PAUL SCHERRER INSTITUT
PSI

D. Rochman

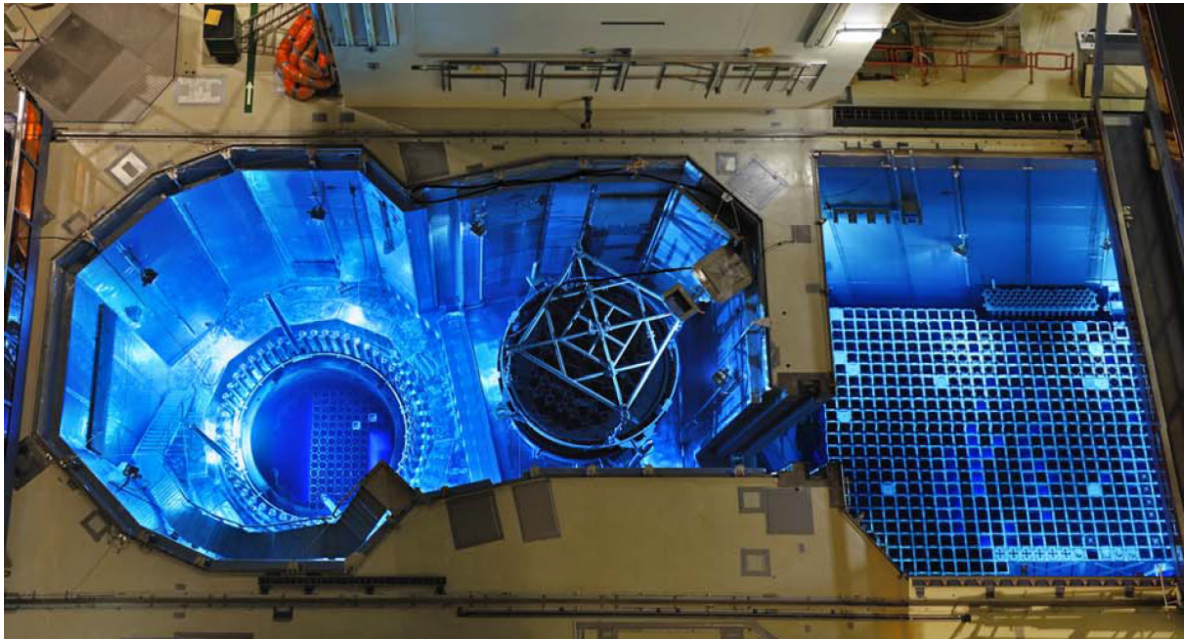
Nuclear data libraries (and insights on evaluations)

Joint ICTP-IAEA workshop, Trieste, Italy, October 9th, 2017

Zertifiziertes Managementsystem STARS ISO 9001

Summary

- What are nuclear data
- Are they important ?
- How can they be produced for application ?
- Some modern methods of evaluation: TMC, BMC, GLLS and MOCABA



