross sections (and $\overline{\nu}$ and χ) for the post-adjusted (*a posteriori*) over the prior. The cross sections, $\overline{\nu}$ and χ are presented from 100 keV to 6 MeV on a logarithmic scale.

Example with imf7 (bigten) - BMC

- Updated correlations



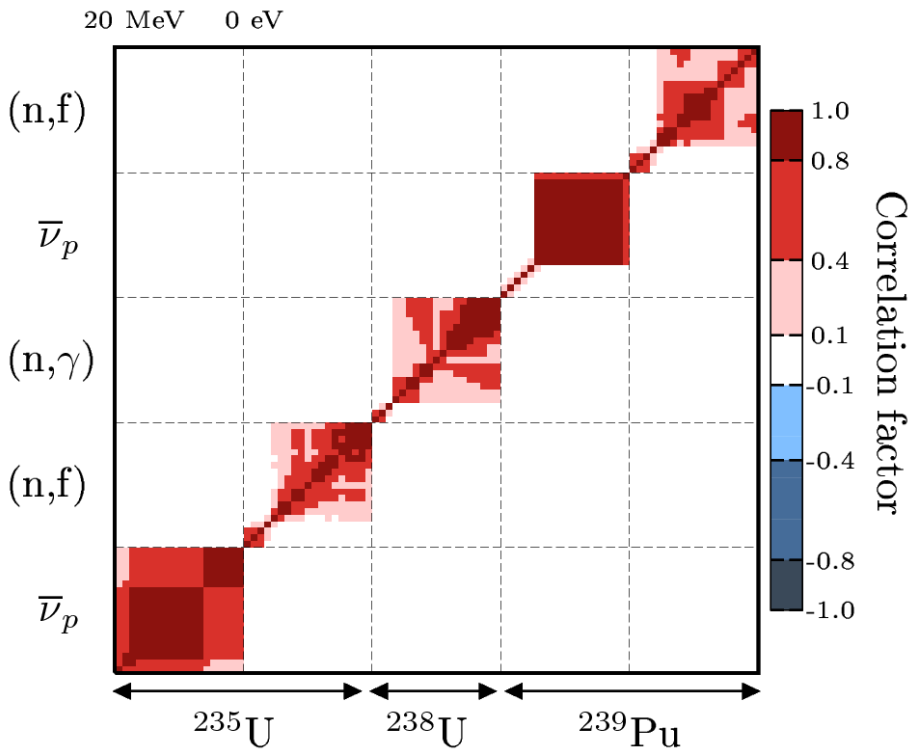
Prior



Posterior

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)



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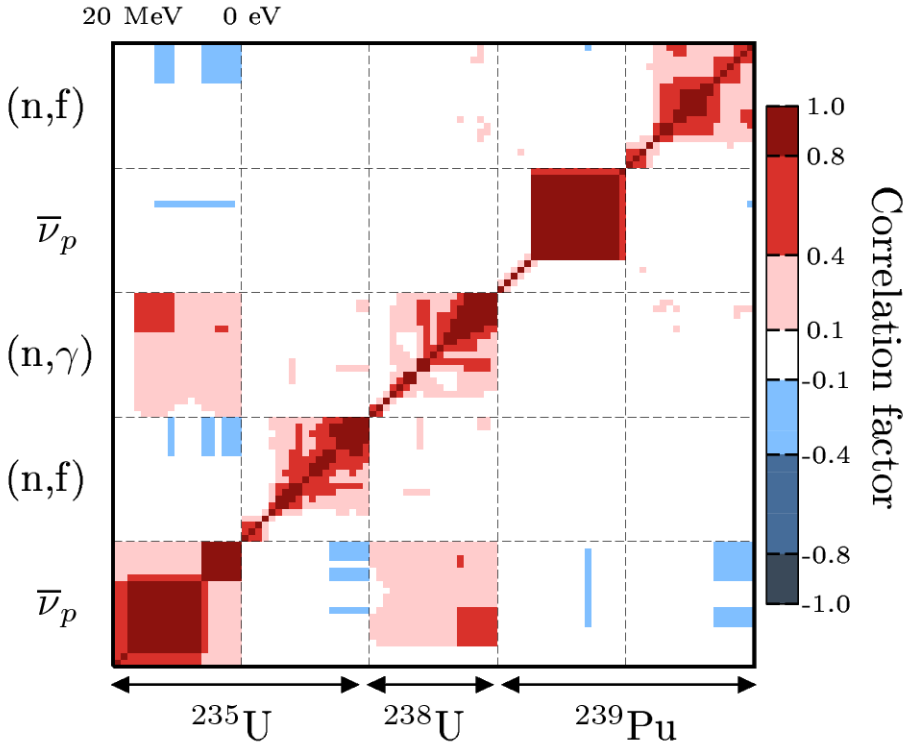


