A Comparison of Sensitivity/Uncertainty Methodologies for the Tritium Production in

1) the HFTM/IFMIF Specimen Cells
&
2) measurements in Tritium activity in HCLL TBM mock-up LiPb

O. Cabellos[1,2], C.J. Diez[2], J.S. Martínez [2]

[1] ***Instituto de Fusión Nuclear***
[2] ***Departamento de Ingeniería Nuclear***

Universidad Politécnica de Madrid (UPM)

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OUTLINE

1. **Motivation of this presentation**
   - HFTM/IFMIF Specimen Cells
   - Measurements of tritium activity in HCLL TBM mock-up LiPb
2. **Error propagation techniques for activation**
   - Sensitivity/Uncertainty analysis
   - Monte Carlo method
3. **Nuclear Data Uncertainties**
   - ^{23}Na and ^{56}Fe
   - ^{7}Li and ^{6}Li
4. **Uncertainty Results**
   - HFTM/IFMIF Specimen Cells
   - Measurements of tritium activity in HCLL TBM mock-up LiPb
5. **Conclusion**

1. Motivation of this work: (1) HFTM/IFMIF Specimen Cells

The prediction of the tritium production is required for handling procedures of samples, safety&maintenance and licensing of the International Fusion Materials Irradiation Facility (IFMIF).

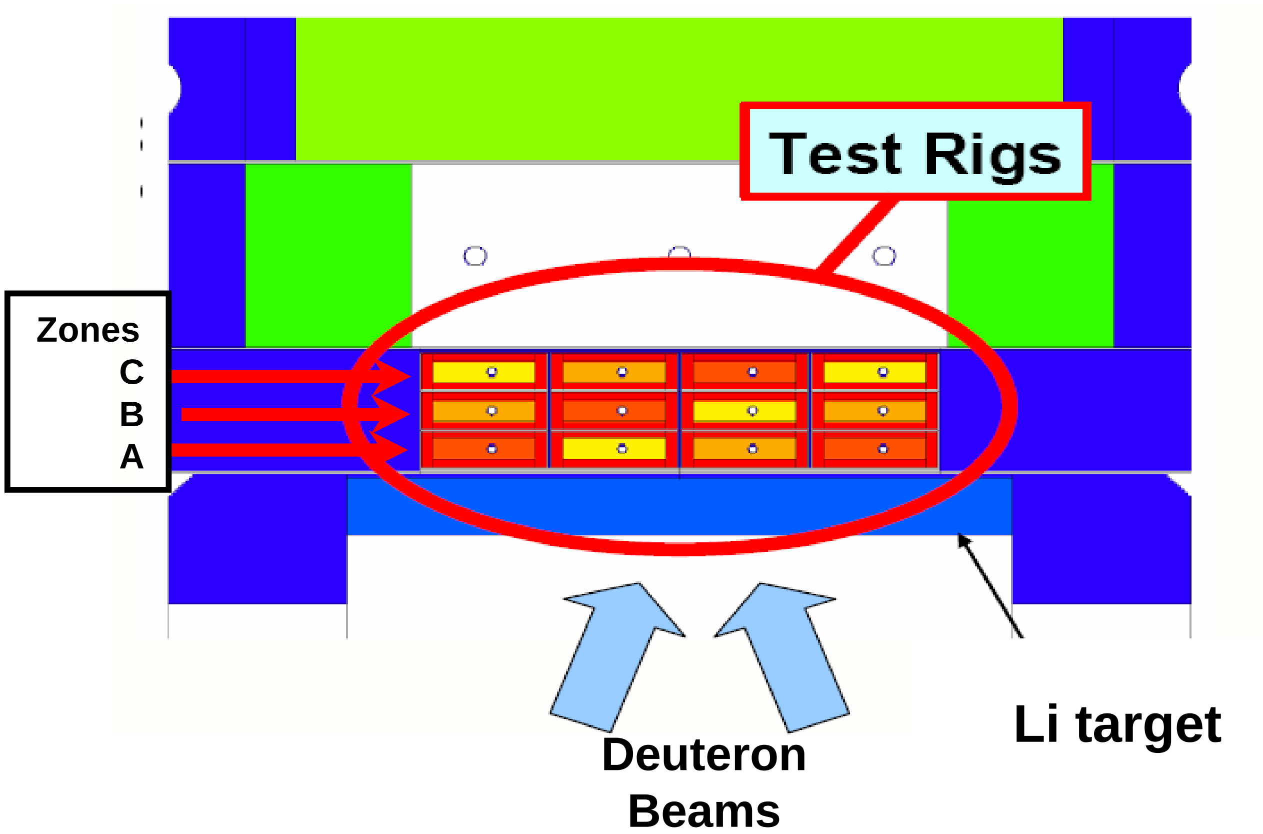

Table 1. Initial composition (in % atom fraction) for the three test rigs

Element	Rig-1	Rig-2	Rig-3
Cr	7.1	9.3	7.9
C	0.40	0.5	0.4
Mn	0.30	0.39	0.33
V	0.26	0.21	0.18
W	0.22	0.29	0.25
Ta	0.016	0.021	0.018
Fe	65.50	86.0	73.4
Na	18.0	2.3	12.0
K	8.30	1.0	5.5

1. Motivation of this work: (1) HFTM/IFMIF Specimen Cells

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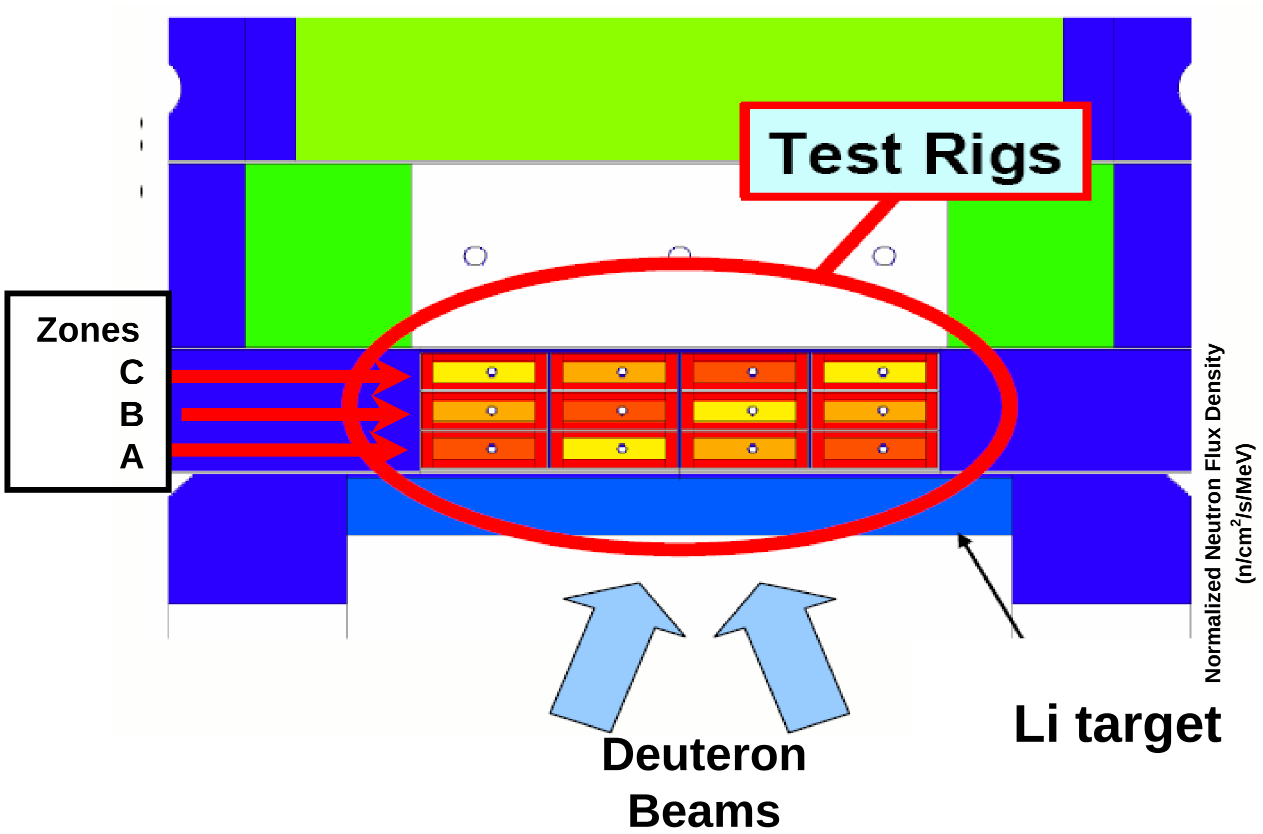
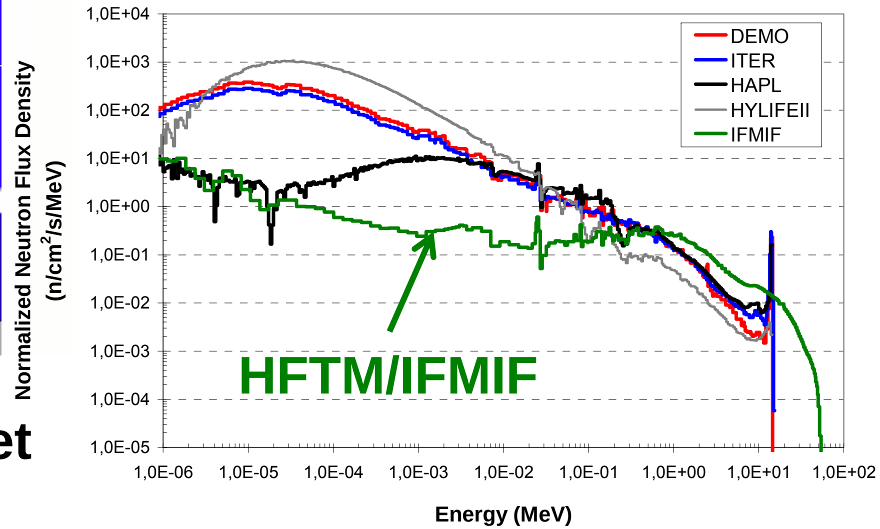


Figure 1. Neutron flux density in the high flux test module (HFTM) of IFMIF and the first wall of the magnetic (ITER and DEMO) and inertial (HYLIFE-II and HAPL) fusion energy neutron environments



1. Motivation of this work: (1) HFTM/IFMIF Specimen Cells

- **EFFDOC – 1054: "Estimation of the tritium production in the HFTM specimen cells"(by A. Klix) JEFF/EFF Meeting Paris, 18-20 Nov 2008**

Ci/fpy	1.0	2.1	1.5	1.0
Ci/fpy	2.3	1.9	1.6	2.3
Ci/fpy	2.2	2.1	3.4	2.2

Tritium production Ci / fpy (sum over all isotopes)

Total tritium production in all rigs is **23.4 Ci/fpy** (calc. with IEAF-2001)
Largest contribution from iron, but...

Ci/fpy	0.6	0.8	0.7	0.6
Ci/fpy	0.9	1.0	0.9	0.9
Ci/fpy	1.1	1.2	1.3	1.1

Tritium production Ci / fpy (sum over all isotopes)

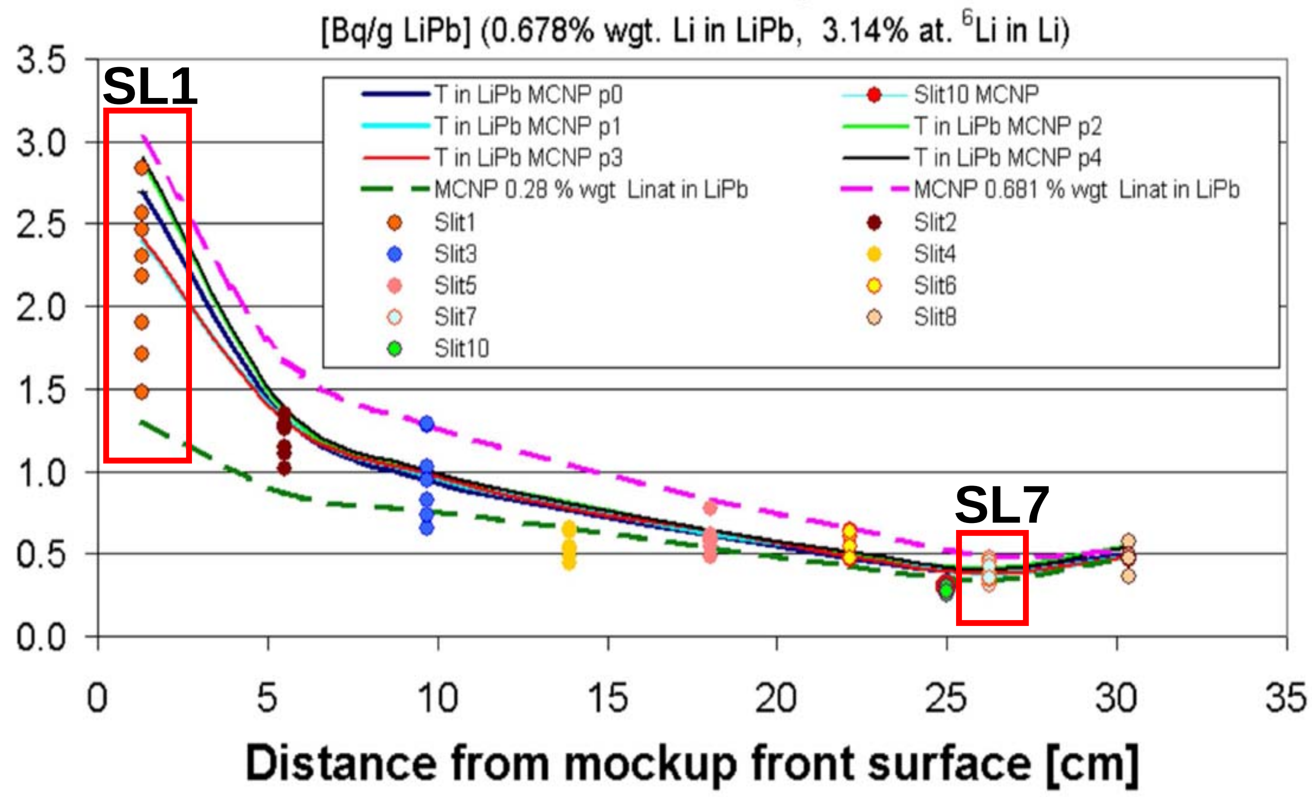
Total tritium production in all rigs is **11.2 Ci/fpy,**
calc. with EAF-2007 (Na, K, Fe) and IEAF-2001 (Rest)

1. Motivation of this work: (2) Measurem. of tritium activity

- **EFFDOC – 1113: "Measurements of tritium activity in HCLL TBM mock-up LiPb material irradiated in the Frascati experiment" (by W. W.Pohorecki) JEFF/EFF Meeting Paris, 31 May-2 June 2010**

- **T activity in LiPb mock-up material irradiated in Frascati: measurement and MCNP results.**