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

Some general facts

Kernkraftwerke weltweit

Les centrales nucléaires dans le monde

Stand 31.12.2016* / Etat au 31 décembre 2016*

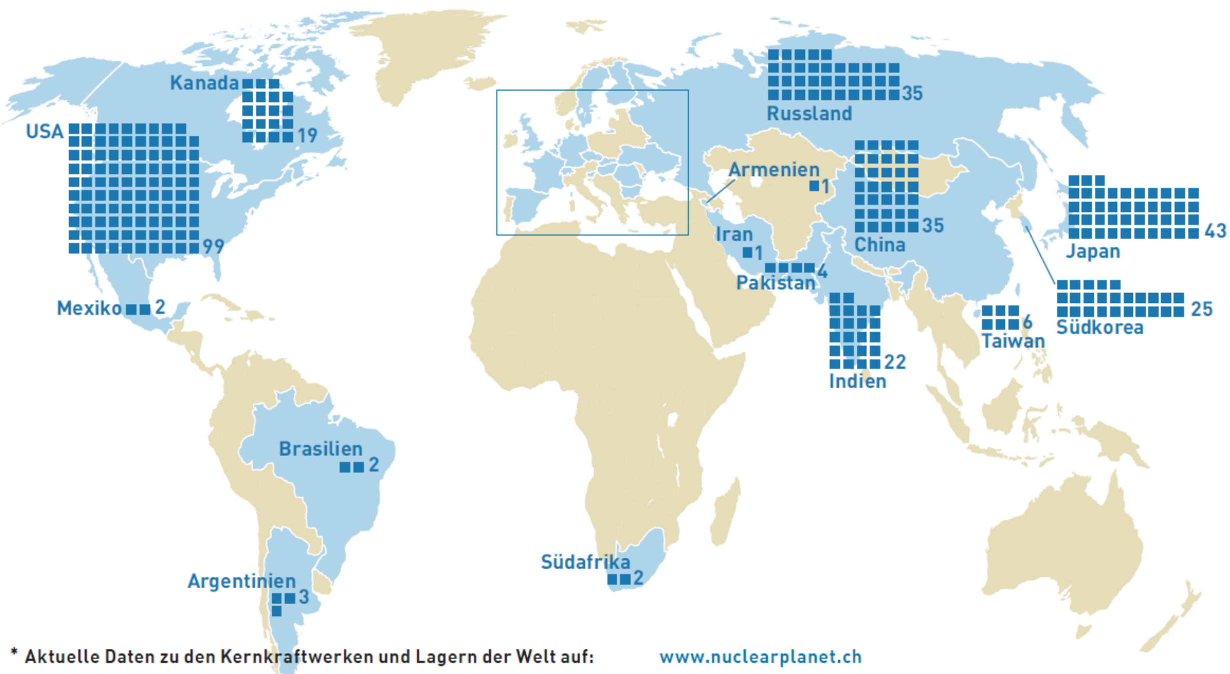
Ganze Welt

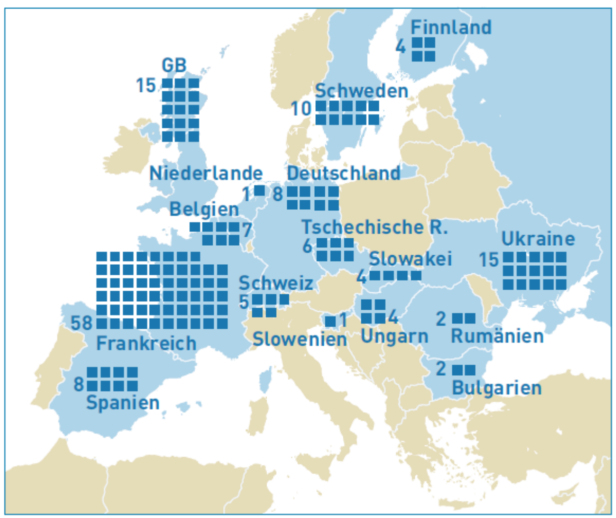
Monde entier

449

391 800 MW

11 %

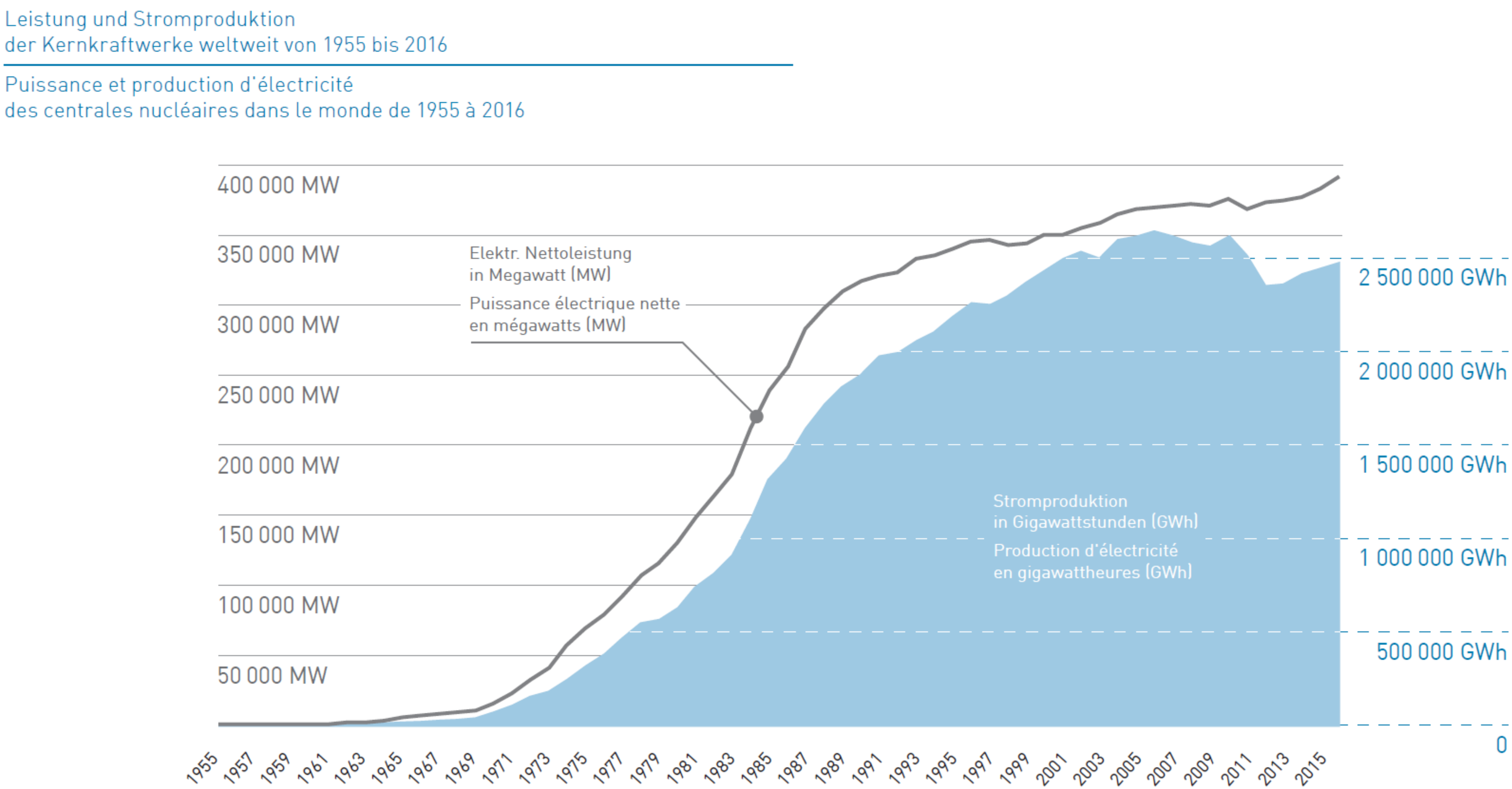




* Aktuelle Daten zu den Kernkraftwerken und Lagern der Welt auf: www.nuclearplanet.ch