Posterior

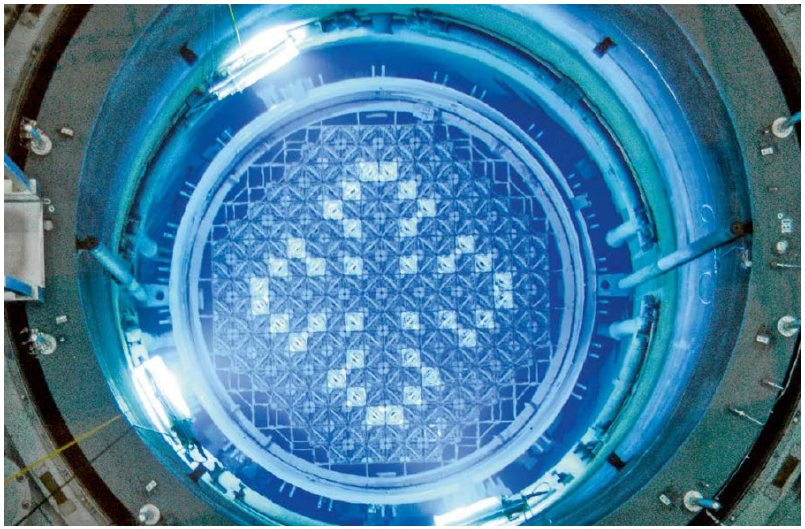
Making use of T6/TENDL: uncertainty propagation