Figure 2: Slit 1-8, ^{3}H activity in LiPb



Average neutron energy
SL1: ~ 7.7 MeV
SL7: ~ 1.2 MeV

1. Motivation of this work: (3) XSs Uncertainties on TPR calc.

- **EFFDOC – 1135: "Analysis of the HCLL Blanket Mock-up Experiment" (by R. Villari et al.) JEFF/EFF Meeting Paris, 9-11 May 2011**

Uncertainties on TPR determination

- Proposed definitive uncertainty on C/E comparison

✓ experimental errors (Li-6)	3.7%
✓ uncertainty on FNG source intensity	3%
✓ Monte Carlo calculation statistics	< 1%
✓ cross sections	< 2%
✓ Pb-Li composition	1%*

$$\Delta\,(C/E) \sim 5.3\,\% \quad (1\sigma)$$

- As a general result C/E are close to one within the total combined uncertainties (~±10% at 2σ level)

**Sensitivity of TPR to Li6 content : -0.5%/%*

2. Error propagation techniques for activation

Goal: "to analyse how ND uncertainty is transmitted to N"

$$\frac{d}{dt}N = AN \qquad N = (N_1, N_2, \dots) \quad \sigma = (\sigma_1, \sigma_2, \dots) \quad \Rightarrow \quad N_i = N_i(\sigma)$$

1) Sensitivity / Uncertainty Analysis (S/U)

- Method based on the first order Taylor series to estimate uncertainty indices for each reaction cross section in a continuous irradiation scenario ***(linear approximation)***

2) Monte Carlo Uncertainty Analysis (MC)

- To treat the global effect of all cross sections uncertainties in activation calculations, we have proposed an uncertainty analysis methodology based on Monte Carlo random sampling of the cross sections

- Assignment of a Probability Density Function (PDF) to each cross section

2.1. Sensitivity/Uncertainty Analysis

We assume only XS uncertainties:

$$N_i = N_i(\sigma, \not{\lambda}, \not{\phi}(E), \not{N}_0) \quad \Rightarrow \quad N_i(\sigma) \approx N_i(\sigma_0) + \sum_{j=1}^{m} \left[\frac{\partial N_i}{\partial \sigma_j}\right]_{\sigma_0} (\sigma_j - \sigma_{j0}) + \ldots$$

$$\underbrace{\frac{N_i(\sigma) - N_i(\sigma_0)}{N_i(\sigma_0)}}_{e_i} \approx \sum_{j=1}^{m} \underbrace{\frac{\sigma_{j0}}{N_i(\sigma_0)} \left[\frac{\partial N_i}{\partial \sigma_j}\right]_{\sigma_0}}_{\rho_{ij}} \underbrace{\frac{(\sigma_j - \sigma_{j0})}{\sigma_{j0}}}_{\varepsilon_j}$$

e_i: Relative error in N_i due to changes in cross-sections

ρ_{ij}: Cross-section sensitivity coefficient (FSAP, ASAP, …)

ε_j: Relative error in cross-sections

$$e_i = \rho_{i1}\varepsilon_1 + \rho_{i2}\varepsilon_2 + \cdots + \rho_{im}\varepsilon_m$$

$$Var[e_i] = \rho_{i1}^2\Delta_1^2 + \rho_{i2}^2\Delta_2^2 + \cdots + \rho_{im}^2\Delta_m^2$$

$$Var[e_i] = \rho_i^T V \rho_i$$

$$\rho_i = (\rho_{i1}, \quad \rho_{i2}, \quad \cdots \quad \rho_{im})$$

(sandwich formula)

$$Var(\varepsilon) = V$$

Information obtained processing ND

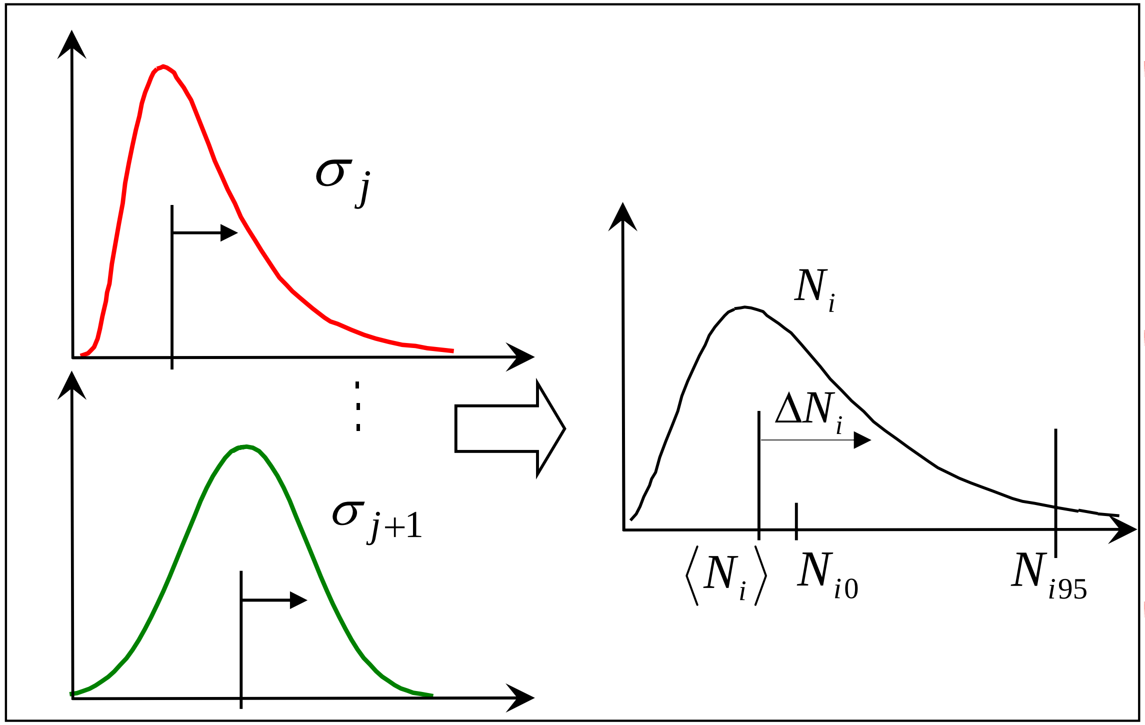
2.2. Monte Carlo Method

- We use simultaneous random sampling of all the XS PDFs involved in the problem. PDF is assigned to each σ_j: $\sigma_j \rightarrow N(\sigma_{j0}, \mathrm{var}(\sigma_j)) \Longrightarrow \varepsilon_j \rightarrow N(0, \Delta_j^2)$

$$\log\begin{pmatrix}(\sigma_1/\sigma_{10})\\(\sigma_2/\sigma_{20})\\\vdots\\(\sigma_m/\sigma_{m0})\end{pmatrix} \rightarrow N(0,V)$$

$\Rightarrow$ For large values of Δ_j, σ_j could be negative!

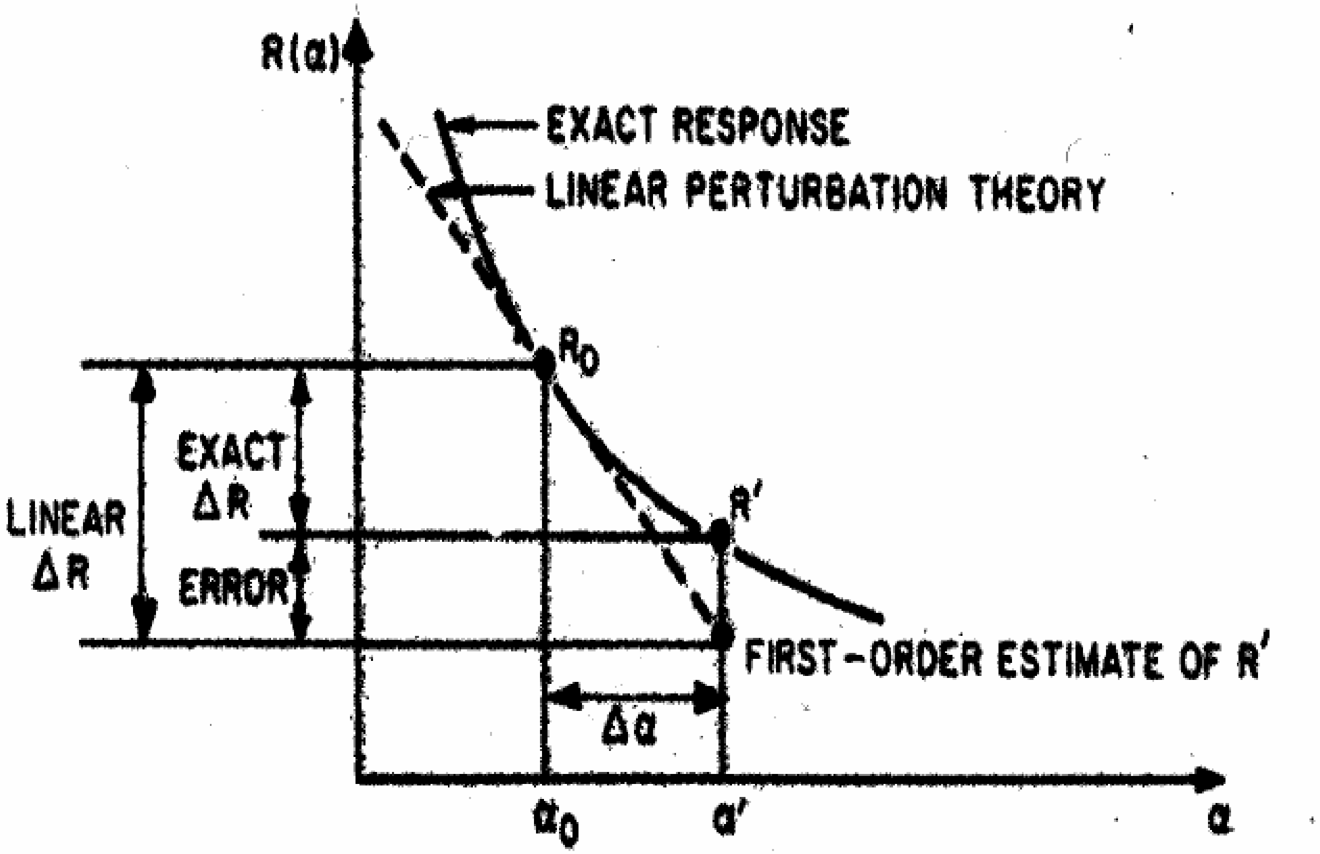
- PDF assumed to be lognormal: $\log(\sigma_j/\sigma_{j0}) = \log(1+\varepsilon_j) \approx \varepsilon_j \rightarrow N(0, \Delta_j^2)$



- From the sample of the random vector σ, $\sigma = (\sigma_1 ..., \sigma_j ..., \sigma_m)$ the matrix **A** is computed and the vector of nuclide quantities ***X*** is obtained $N = (N_1 ..., N_i ..., N_n)$
- Repeating the sequence, we obtain a sample of isotopic concentration vectors. The statistic estimators of the sample can be estimated
- Enables to investigate the global effect of the complete set of $\Delta\sigma$ on N

2.3 S/U versus Monte Carlo

Applicability of 1st Taylor-series expansion



- ✓ "The deterministic S/U approach should be used wherever it provides sufficiently accurate results"
- ✓ "Normally, this will be the case when errors are relatively small and the conditions not extreme"

3. Nuclear Data Uncertainties (EAF/UN)

Review of available uncertainty cross-section data

➔ **Activation-oriented nuclear data libraries**

- **FENDL UN/A-2.0, EAF2003/5/7/10-UN**

e.g.: EAF2007 Na^{23}(n,T)

```
NA- 23N,T                                                         112333105
 1.10230E+4 2.2792E+01          0          0          0          1112333105
 0.0000E+00 0.0000E+00          0        105          0          1112333105
 0.0000E+00 0.0000E+00          0          1          8          4112333105
 1.0000E-05 0.0000E+00 1.1150E+07 4.4100E-02 2.0000E+07 4.4100E-02112333105
 6.0000E+07 0.0000E+00                                            112333105
```

E_i (eV) $\Delta^2_{I=1,EAF}$ E_{i+1}(eV)

(relative error, Δ)~ $\Delta_{I=1,EXP}= \Delta_{I=1,EAF}/3 = 7\%$

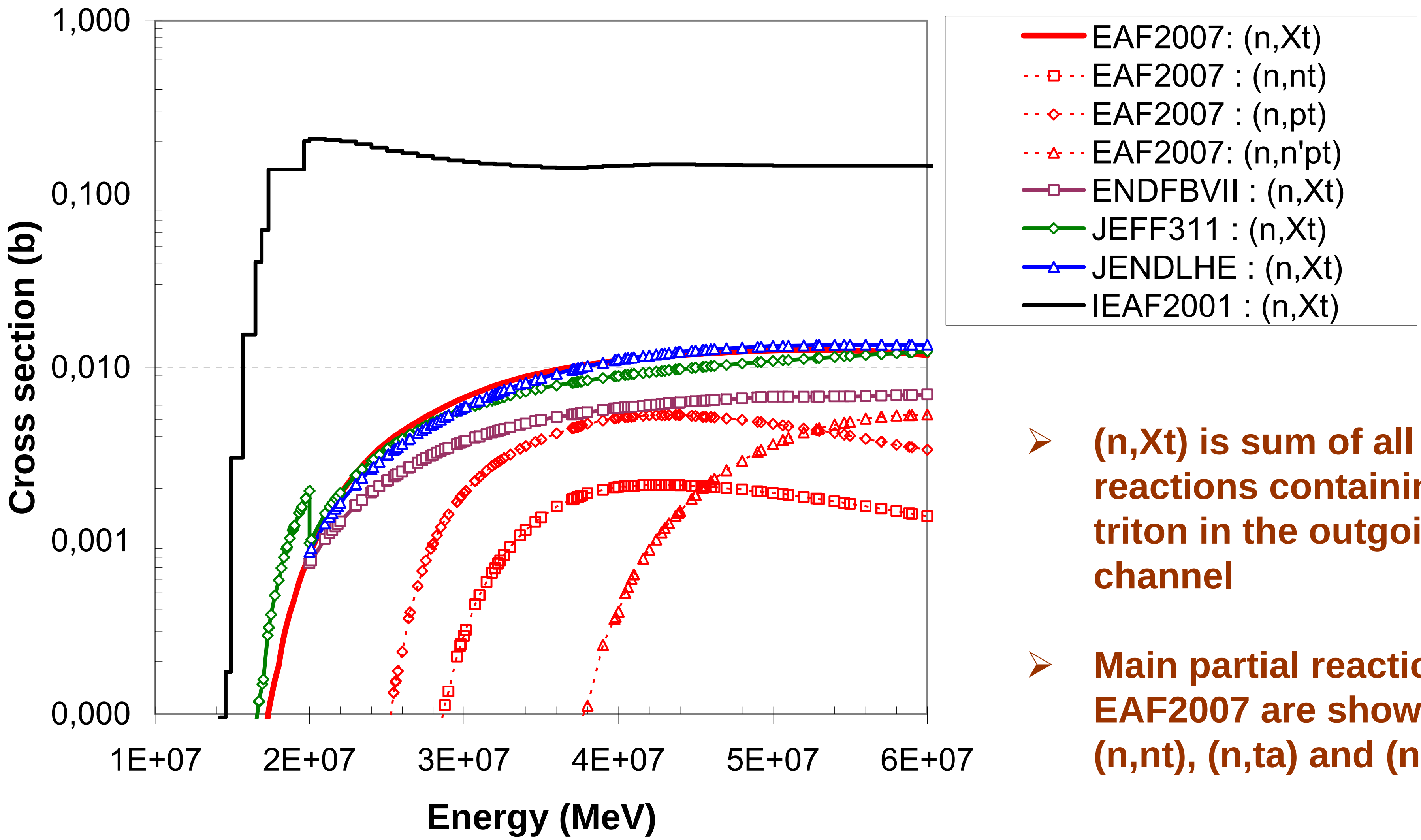
➢ **The PDF for each XS is assumed to be lognormal: $\log(\sigma/\sigma_0) \sim N(0,\Delta)$**