Les données relatives aux centrales nucléaires et aux dépôts de déchets radioactifs dans le monde entier sont mises à jour sur:

Some general facts



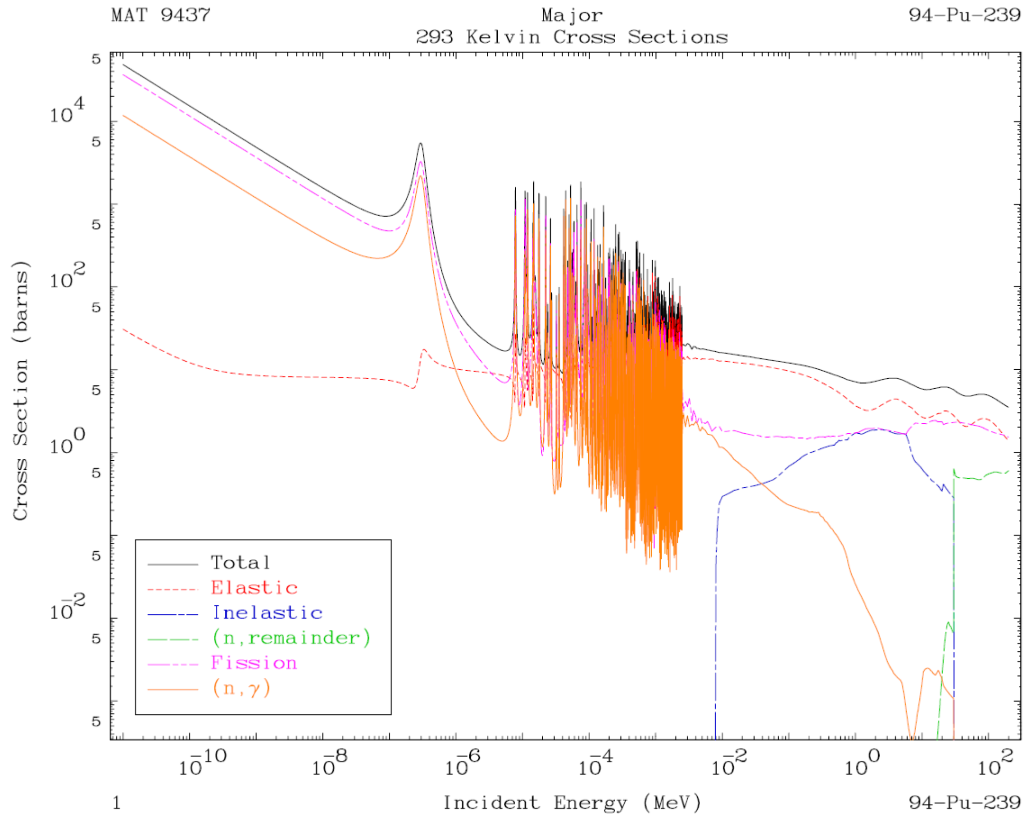
What is “nuclear data” ?

The term “Nuclear data” can have different meaning:

- Old and dusty books, constants, mature field, code inputs, parameters
- Listing, Schrodinger equation, unexciting…
- But it is not !

What are nuclear data in this presentation ?

- From ^{1}H to ^{280}Ds,
- From 0 to 20(0) MeV neutron induced,
- Cross sections, particle emission,
- Angular and energy distributions
- Decay data (half-lives, gamma-ray,…), fission yields, neutron yields,
- And uncertainties



- All these data are nicely condensed in text files in ENDF-6 format (80 columns)

