DE LA RECHERCHE À L'INDUSTRIE

GENERATION AND USE OF TSL COVARIANCE MATRIX : H(H2O)

CONTRIBUTION CEA, DEN CADARACHE

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15 May 2018, NEA, Paris

www.cea.fr

Generation of covariance matrix between model parameters

Description of the method implemented in the CONRAD code for calculating covariance matrix between model parameters ⇒ **LEAPR parameters (JEFF-3.1.1)**

Annals of Nuclear Energy 104 (2017) 132–145

Contents lists available at ScienceDirect

Annals of Nuclear Energy

journal homepage: www.elsevier.com/locate/anucene

Covariance matrices of the hydrogen neutron cross sections bound in light water for the JEFF-3.1.1 neutron library

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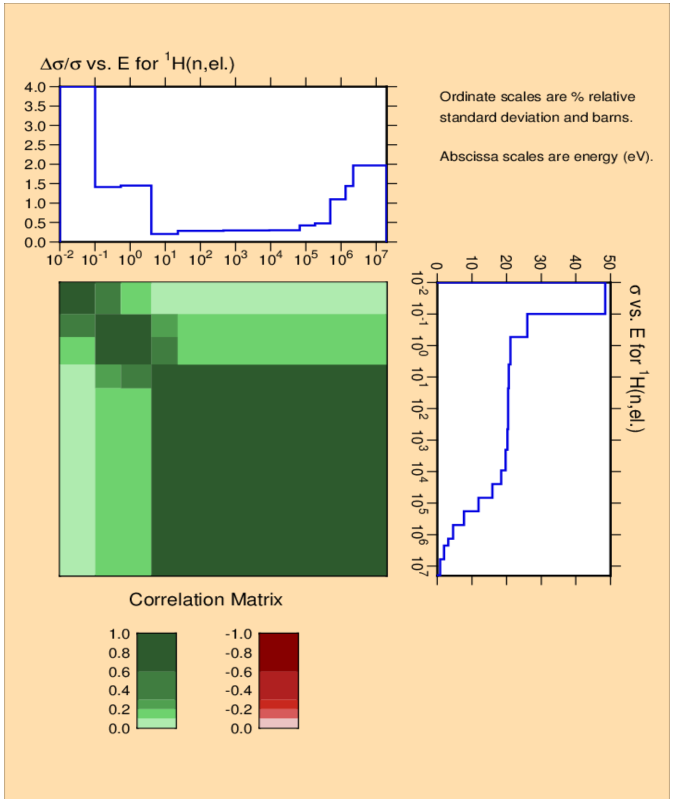
Full covariance matrix on the elastic scattering cross section of H1 in H2O from thermal to MeV energy range by using **contraints on the bound cross section**



Covariance matrix between the LEAPR parameters

Final results after the retroactive analysis and ZVP treatment

- Free model parameters x
- Fixed model parameters θ with known uncertainties

Parameters	Values	Rel. unc.	Correlation matrix					
Δ	1.000 ± 0.241	(24.1%)	100.0					
σ_s	20.478 ± 0.041	(0.2%)	−1.2	100.0				
F	1.000 ± 0.186	(18.6%)	15.3	14.2	100.0			
E_1	205.0 ± 6.0	(2.9%)	−1.2	0.0	6.0	100.0		
E_2	436.0 ± 36.0	(8.3%)	2.3	0.0	45.7	0.0	100.0	
c	0.0 ± 1.5	–	0.0	0.0	0.0	0.0	0.0	100.0

- Defect model parameter added after the ZVP treatment

- Experimental parameters not included in the covariance matrix (marginalization)