- **σ_0= the best-estimate XS value contained in the EAF-XS library**
- **$\Delta = \Delta^2_{LIM}/9$, being Δ^2_{LIM} the variance included in the EAF-UN library**

e.g.: FISPACT2007 Manual	**$\log(\sigma_{exp}/\sigma_{calc}) \sim N(0,\Delta)$, and $f=1+\Delta$** **$\sigma_{cal}/f < \sigma < \sigma_{cal}*f$**

3.1 HFTM/IFMIF Tritium prediction cross-sections

Figure 3. **Tritium production cross section for Fe54**

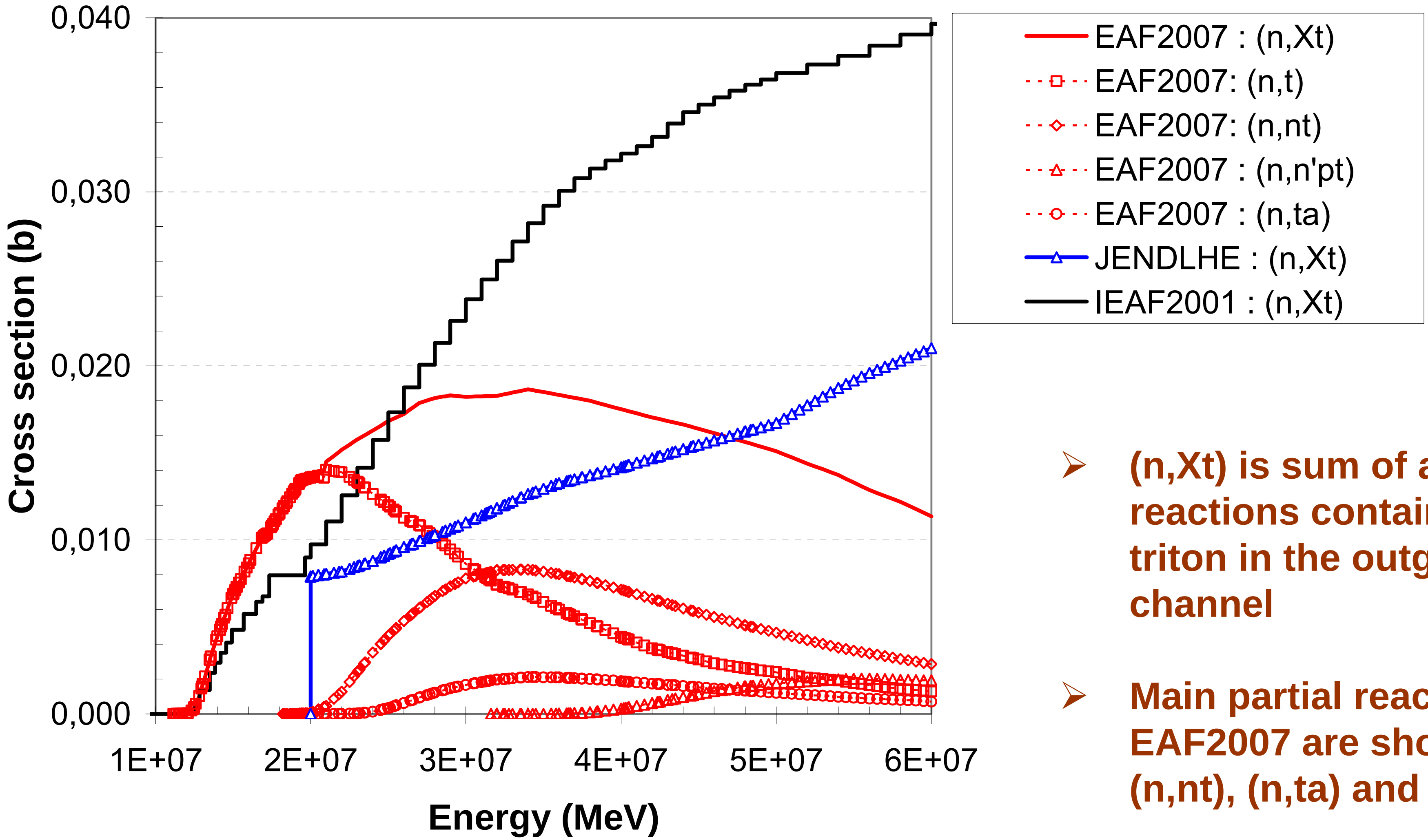


- **(n,Xt) is sum of all reactions containing a triton in the outgoing channel**
- **Main partial reactions for EAF2007 are shown: (n,t), (n,nt), (n,ta) and (n,npt).**

- **Fe54: Large discrepancy between IEAF2001 and the other evaluated ND libraries.**

3.1 HFTM/IFMFIF Tritium prediction cross-sections

Figure 4. **Tritium production cross section for Na23**

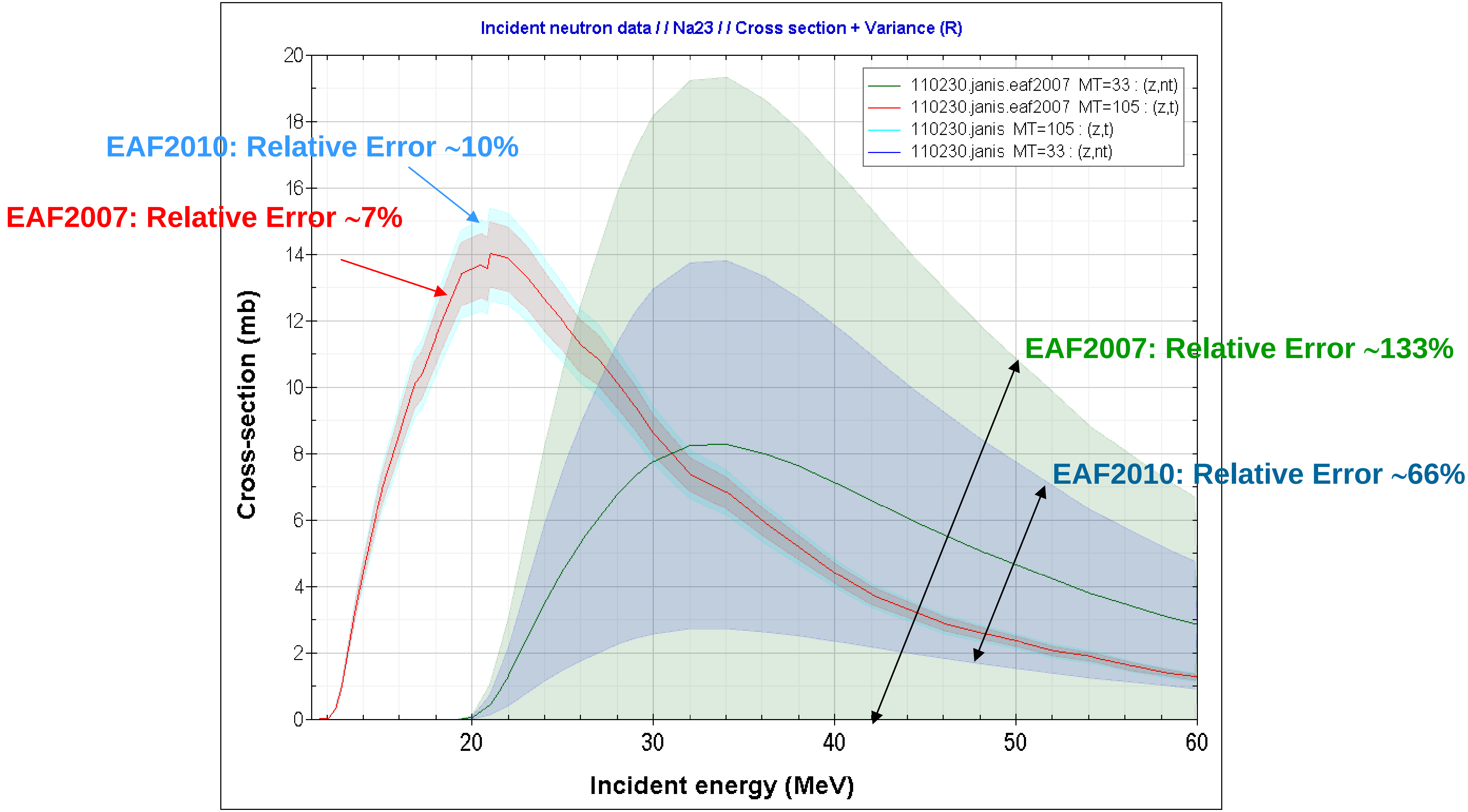


- **(n,Xt) is sum of all reactions containing a triton in the outgoing channel**
- **Main partial reactions for EAF2007 are shown: (n,t), (n,nt), (n,ta) and (n,npt).**

- **Na23: many evaluated data libraries do not contain tritium producing reactions, and large discrepancy between libraries**

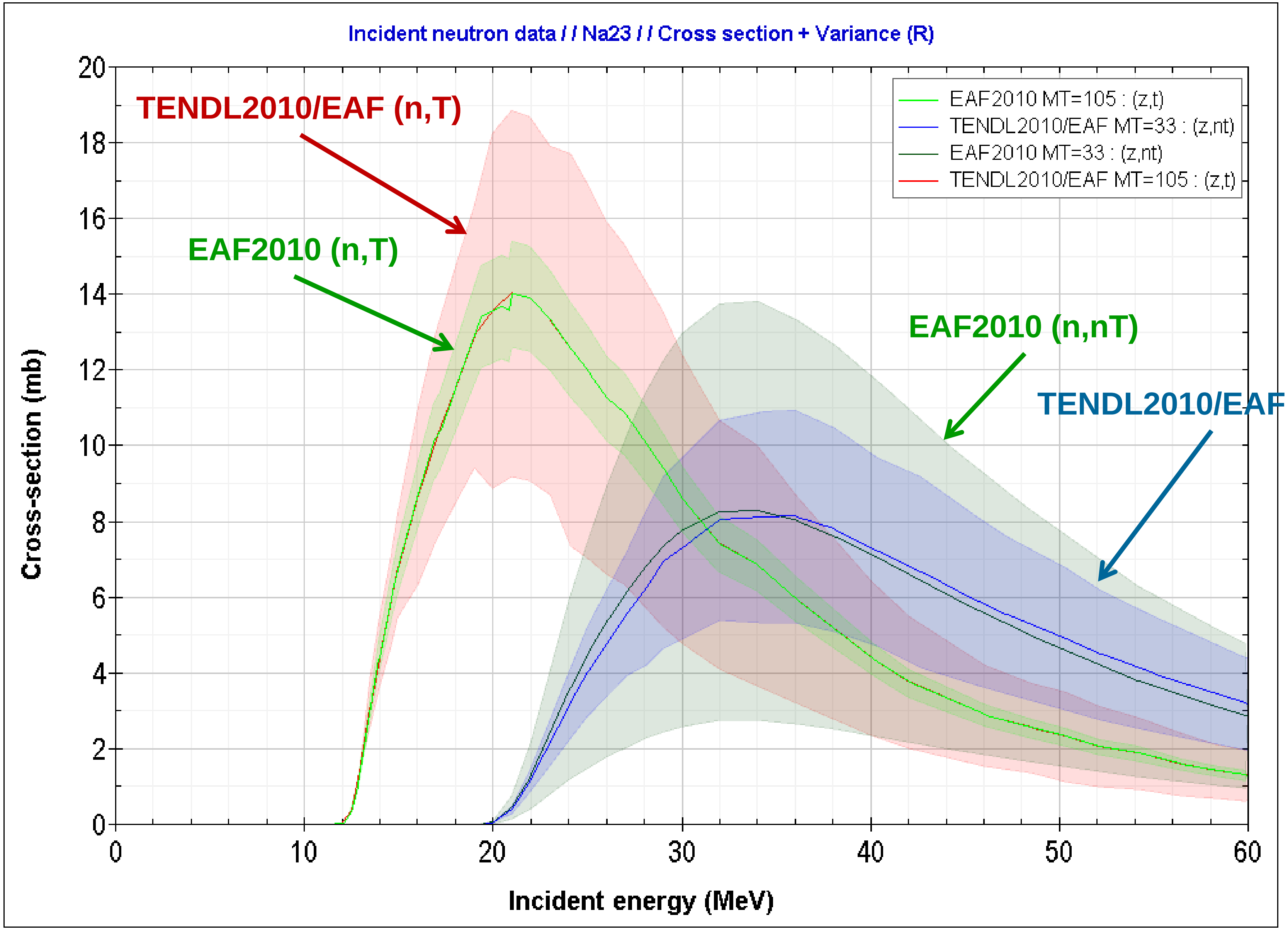
3.1 Uncertainties in Tritium prediction: EAF2007&2010/UN