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,

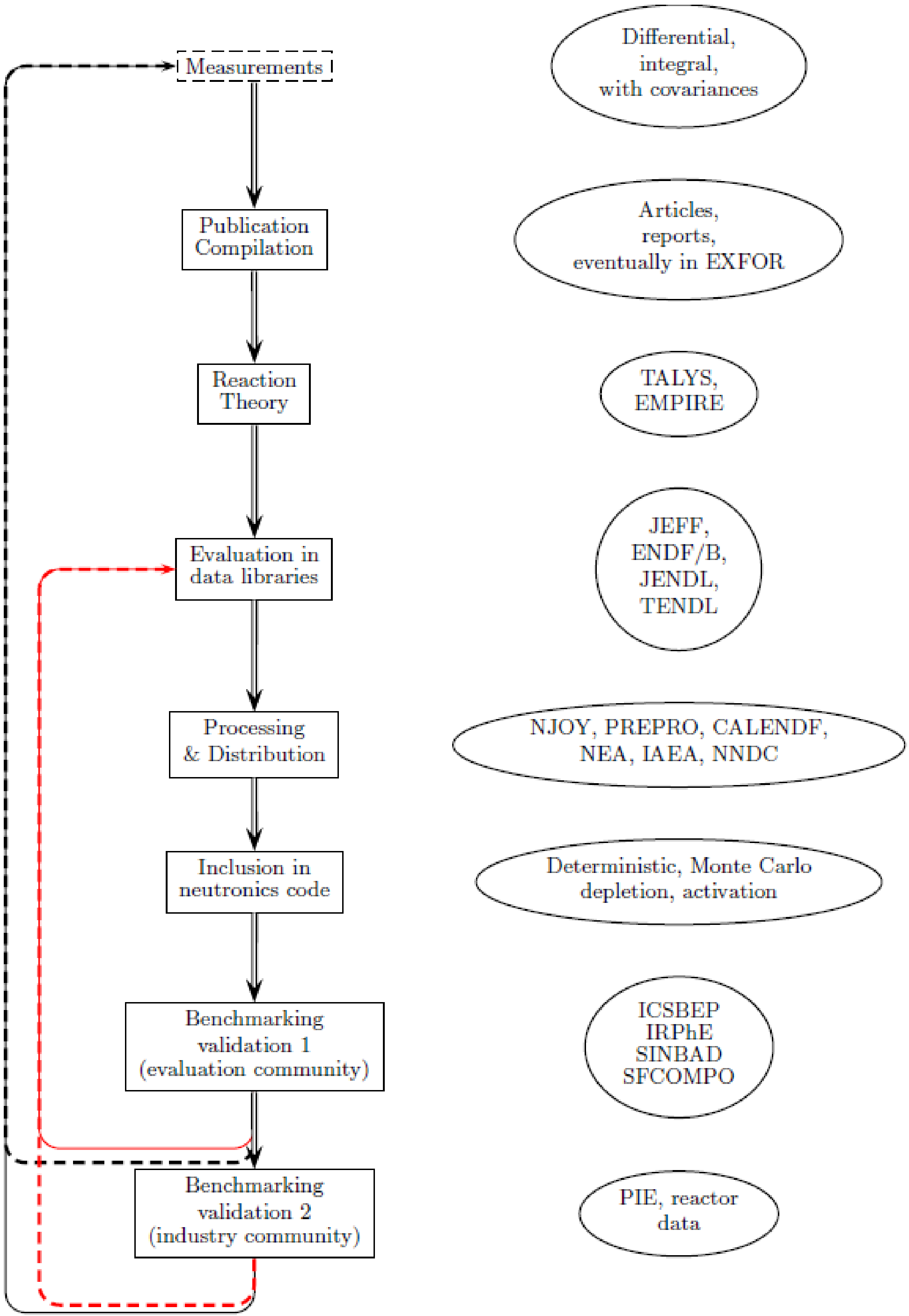
Dry fuel storage, Zwilag, Switzerland

Better nuclear data have a limited effect on:

- Current reactor operation,
- Current reactor safety,
- Accident simulation,
- Proliferation,
- Chernobyl, TMI, Fukushima and other accident.

Nuclear data life cycle

- **Evaluated data**
  - Recommended data, based on all data available from experiments and/or theory (critical analysis of experimental data and their uncertainties, inter- and extrapolation, supplemented with nuclear model calculations)



How to produce nuclear data ?

Independently of the quality of the data, there are 2 ways to produce them:

First solution: manual production

- Widely used for decades up to 2100,
- Concerns all major libraries,
- Questionable QA practices (≠ than the industry standards),
- Has produced very good data,
- We know less and less why.

Second solution: "computer-assisted" production

- One word: "reproducibility",
- Concerns only one library: TENDL
- Much better QA,
- Spent your time on the physics (evaluation), not on the format

The world perception is changing and the second solution might spread around.
See TALYS lab for practical exercises.

How to use nuclear data ?

In general, nuclear data files/evaluations are used by simulation codes:

Neutron transport,
- Monte Carlo: MCNP, SERPENT, TRIPOLI, MONK…
- Fuel assembly (lattice) deterministic: SCALE, DRAGON, CASMO, APPOLO…
- Full core deterministic: SCALE, PANTHER, SIMULATE, DARWIN…
- Transient: S3K, RELAP…

Isotope inventory, radioprotection
- Depletion: FISPACT, ORIGEN, CASMO, SERPENT,…
- Fuel inventory/decay heat: SNF, FISPACT,…

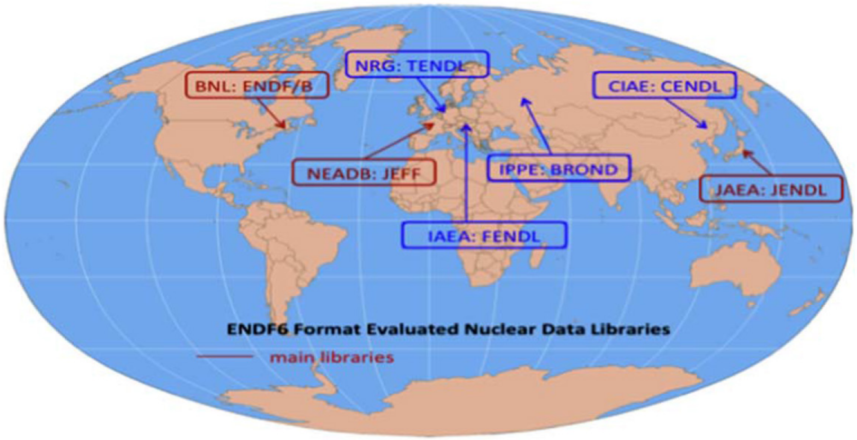
But prior to use them, some processing of the nuclear data is needed:
- NJOY (USA LANL),
- CALENDF (France CEA),
- PREPRO (USA LLNL),
- AMPX, PUFF (USA ORNL),
- WIMS (UK), and many other.