3nd Example: Application to users' quantities

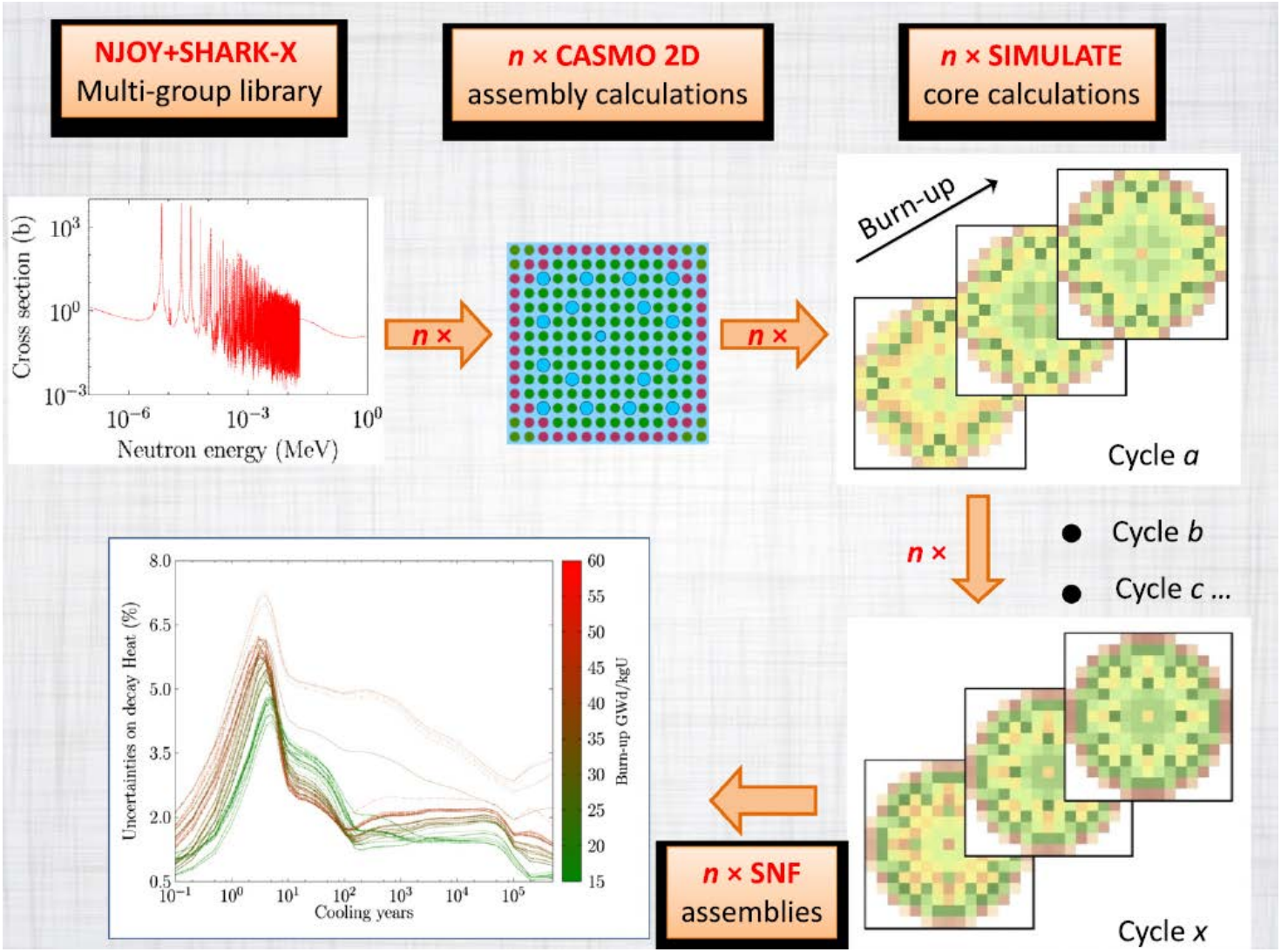
Some studied cases so far at PSI

The following cases have been studied, some of them following user's demands, showing the importance of nuclear data and their uncertainties

- Criticality: ANE 116 (2018) 57, ANE 92 (2016) 150, ANE 36 (2009) 810
- Full core: ANE 110 (2017) 547
- Pin peak power: ANE 112 (2018) 236
- Decay heat: EPJ N4 (2018) 6
- Dosimetry
- Transient: ANE 118 (2018) 178
- Canister loading curves: Jour. of Haz. Mat. 357 (2018) 384
- DNBR
- Geological repository
- dpa: Nucl. Mat. Ener 15 (2018) 244
- PIE and penalty factors