Figure 5. ^{23}Na (n,T) and (n,nT) cross-sections: EAF2007/2010

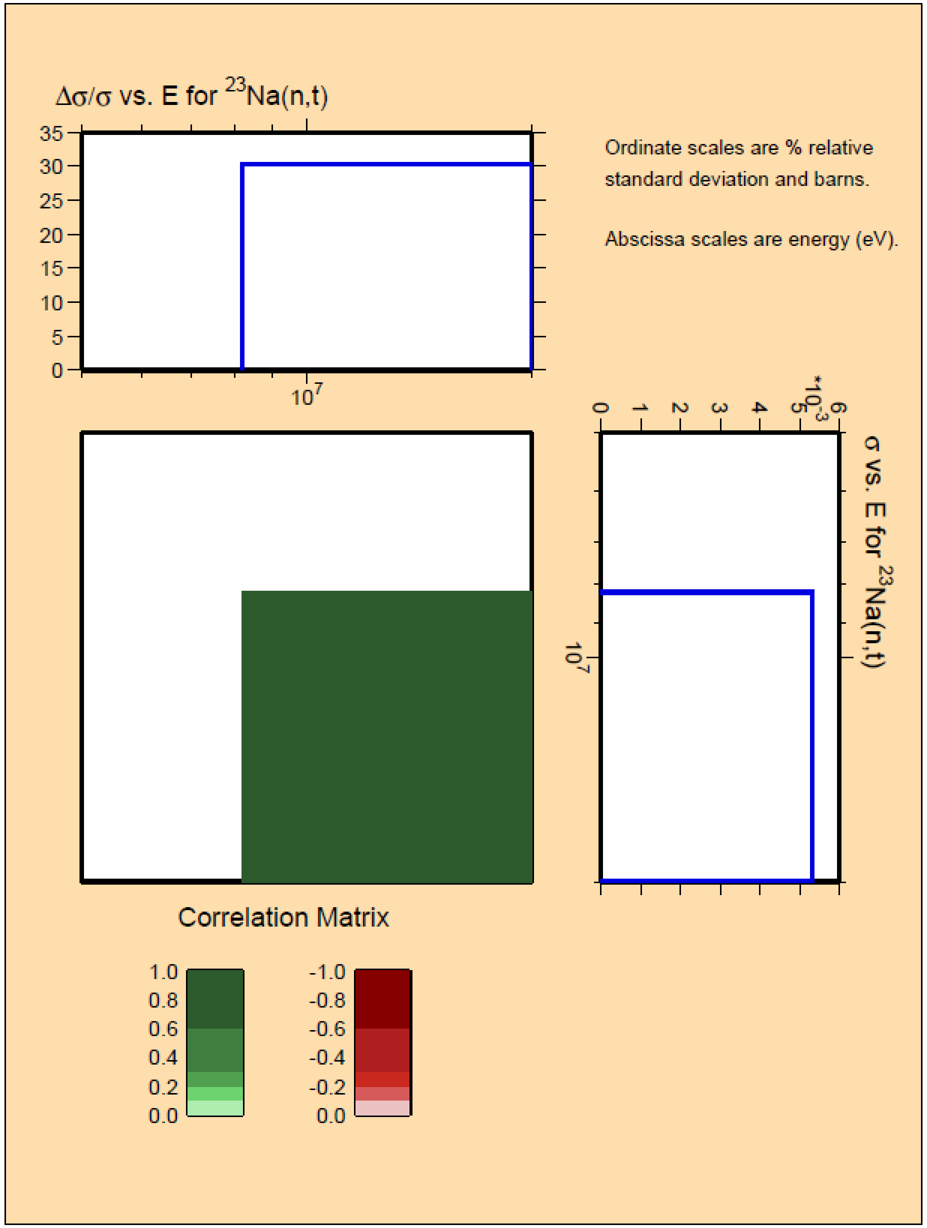


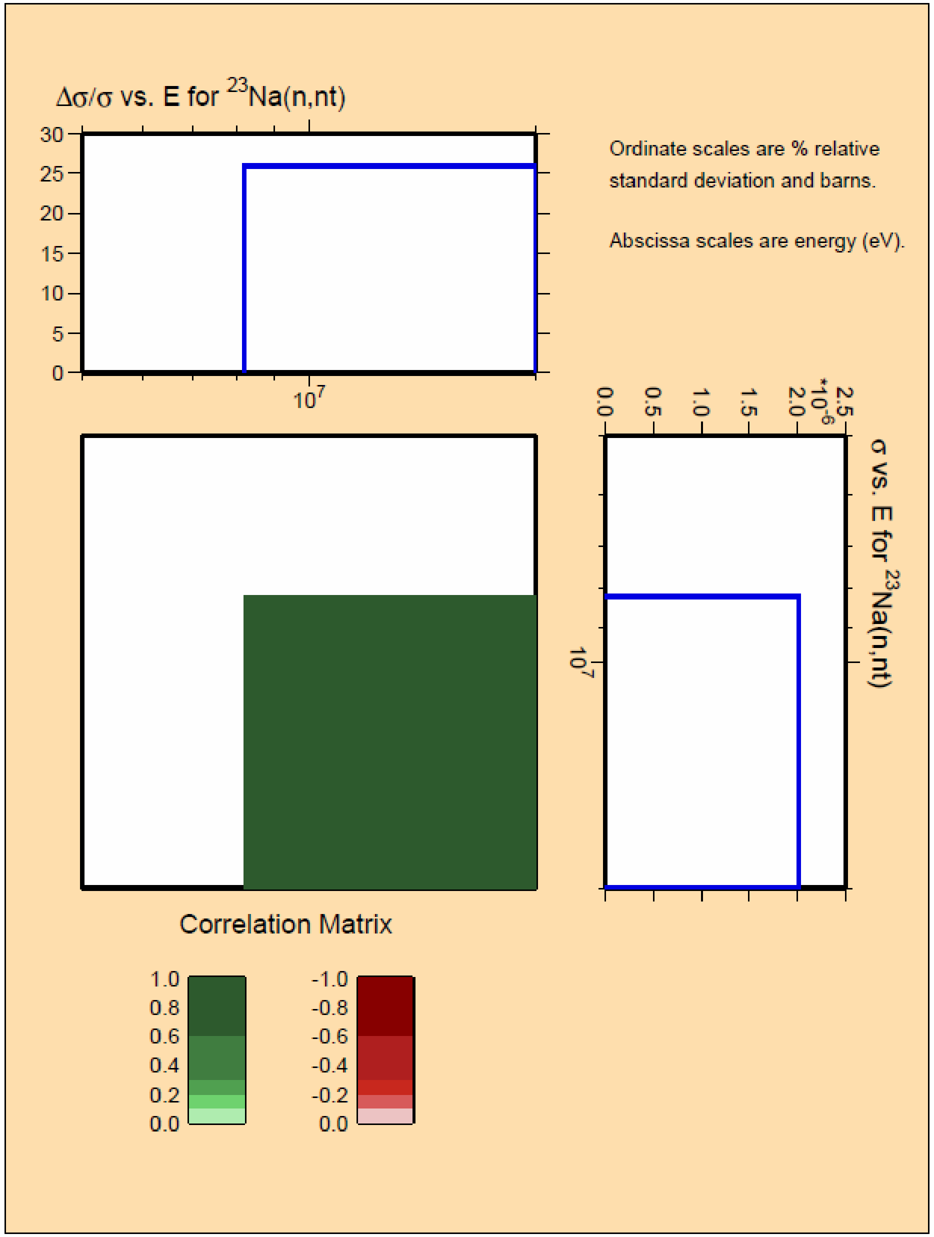
3.1 TENDL2010: ^{23}Na(n,xT)