PAUL SCHERRER INSTITUT

Nuclear data libraries

Historically, there exists today many nuclear data libraries:

- General purpose
  - JEFF, mostly towards reactor applications
  - JENDL, mostly towards reactor applications
  - ENDF/B, mostly towards reactor applications
  - TENDL
  - BROND, mostly towards reactor applications
  - CENDL, mostly towards reactor applications
- For fusion application
  - FENDL
  - TENDL
- For dosimetry
  - IRDFF
  - TENDL
  - EAF
- Plus all derived libraries



Nuclear data libraries: what's inside

– In traditional library

❶ ENDF files

– in TENDL

❶ Tabular angular distributions
❷ Tabular Gamma-ray intensities
❸ Tabular partial cross sections to discrete levels
❹ Tabular residual cross sections
❺ Tabular cross sections
❻ ENDF files including covariances
❼ EAF cross section and variance files
❽ Processed ACE files (with NJOY)
❾ Processed covariances (tabular and plots)
❿ Random ENDF files (to get uncertainties on anything with TMC)

Nuclear data libraries: what's inside an ENDF file

- 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.

Nuclear data libraries: format

- ENDF-6 format: all current libraries

```
1.112846+5 4.000000+0 6.947395+0 3.549072-1 0.000000+0 0.000000+02525 2151  182
1.117475+5 4.000000+0 5.085219+0 1.027339-1 0.000000+0 0.000000+02525 2151  183
1.118390+5 3.000000+0 9.557557-1 3.608416-1 0.000000+0 0.000000+02525 2151  184
1.119557+5 1.000000+0 2.396252+1 2.622365-1 0.000000+0 0.000000+02525 2151  185
1.149003+5 2.000000+0 8.845672+1 3.624525-1 0.000000+0 0.000000+02525 2151  186
1.155829+5 2.000000+0 3.233438+1 2.248352-1 0.000000+0 0.000000+02525 2151  187
1.169387+5 3.000000+0 2.620988+1 2.669427-1 0.000000+0 0.000000+02525 2151  188
1.202353+5 2.000000+0 1.372418+2 3.792647-1 0.000000+0 0.000000+02525 2151  189
1.207319+5 3.000000+0 2.723689+1 2.849488-1 0.000000+0 0.000000+02525 2151  190
1.213819+5 4.000000+0 1.809683+1 1.177020-1 0.000000+0 0.000000+02525 2151  191
1.218669+5 3.000000+0 2.984662+1 5.810848-1 0.000000+0 0.000000+02525 2151  192
1.238063+5 1.000000+0 4.002582+1 5.298469-1 0.000000+0 0.000000+02525 2151  193
                                                                  2525 2  099999
                                                                  2525 0  0    0
2.505500+4 5.446610+1          0          0          0          02525 3  1    1
0.000000+0 0.000000+0          0          0          1        7862525 3  1    2
       786          2                                           2525 3  1    3
1.000000-5 0.000000+0 1.000000+0 0.000000+0 5.000000+0 9.000000-32525 3  1    4
1.000000+1 1.100000-2 3.000000+1 2.400000-2 6.000000+1 2.800000-22525 3  1    5
1.000000+2 3.300000-2 2.000000+2 3.900000-2 4.000000+2 3.550000-22525 3  1    6
8.000000+2 3.100000-2 3.150000+3 1.260000-2 9.750000+3 6.540000-32525 3  1    7
1.950000+4 5.760000-3 2.750000+4 4.030000-3 3.500000+4 2.480000-32525 3  1    8
4.500000+4 3.600000-3 5.450000+4 3.800000-3 6.375000+4 2.430000-32525 3  1    9
7.425000+4 3.520000-3 8.750000+4 3.440000-3 1.015700+5 3.140000-32525 3  1   10
1.100000+5 2.500000-3 1.150000+5 2.200000-3 1.211830+5 2.000000-32525 3  1   11
```

- New format: XML based, might come soon

Processing nuclear data libraries

This is a very specific task, sometimes secretive, sometimes with specific parameters

Most simple processing: nothing done

- Fission yields, decay data,
- Libraries are read as they are by simulation codes