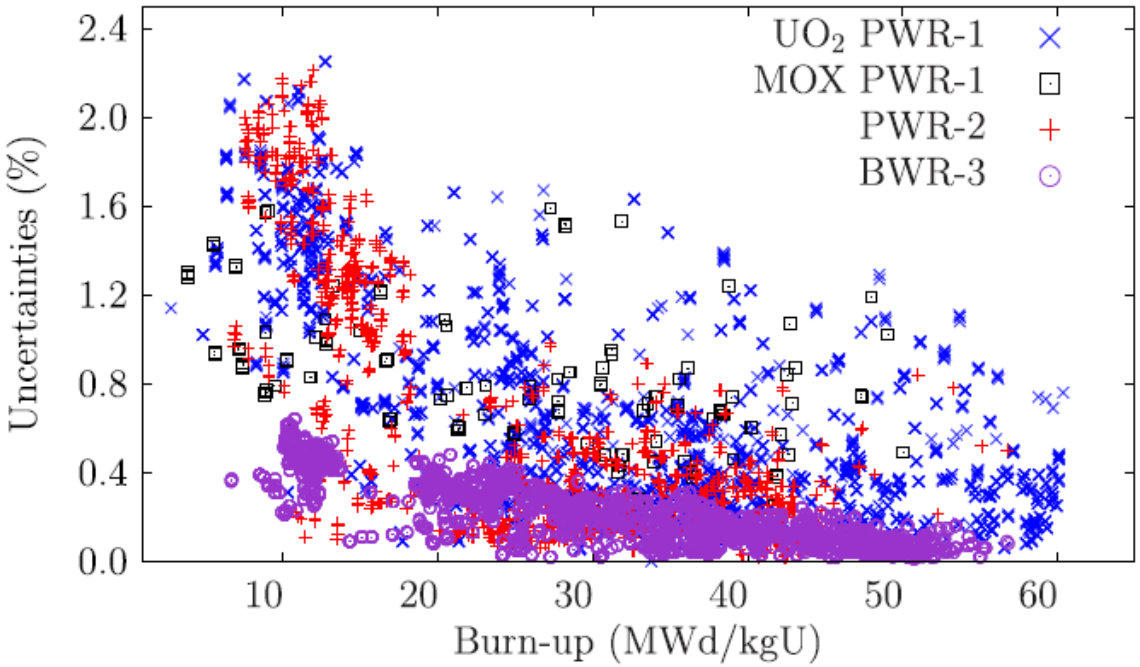


Example for PWR/BWR spent fuel

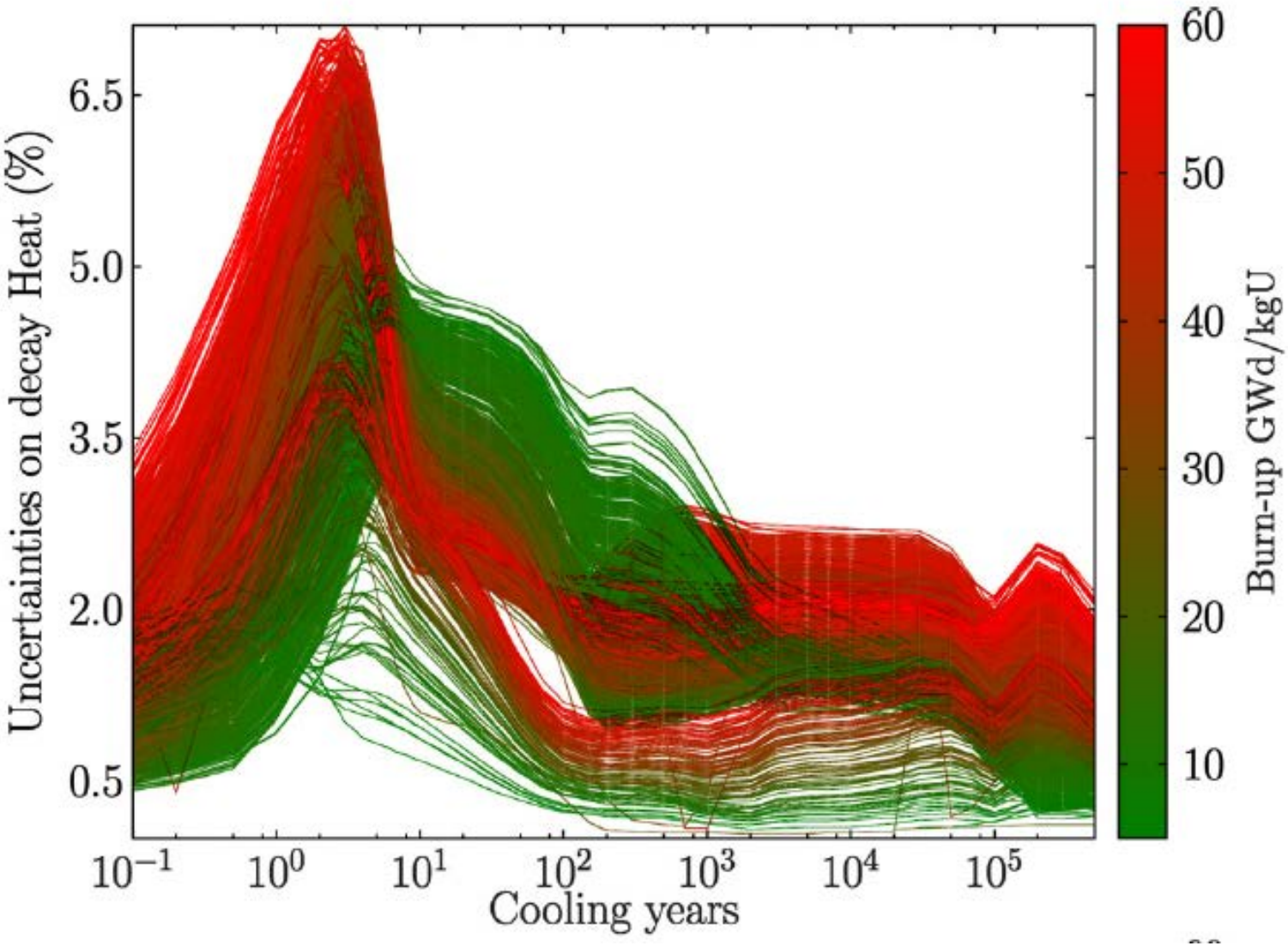


Example for PWR/BWR spent fuel

Core label	Type	Fuel	Enrichment %	Cycles	Assembly-cycles	Burn-up MWd/kgU
PWR-1	PWR	UO_2	2.9–4.7	17–42	2542	4–60
PWR-1	PWR	MOX	2.2–5.8	17–42	297	4–50
PWR-2	PWR	UO_2	1.9–3.5	1–16	2647	7–55
BWR-1	BWR	UO_2	0.7–4.5	19–44	3746	10–45



Example for PWR/BWR spent fuel



Conclusion

- The TENDL library is improving year after year,
- The T6 code package allows to produce TENDL, random files and to go further,
- Automation is a key thing, but does not replace dedicated work
- We believe that we are slowly changing the evaluation process,
- The integration evaluation-application is stronger than before. Is that good ?
- Future: more in-depth evaluation,
  more model defect,
  more use of integral data (??)

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PSI

Wir schaffen Wissen – heute für morgen