Figure 6. ^{23}Na (n,T) and (n,nT) cross-sections: EAF2010 and TENDL2010/EAF



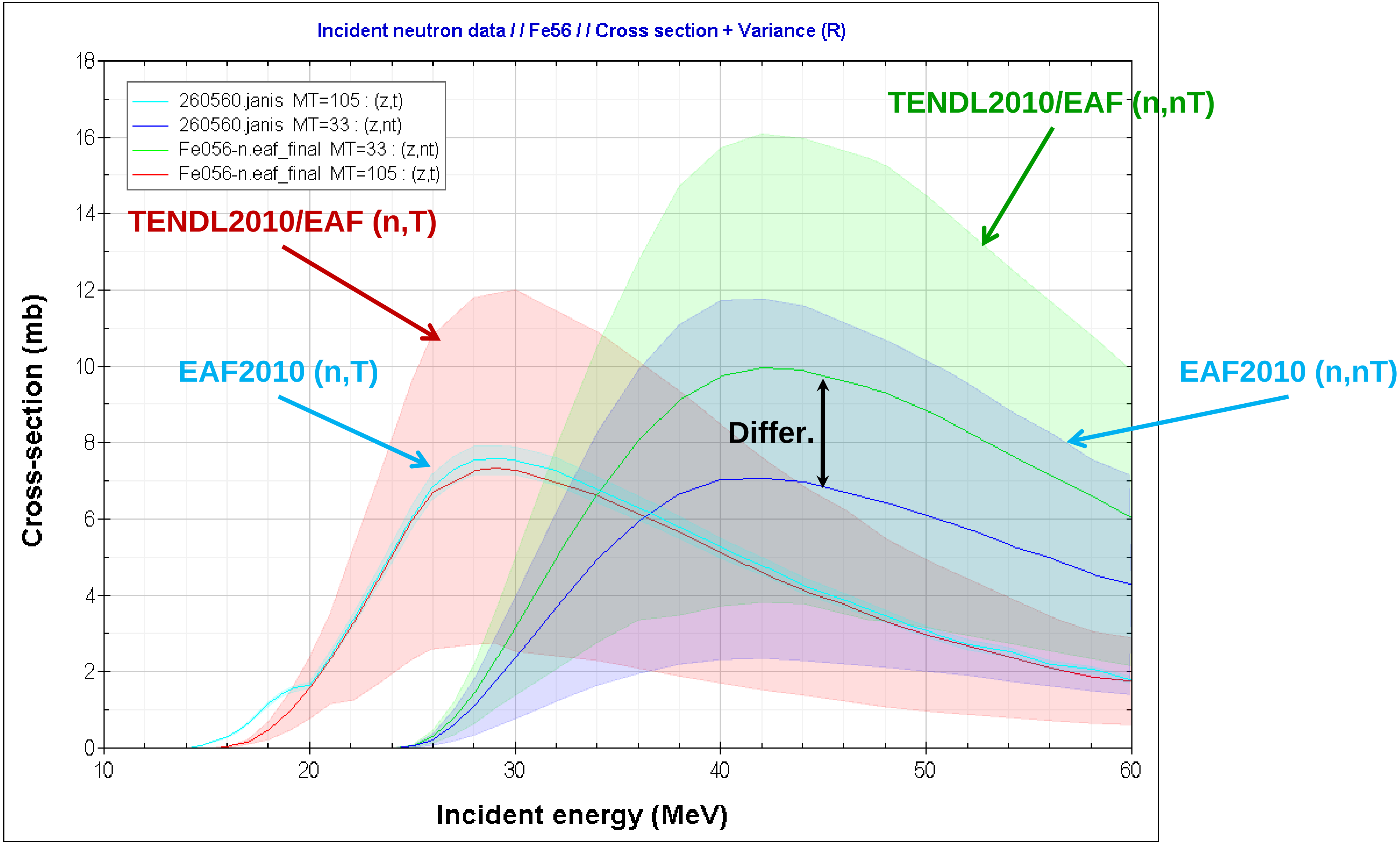
3.1 TENDL2010: $^{23}Na(n,xT)$



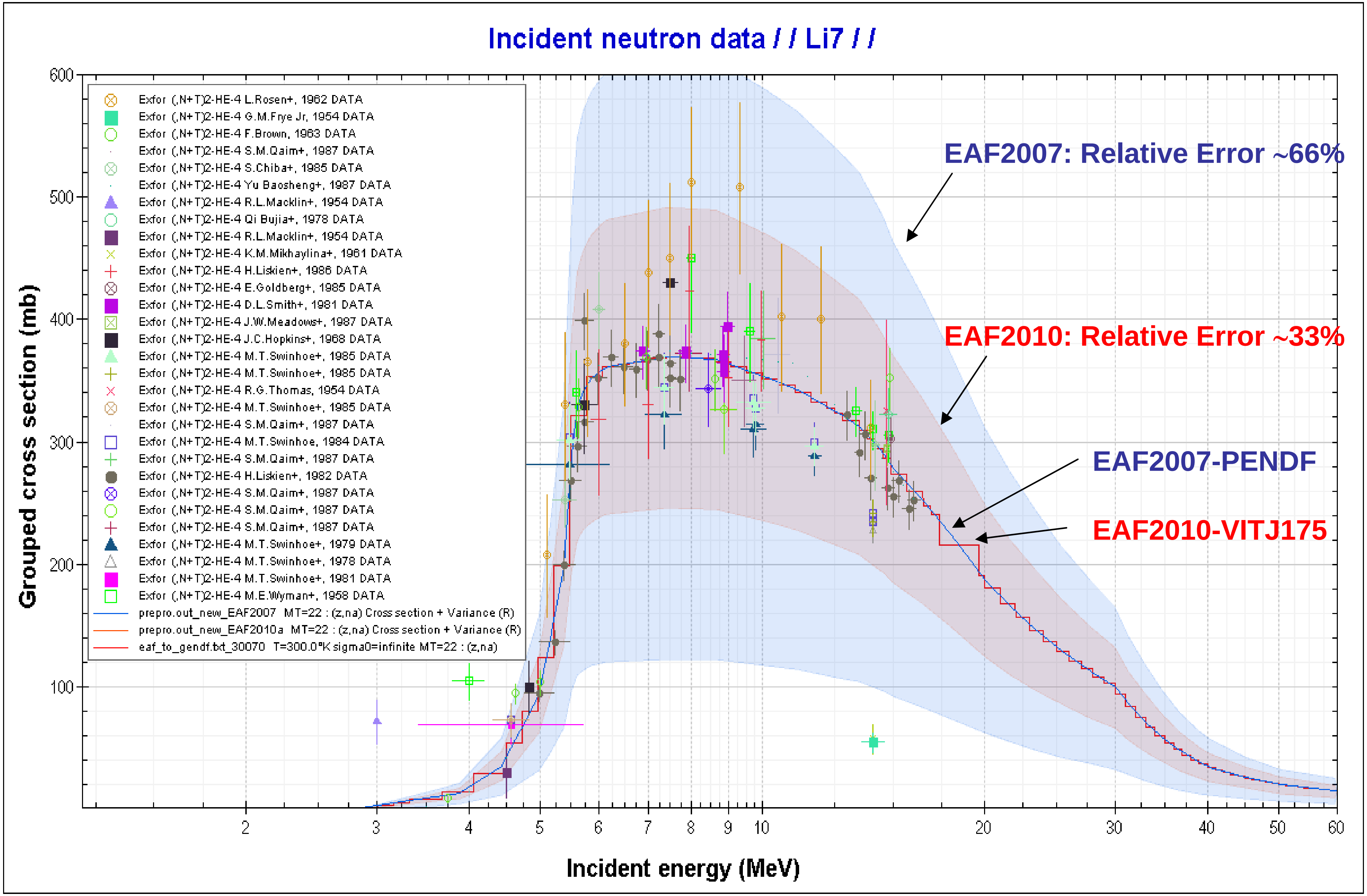


3.1 TENDL2010: $^{56}Fe(n,xT)$

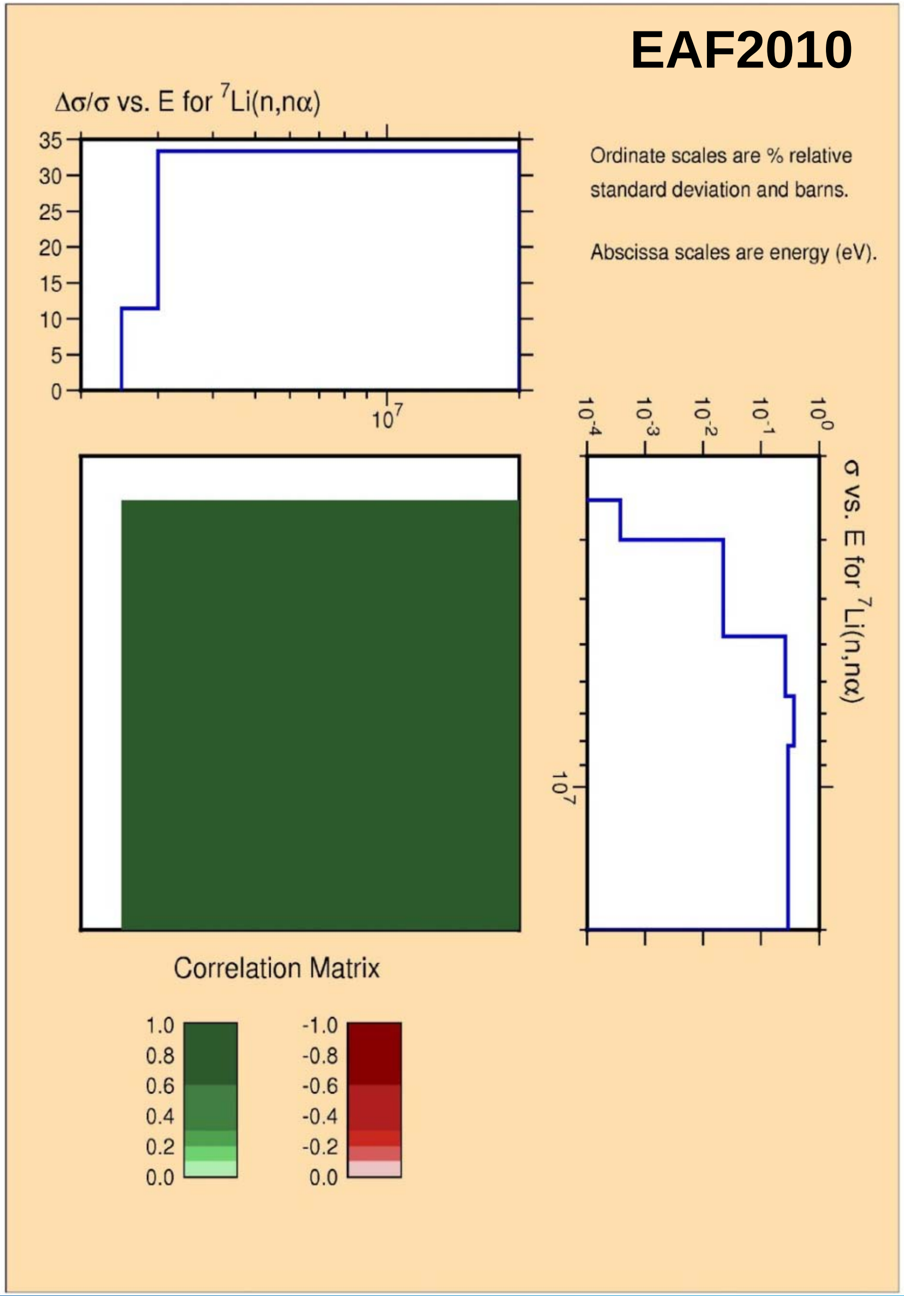
Figure 7. ^{56}Fe (n,T) and (n,nT) cross-sections: EAF2010 and TENDL2010/EAF



3.2 EAF 2010&2007 Uncertainties: ^{7}Li(n,T)



3.2 EAF 2010&2007: Covariance matrix: ^{7}Li(n,T)



- Given ***V*** the G-by-G variance matrix of the relative XSs vector, **the variance Δ^2 of the relative spectrum-averaged cross section** is:

$$\Delta^2 = \omega^T V \omega \quad \text{; with} \quad \omega = \left[\frac{\phi_1}{\bar{\phi}}\frac{\sigma_1}{\sigma^{eff}}, \cdots, \frac{\phi_G}{\bar{\phi}}\frac{\sigma_G}{\sigma^{eff}}\right]^T$$

- Assuming $\Delta^2_{I=1,EAF}$ (relative error, Δ)

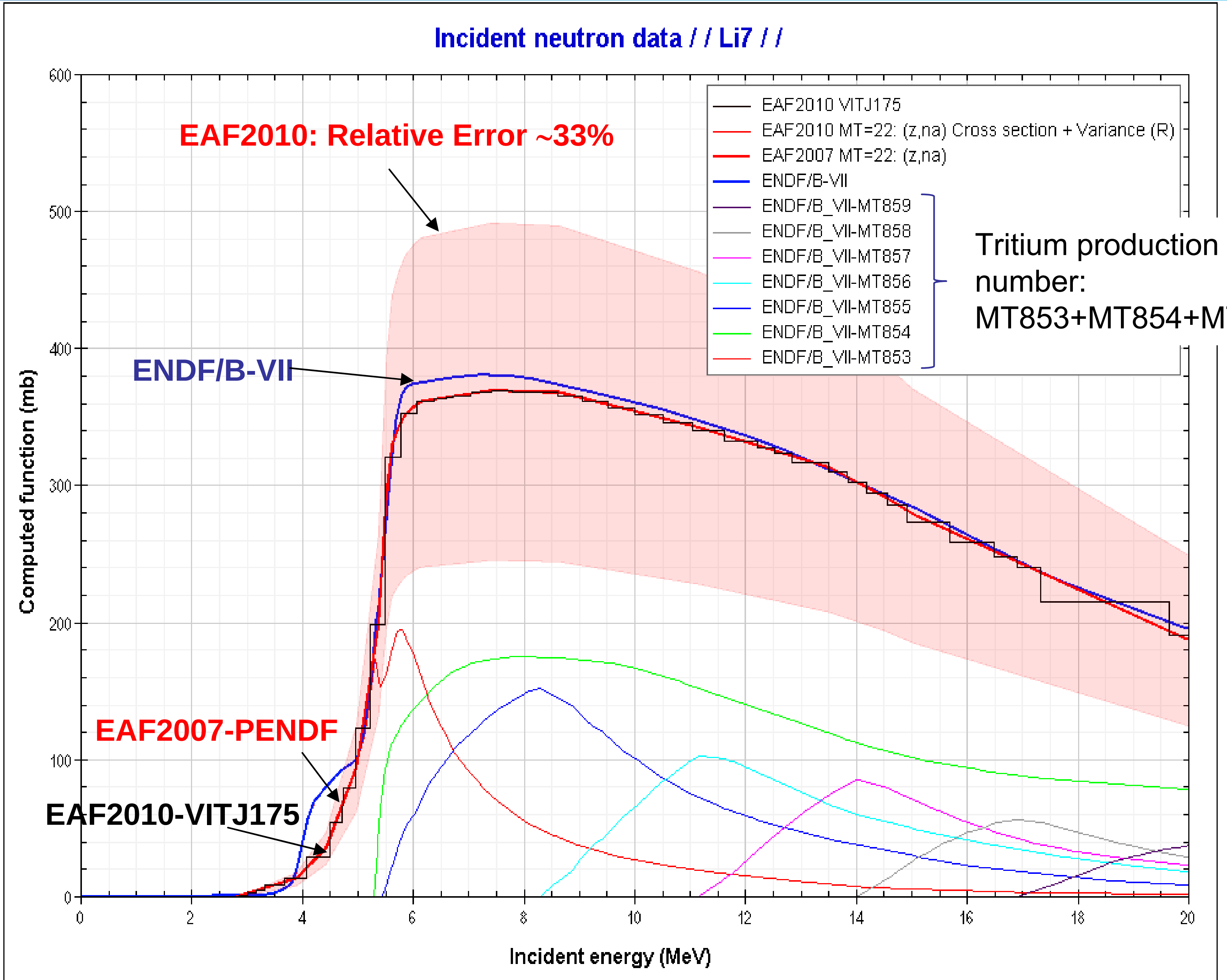
  $\rightarrow \Delta_{I=1,EXP} = \Delta_{I=1,EAF}/3$

1group uncertainty for SL1

Uncert_1group (EAF2007) = Δ	$\Delta^2_{EAF2007}$	Relative Exp Error (%)
Li6(n,T)He4	0.01	3.33
Li7(n,na)T	4.00	66.67
F19(n,T)	0.36	20.00
…		
F19(n,nT)	16.00	133.33

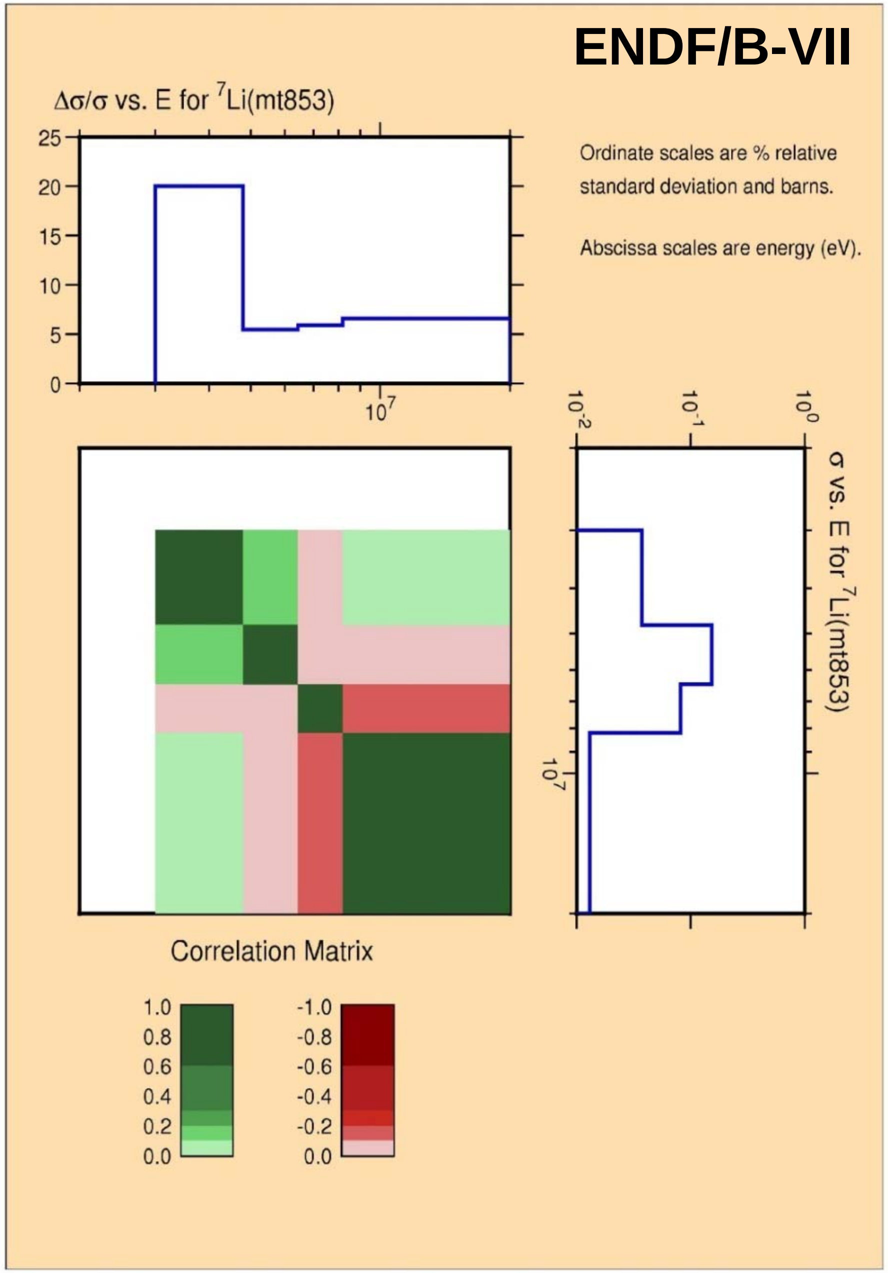
Uncert_1group (EAF2010) = Δ	$\Delta^2_{EAF2010}$	Relative Exp Error (%)
Li6(n,T)He4	0.01	3.33
Li7(n,na)T	1.00	33.33
F19(n,T)	0.36	20.00
…		
F19(n,nT)	4.00	66.67

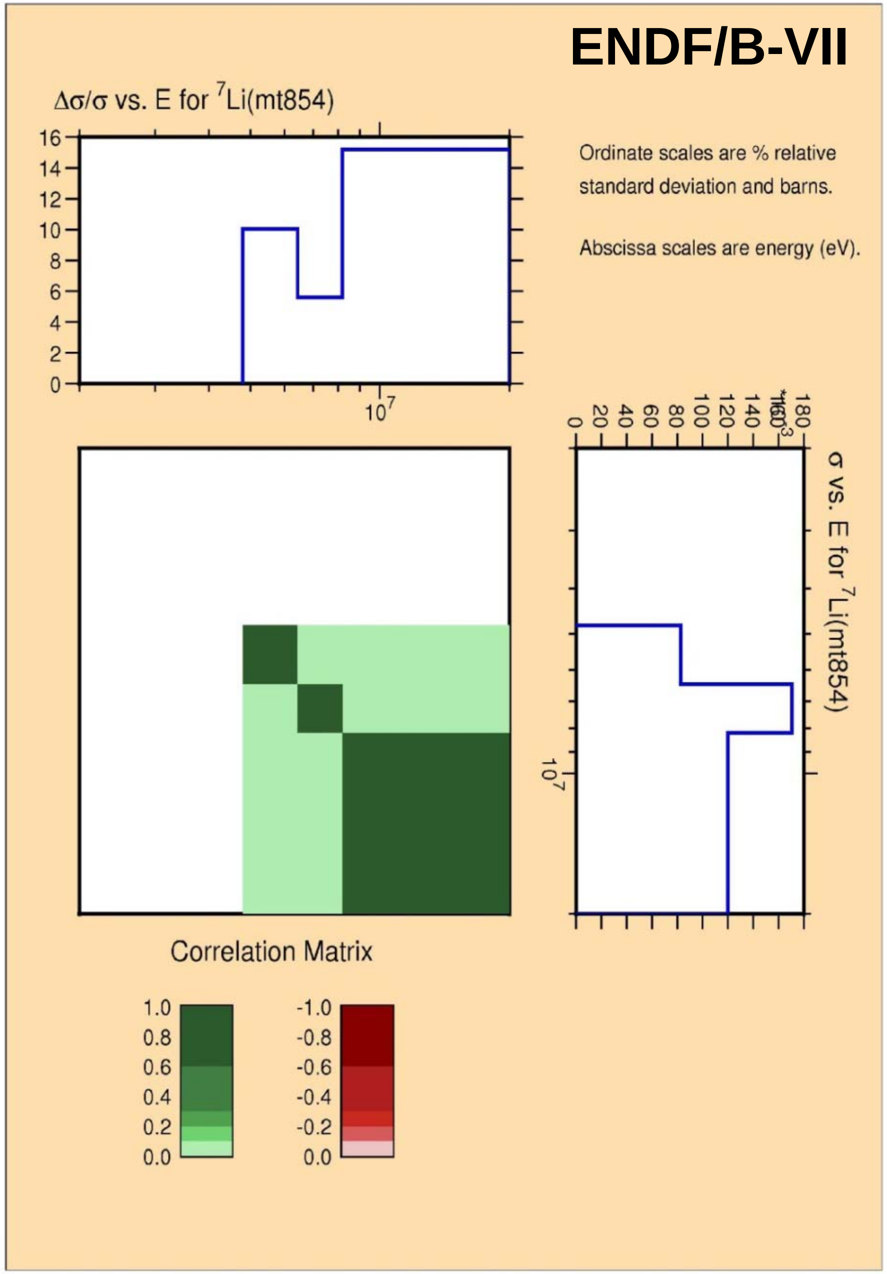
3.2 ENDF/B-VII vs EAF2010: ^{7}Li(n,T)