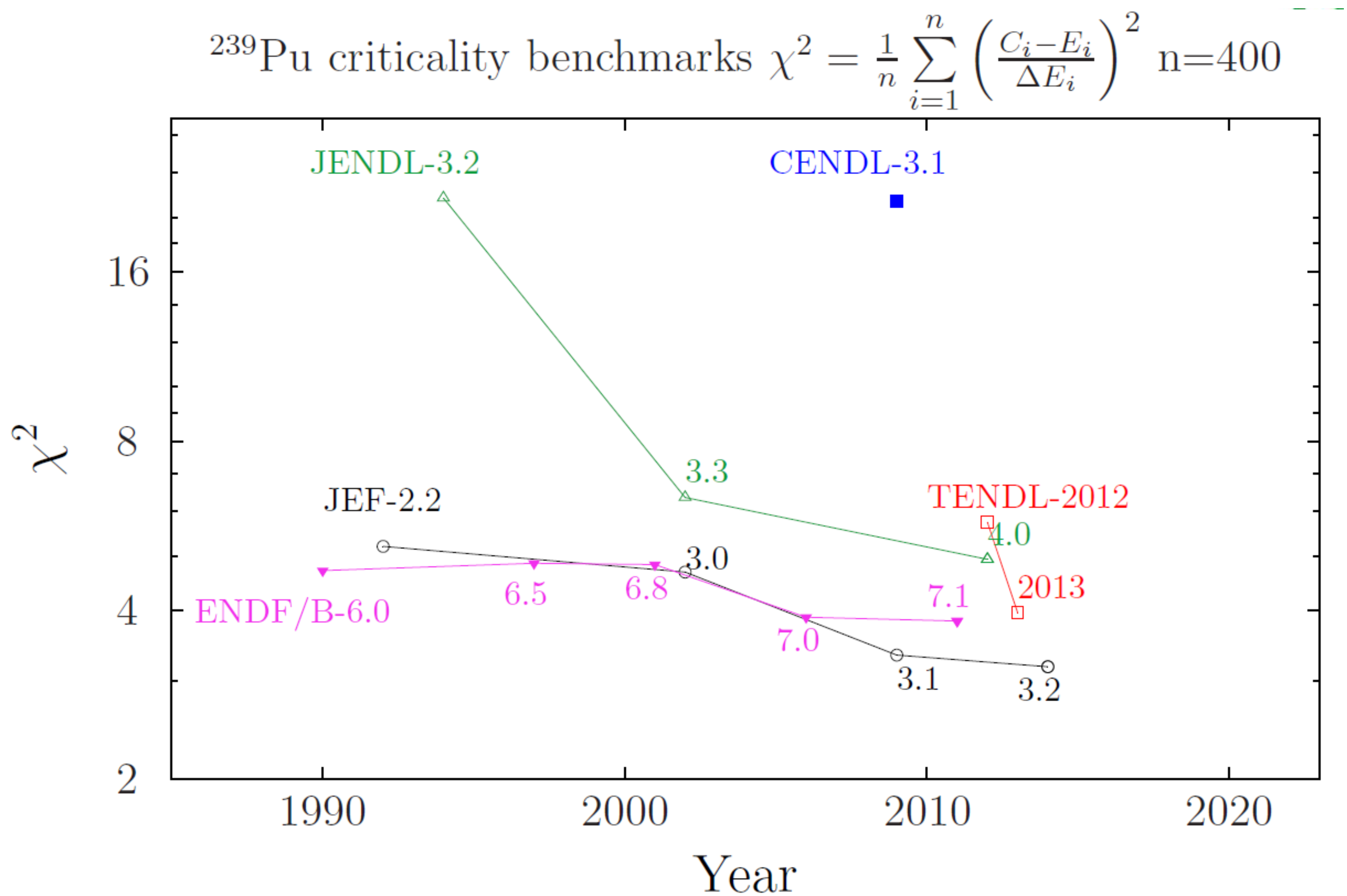
More sophisticated:

- For Monte Carlo transport calculation (MCNP, SERPENT)
- Usually performed with NJOY
- Can take hours: pointwise, groupwise data, Doppler broadening, reconstruction of emission spectra…

One step further:

- For Deterministic transport calculation,
- Performed with many processing codes,
- As for Monte Carlo, + self-shielding factors,
- Not always in the open literature (expert knowledge).

Library performance, how to assess it ?



Some modern methods of evaluation: 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 less fast, 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).

Some modern methods of evaluation: TMC, BMC, GLLS and MOCABA

- GLLS: Generalized Linear Least Square

The goal of the GLLS method is to vary nuclear data and integral responses so that they are most consistent with their uncertainty matrices. This is done by minimizing the chi-square, expressed as

$$\chi^2 = \left(\boldsymbol{E} - \boldsymbol{C}(\boldsymbol{\sigma})\right)^T \boldsymbol{M}_{\boldsymbol{EC}}^{-1}\left(\boldsymbol{E} - \boldsymbol{C}(\boldsymbol{\sigma})\right) + (\boldsymbol{\sigma} - \boldsymbol{\sigma_0})^T \boldsymbol{M}_{\boldsymbol{\sigma}}^{-1}(\boldsymbol{\sigma} - \boldsymbol{\sigma_0})$$

Adjusted, or posterior, nuclear data **σ'** and $\mathbf{M}_{\boldsymbol{\sigma}}$' after minimization given as

$$\boldsymbol{\sigma}' = \boldsymbol{\sigma} + \boldsymbol{M}_{\boldsymbol{\sigma}}\boldsymbol{S}^{\boldsymbol{T}}[\boldsymbol{S}\boldsymbol{M}_{\boldsymbol{\sigma}}\boldsymbol{S}^T + \boldsymbol{M}_{\boldsymbol{EC}}]^{-1}[\boldsymbol{E} - \boldsymbol{C}(\boldsymbol{\sigma})]$$

$$\boldsymbol{M}'_{\boldsymbol{\sigma}} = \boldsymbol{M}_{\boldsymbol{\sigma}} - \boldsymbol{M}_{\boldsymbol{\sigma}}\boldsymbol{S}^{\boldsymbol{T}}[\boldsymbol{S}\boldsymbol{M}_{\boldsymbol{\sigma}}\boldsymbol{S}^T + \boldsymbol{M}_{\boldsymbol{EC}}]^{-1}\,\boldsymbol{S}\boldsymbol{M}_{\boldsymbol{\sigma}}$$

Some modern methods of evaluation: TMC, BMC, GLLS and MOCABA

- MOCABA: Monte Carlo version of the GLLS
- Just like GLLS, but S replace by a Monte Carlo estimation M_c

$$\mathbf{C}' = \mathbf{C} + \mathrm{M}_{\mathbf{C}}\left(\mathrm{M}_{\mathbf{C}} + \mathrm{M}_{\mathbf{E}}\right)^{-1}\left(\mathbf{E} - \mathbf{C}\right)$$

$$\mathrm{M}'_{\mathbf{C}} = \mathrm{M}_{\mathbf{C}} - \mathrm{M}_{\mathbf{C}}\left(\mathrm{M}_{\mathbf{C}} + \mathrm{M}_{\mathbf{E}}\right)^{-1}{\mathrm{M}_{\mathbf{C}}}^{T}$$

$$\boldsymbol{\sigma}' = \boldsymbol{\sigma} + \mathrm{M}_{\sigma,\mathbf{C}}\left(\mathrm{M}_{\mathbf{C}} + \mathrm{M}_{\mathbf{E}}\right)^{-1}\left(\mathbf{E} - \mathbf{C}\right)$$

$$\mathrm{M}'_{\sigma} = \mathrm{M}_{\sigma} - \mathrm{M}_{\sigma,\mathbf{C}}\left(\mathrm{M}_{\mathbf{C}} + \mathrm{M}_{\mathbf{E}}\right)^{-1}{\mathrm{M}_{\sigma,\mathbf{C}}}^{T}$$