Tritium production is not in one MT number:
MT853+MT854+MT855+ …=(n,n'at)

3.2 ENDF/B-VII Covariance Matrix in 44g: ^{7}Li(n,T)





3.2 ENDF/B-VII: in Δ_{1g} for SL1: ^{7}Li (n,T)

Cross-sections collapsed in 1 group with SL1

	MT853	MT854	MT855	MT856	MT857	MT858	MT859
XS MTs_1g	7.12E-03	4.76E-02	1.48E-02	2.10E-02	2.71E-02	1.53E-02	2.19E-33
MTs/MTtotal	0.05	0.36	0.11	0.16	0.20	0.12	0.00

Relative cocariance matrix

	MT853	MT854	MT855	MT856	MT857	MT858	MT859
MT853	2.49E-03	0.00E+00	2.02E-04	-2.17E-06	-3.54E-05	-2.22E-05	-5.78E-20
MT854	0.00E+00	1.15E-03	-3.16E-04	-4.86E-04	-6.74E-04	-3.38E-04	-7.81E-18
MT855	2.02E-04	-3.16E-04	1.56E-03	1.70E-04	-1.42E-04	-7.21E-05	-5.10E-19
MT856	-2.17E-06	-4.86E-04	1.70E-04	2.07E-03	-2.60E-04	-1.25E-04	-1.36E-18
MT857	-3.54E-05	-6.74E-04	-1.42E-04	-2.60E-04	2.11E-03	2.24E-04	-2.97E-18
MT858	-2.22E-05	-3.38E-04	-7.21E-05	-1.25E-04	2.24E-04	3.16E-03	3.10E-17
MT859	-5.78E-20	-7.81E-18	-5.10E-19	-1.36E-18	-2.97E-18	3.10E-17	0.00E+00

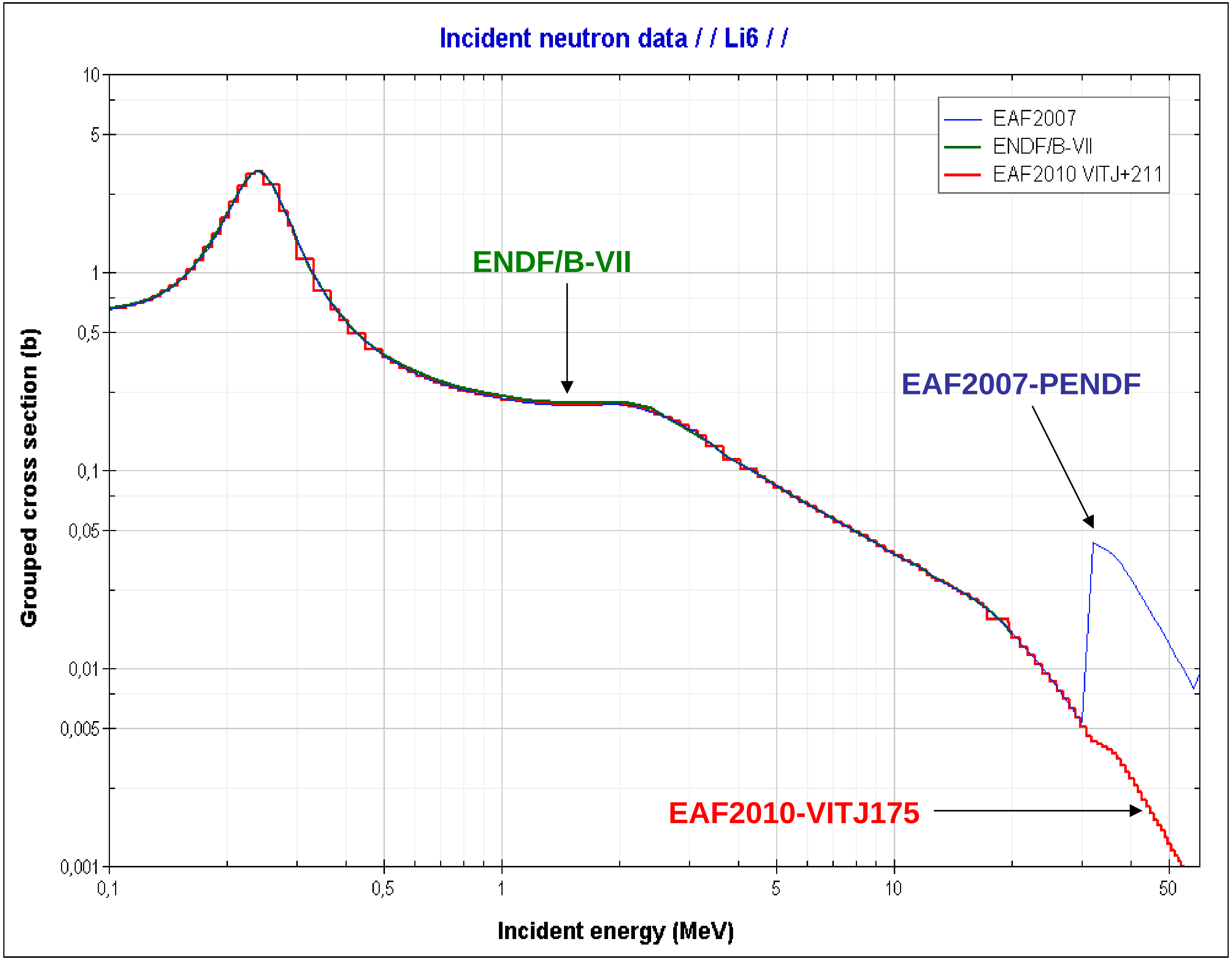
Relative error(%) covariance matrix

	MT853	MT854	MT855	MT856	MT857	MT858	MT859
MT853	4.99	0.00	1.42	0.15	0.59	0.47	0.00
MT854	0.00	3.39	1.78	2.20	2.60	1.84	0.00
MT855	1.42	1.78	3.95	1.31	1.19	0.85	0.00
MT856	0.15	2.20	1.31	4.55	1.61	1.12	0.00
MT857	0.59	2.60	1.19	1.61	4.59	1.50	0.00
MT858	0.47	1.84	0.85	1.12	1.50	5.62	0.00
MT859	0.00	0.00	0.00	0.00	0.00	0.00	0.00

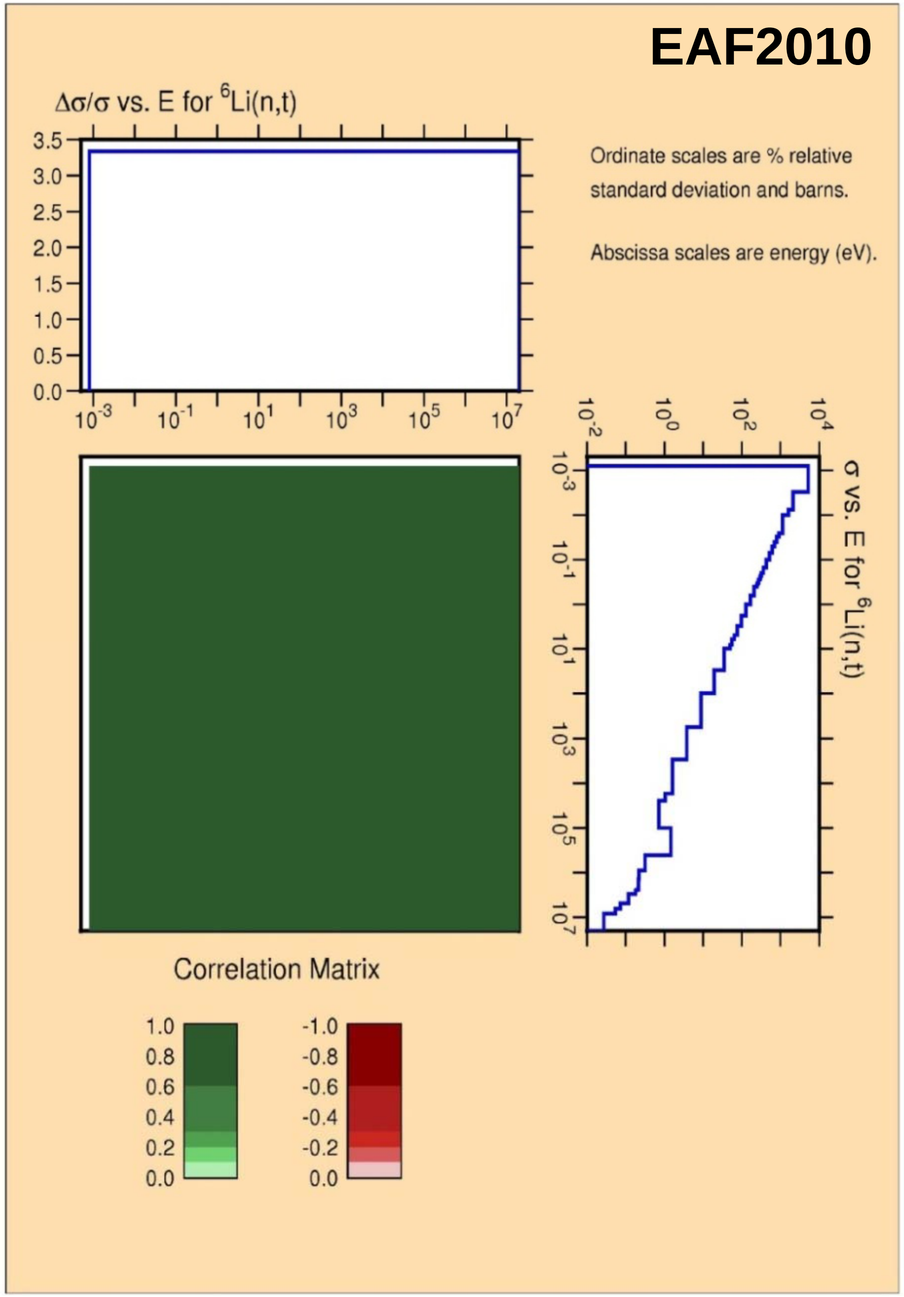
Rel. Err. in 1g (%)	1.17

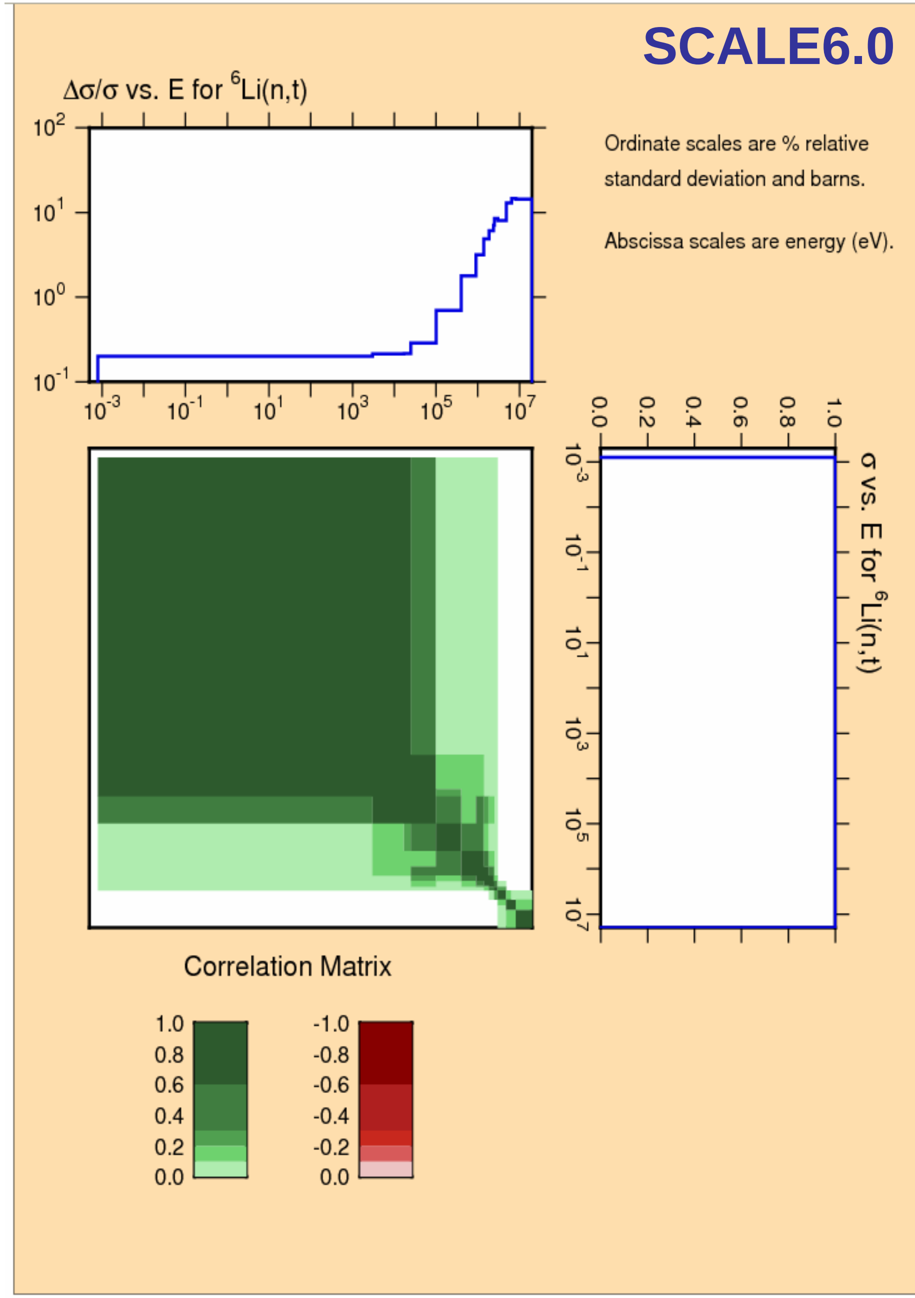
The relative error in 1group “lumped XS“ is only **1.17%** !!!

3.2 ENDF/B-VII vs EAF2010: ^{6}Li(n,T)

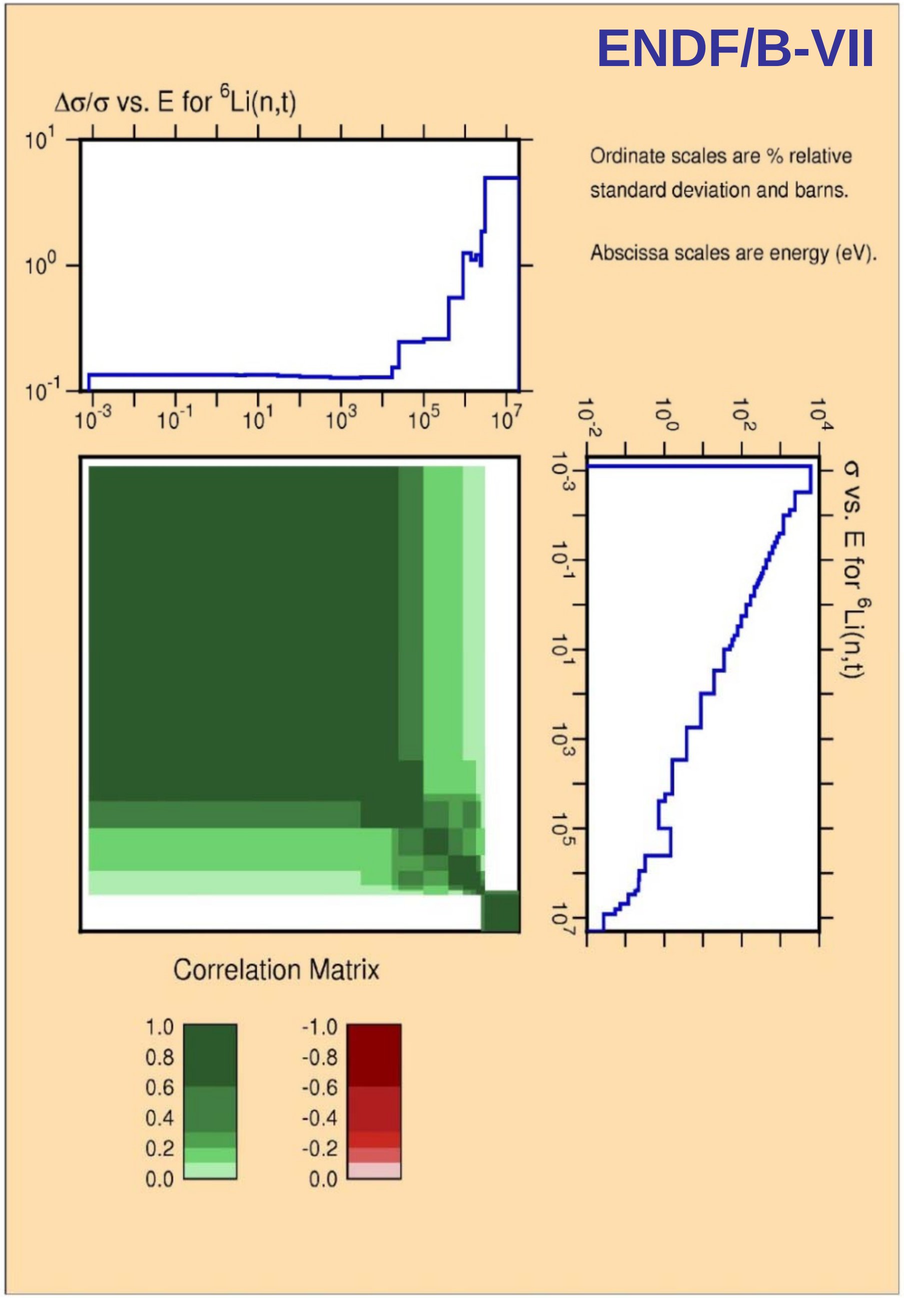


3.2 EAF 2010/2007 and SCALE6.0: Covariance matrix: $^{6}Li(n,T)$





3.2 ENDF/B-VII : Covariance Matrix in 44g: ^{6}Li(n,T)

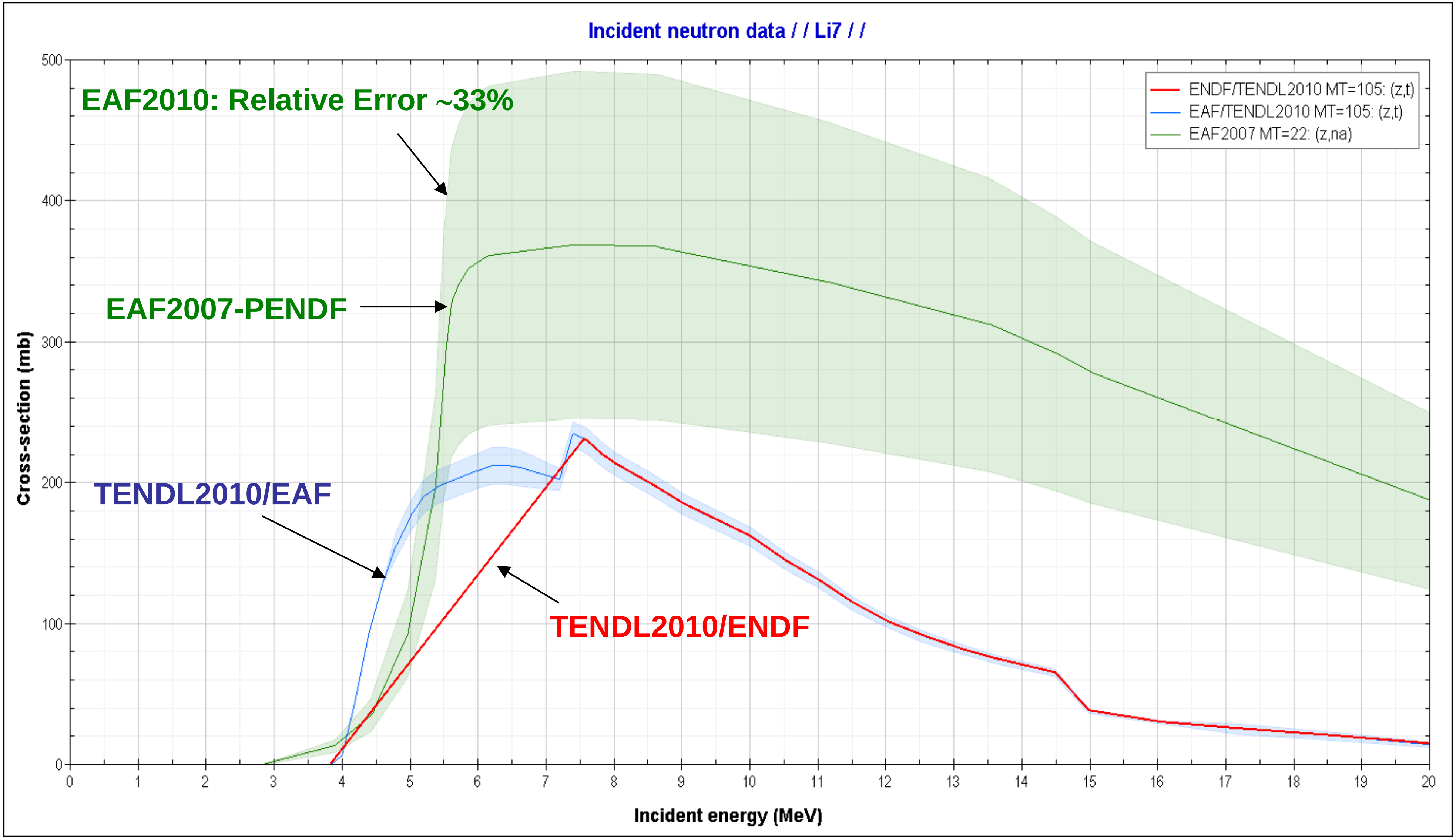


	SL1	
Uncert_1group (ENDF/B-VII) = Δ	$\Delta^2_{ENDF/B-VII}$	Relative Exp Error (%)
Li6(n,T)He4	6.64E-06	0.26

	SL7	
Uncert_1group (ENDF/B-VII) = Δ	$\Delta^2_{ENDF/B-VII}$	Relative Exp Error (%)
Li6(n,T)He4	1.59E-06	0.13

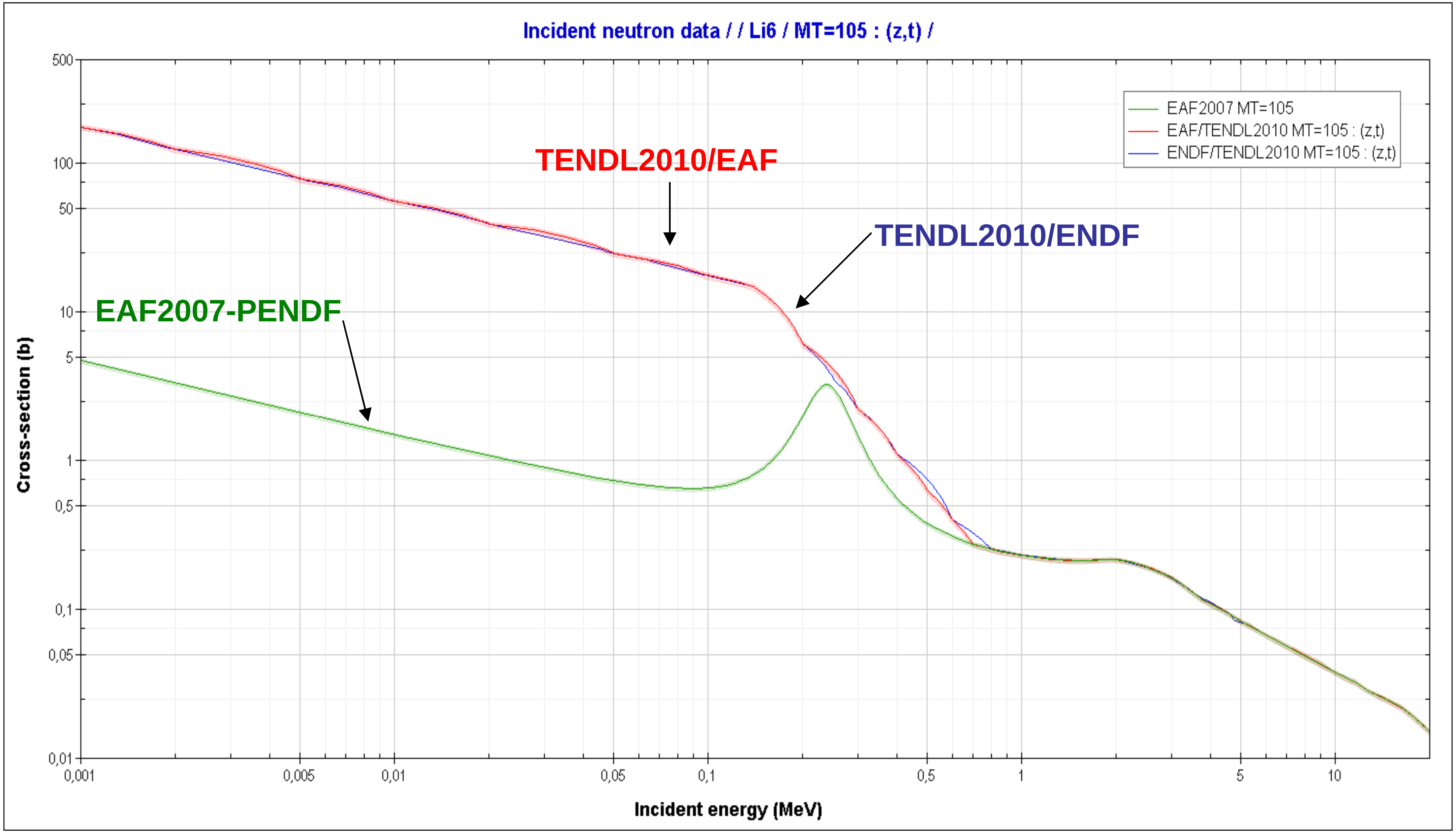
3.2 TENDL2010: $^{7}Li(n,T)$

Figure 8. ^{7}Li (n,T) cross-sections: EAF2010 and TENDL2010/EAF



3.2 TENDL2010: $^{6}Li(n,T)$

Figure 9. **^{6}Li (n,T) cross-sections: EAF2010 and TENDL2010/EAF**



4. Uncertainty Results

- Sensitivity / Uncertainty Analysis (S/U)

  - Method based on the first order Taylor series to estimate uncertainty indices for each reaction cross section

    Is it necessary to take into account non-linear effects ?

    How many sensitivity coefficients should be calculated ?

- Monte Carlo Uncertainty Analysis (MC)

  - To treat the global effect of all cross sections uncertainties in activation calculations, we have proposed an uncertainty analysis methodology based on Monte Carlo random sampling of the cross sections

  - Assignment of a Probability Density Function (PDF) to each cross section

    Which PDFs should be taken ?