Some modern methods of evaluation: TMC, BMC, GLLS and MOCABA

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

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

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

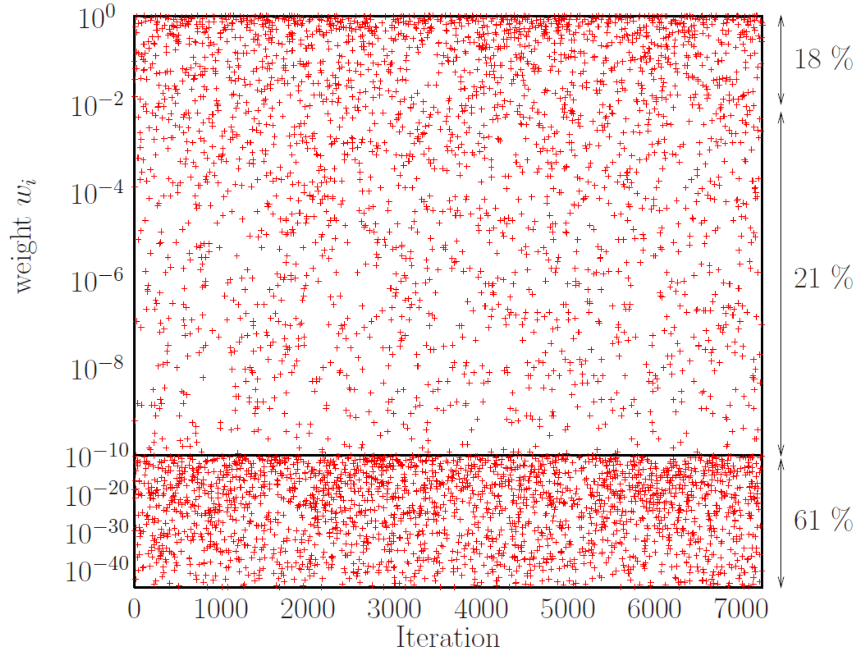


Fig. 1. Calculated weights w_i for the 7000 random cases considered in this work. The number on the right are the percent of weights within the space defined by the arrows.

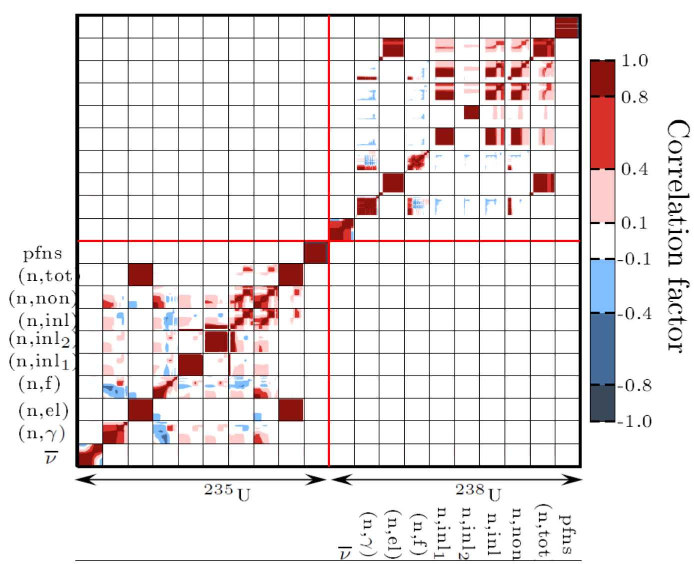
- The best solutions have large weights, leading to updated values.

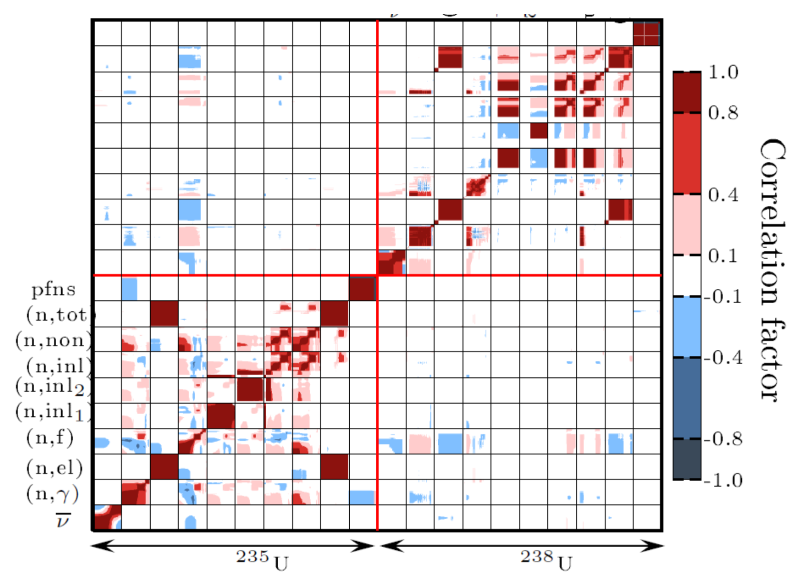
Some modern methods of evaluation: TMC, BMC, GLLS and MOCABA

- BMC: Bayesian Monte Carlo
- Example on U235 and U238

Table 3. Prior and posterior average k_{eff} and uncertainties for four benchmarks. Uncertainties Δk are given in pcm. C/E values are also indicated. The statistical uncertainty for each MCNP6 calculation is in the order of 25 pcm.

Benchmark	Used in Bayesian update	Exp k_{eff}	Exp $\pm\Delta k$	Prior $\bar{k}$	Prior $\pm\Delta k$	Posterior $\bar{k}$	Posterior $\pm\Delta k$	Prior C/E-1 (%)	Posterior C/E-1 (%)
imf7	yes	1.00450	± 70	1.00156	± 850	1.00446	± 71	-0.29	-0.004
hmf1	no	1.00000	± 100	0.99509	± 1120	0.99691	± 960	-0.49	-0.39
imf1-1	no	0.99880	± 90	0.99767	± 900	0.99984	± 670	-0.11	0.10
lct6-1	no	1.00000	± 200	0.99836	± 405	0.99879	± 440	-0.16	-0.12





Some modern methods of evaluation: TMC, BMC, GLLS and MOCABA

- Comparison BMC/MOCABA

system	quantity	Exp.	Exp. unc. (pcm)	Prior C	Prior unc. (pcm)	Posterior (BMC)	Posterior unc. pcm (BMC)	Posterior (MOCABA)	Posterior unc. pcm (MOCABA
mmf1	k_{eff}	1.00000	160	0.99861	670	**0.99971**	**120**	**0.99976**	**146**
pmf2	k_{eff}	1.00000	200	1.00354	663	**1.00172**	**154**	**1.00112**	**177**
pmf2	**F8/F5**	0.20710	2100	0.20618	509	**0.20708**	**557**	**0.20658**	**494**
imf7	k_{eff}	1.00450	70	1.00145	853	**1.00455**	**58**	**1.00443**	**69**
imf1	k_{eff}	0.99880	90	0.99730	912	**0.99890**	**73**	**0.99916**	**83**
hmf1	k_{eff}	1.00000	200	0.99464	1122	**0.99822**	**125**	**0.99815**	**157**
hmf1	**F9/F5**	1.41520	1400	1.39025	2468	**1.39341**	**920**	**1.39650**	**929**
hmf1	**F8/F5**	0.16430	1800	0.15683	445	**0.15522**	**191**	**0.15684**	**348**

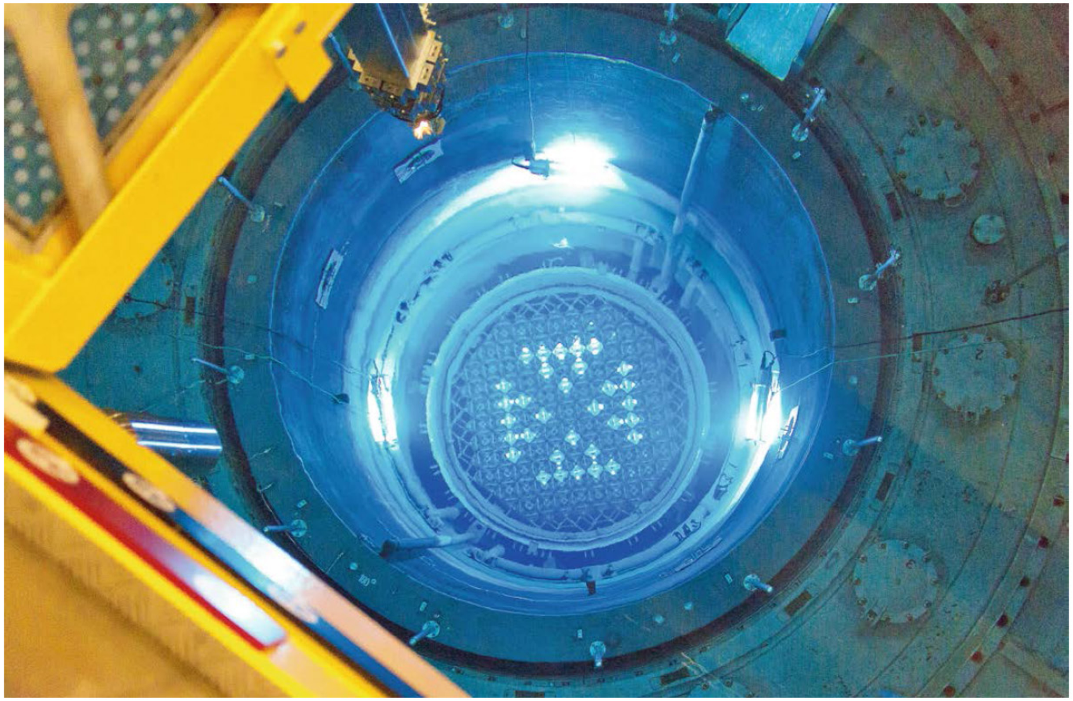
Conclusion

- There are various nuclear data libraries,
- There are various ways of evaluating data,
- There are various applications of libraries (energy, astrophysics, medical),

- All simulations cannot be better than the underlying nuclear data

- Is all of that important for specific applications ? See the next presentation

Kern im offenen Reaktor. Foto: KKM



Wir schaffen Wissen – heute für morgen