4.1 HFTM/IFMIF Tritium Prediction Uncertainties

Uncertainty calculation

Table 2. Tritium production calculated with EAF2007

0.6 0.7±0.3	0.8 1.0±0.5	0.7 0.9±0.3	0.6 0.7±0.3
0.9 1.1±0.6	1 1.2±0.5	0.9 1.1±0.4	0.9 1.1±0.6
1.1 1.4±0.5	1.2 1.4±0.5	1.3 1.6±0.9	1.1 1.4±0.5

Nominal value (Ci/fpy)
Mean ± s.d. (Ci/fpy)

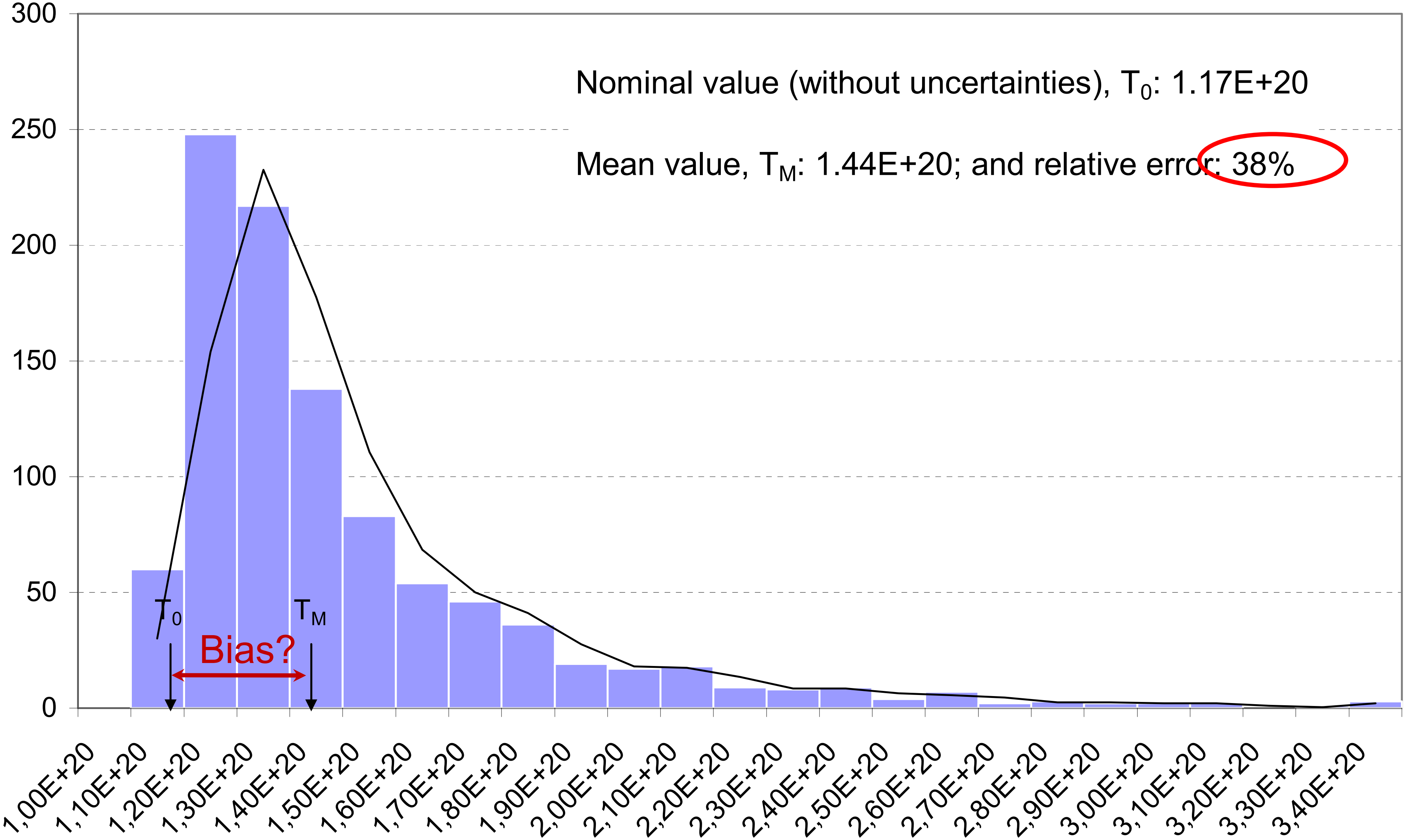
- **nominal value (Ci/fpy) calculated with the best-estimate XS data**
- **mean value (Ci/fpy) and standard deviation (Ci/fpy) calculated with the uncertainty library using the Monte Carlo method with ACAB code**

Total tritium prediction:

- **IEAF2001: 23.4 Ci/fpy**
- **EAF-2007: 11.2 Ci/fpy (best-estimate)**
- **EAF2007/UN: 13.7± 6 (Uncertainties)**
- **Relative errors up to 51% in tritium prediction can be found in rig 2**
- **Similar relative errors for the same rigs positioned in different locations**
- **Histogram of the Monte Carlo sampling fit to a long tail lognormal distribution**

4.1 HFTM/IFMIF Uncertainty Results

Baseline results: Histogram of the 1000 values by MC method



4.1 Sensitivity analysis in the HFTM specimen cells

Table 3 . Uncertainty and sensitivity information for cross sections that contribute most to the uncertainty in the tritium prediction.

Isotope	ρ_{jT}	Δ (%)	$\rho_{jT}*\Delta$
Fe^{56}(n,nt)	0.07	133.3	9.03
Na^{23}(n,nt)	0.06	133.3	8.39
Na^{23}(n,t)	0.38	4.3	1.86
Fe^{56}(n,t)	0.31	4.3	1.32
K^{39}(n,nt)	0.008	133.3	1.08
Na^{23}(n, tα)	0.01	66.7	0.68
Cr52(n,nt)	0.005	133.3	0.64
….	….	….	….
		Total	???

~ 23% !!!

- ρ_{jT} is the sensitivity coefficient for the tritium production from the activation of an isotope after 1fpy
- Δ is the corresponding relative error
- the index $\rho_{jT}*\Delta$ that can be used to rank cross sections inducing the highest uncertainties in the tritium prediction

4.1 Sensitivity analysis in the HFTM specimen cells

Element-by-element uncertainty analysis

Table 4. Tritium production and standard deviation (in Ci/fpy) due to an initial mass of 1000 grams for each initial element used in HFTM rigs in the three zones A, B and C.

Zone	Cr	C	Fe	K	Mn	Na	Ta	V	W
A	4.2±2.5	46.2±10.8	6.0±3.4	14.0±6.4	9.6±7.6	57.2±40.8	1.8±1.4	6.1±7.4	1.6±0.9
B	2.8±1.6	31.1±7.2	4.1±2.3	9.6±4.3	6.5±5.1	39.2±27.5	1.3±1.0	4.1±4.9	1.1±0.6
C	2.4±1.4	26.3±6.1	3.5±2.0	8.1±3.6	5.5±4.3	33.3±23.2	1.1±0.8	3.5±4.1	0.9±0.5

- **Na is the element with the largest generation of tritium**
- **V is the element with the largest relative error (~120%)**
- **Fe and Na have relative errors of ~56% and ~70%, respectively**

4.2 Uncertainty of tritium activity in HCLL TBM mock-up LiPb

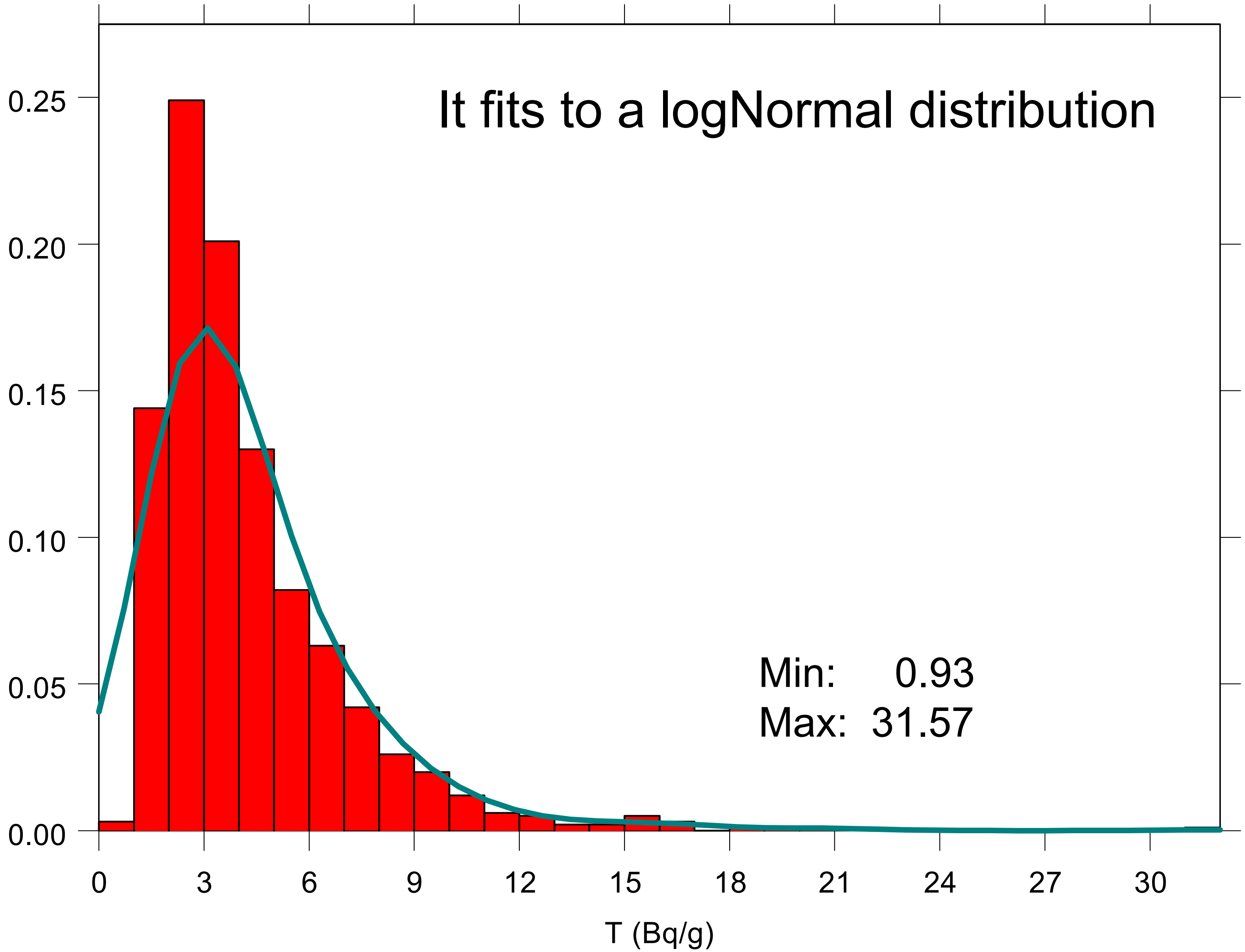
Table 5: Tritium Uncertainty Prediction in SL1 and SL7 using EAF2007/UN

	SL1		SL7	
	Natural Abundance 7.25% Li6 in Li	Depleted Li6 3.14% Li6 in Li	Natural Abundance 7.25% Li6 in Li	Depleted Li6 3.14% Li6 in Li
Total Bq (at shutdown)	3.92	3.47	0.64	0.28
Only due to Li	3.78	3.33	0.64	0.28
Only Li6	0.96	0.40	0.62	0.26
Only Li7	2.82	2.93	0.02	0.02
Sensitivity Coefficiente: ρ = (DN/N) / (DXS/XS) in %				
Li6(n,T)He4	0.25	0.12	0.96	0.91
Li7(n,na)T	0.72	0.84	0.04	0.09
F19(n,T)		0.04		
Mg25(n,T)		1.14E-06		
…	…			
F19(n,nT)		6.36E-03		
Sensitivity/Uncertainty (%) = ρ*Δ				
Li6(n,T)He4	0.82	0.38	3.21	3.03
Li7(n,na)T	47.83	56.21	2.43	5.76
F19(n,T)		0.70		
…				
F19(n,nT)		0.85		
Sensitivity/Uncertainty (%)= (ρ*Δ)	**47.84**	**56.22**	**4.03**	**6.51**
Uncertainty with Monte Carlo				
Mean value	4.67	4.27	0.65	0.29
Relative error (%)	**58.62**	**67.03**	**4.78**	**8.77**

- ρ : is the sensitivity coefficient for the tritium production
- Δ : is the corresponding relative error collapsed in 1 group
- the index "ρΔ" that can be used to rank cross sections inducing the highest uncertainties

4.2 Monte Carlo sampling using a LogN PDF

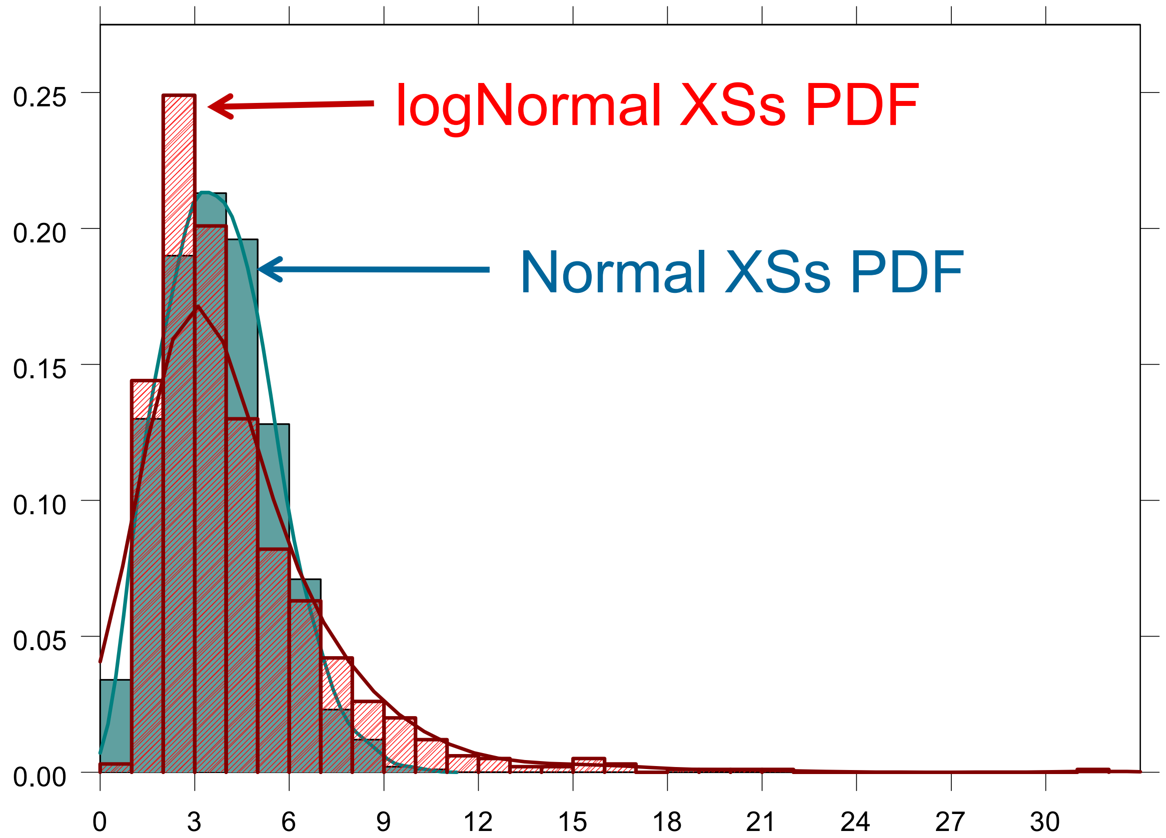
Mean Value: T_M= 4.27 Bq/g; and relative error : 67.03%



4.2 Effect of the selection of PDF

Table 6. Tritium Uncertainty Prediction in SL1 and SL7 using EAF2007/UN

	SL1 (3.47 Bq)		SL7 (0.28 Bq)	
	Normal	Log Normal	Normal	Log Normal
Uncertainty with Monte Carlo				
Mean value	3,79	4,27	0,29	0,29
Relative error (%)	45,10	**67,03**	5,77	**8,77**



5. Conclusions

1. **A Comparison of error propagation methodologies for the Tritium Production has been performed:**
   - ✓ Tritium Production in the HFTM/IFMIF Specimen Cells
   - ✓ Measurements in Tritium activity in HCLL TBM mock-up LiPb

2. **Main (n,xT) cross-section uncertainties are analyzed**
   - ✓ ^{23}Na and ^{56}Fe for HFTM/IFMIF
   - ✓ ^{7}Li and ^{6}Li in HCLL TBM mock-up LiPb

3. **It is shown that Monte Carlo technique is able:**
   - ✓ to deal with non-linear effects or when uncertainties are high
   - ✓ to provide with the global effect of the uncertainties of the complete set of nuclear data

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Processing TENDL2010/EAF

- MT=18 and MT=102 with more than 10000 energy points
- Different channels in the variance and cross section files
- No uncertainties for isomeric/branching reactions

6. References

For this work

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