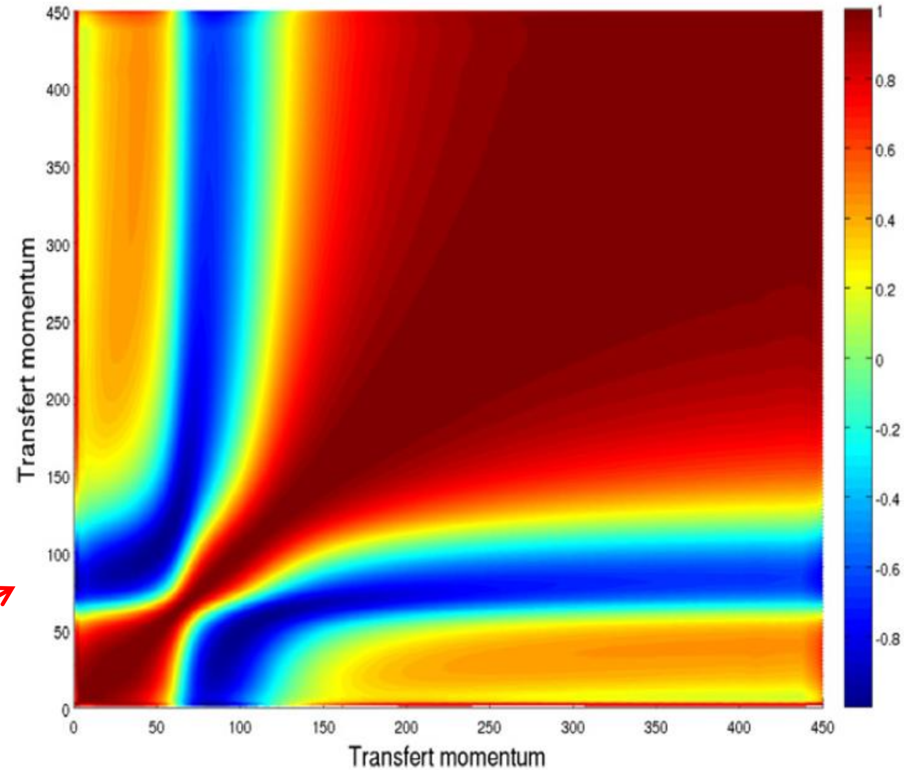
Covariance matrix between the GROMACS parameters

Final results after the retroactive analysis and ZVP treatment

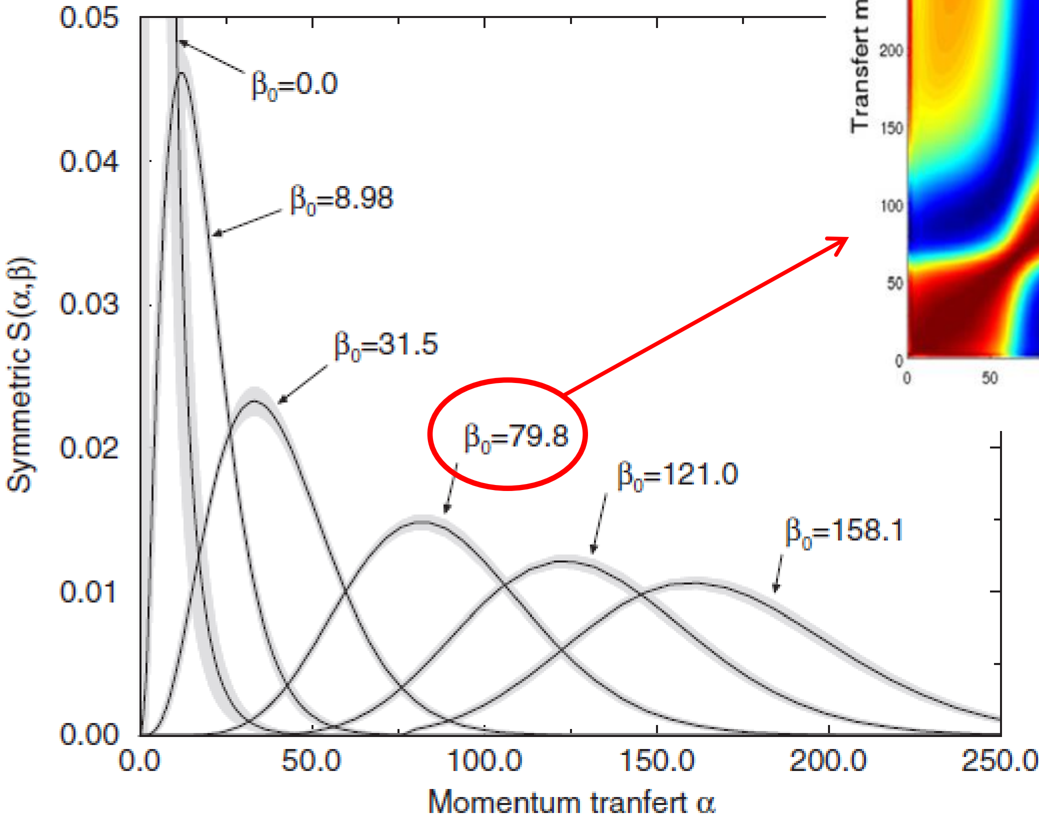
Paramter	Value	Relative posterior uncertainty	Posterior correlation matrix								
σ_O [nm]	0.31644	2.3%	100	-77	93	69	33	-18	-64	83	-14
ε_O [KJ/mol]	0.77491	14.6%		100	-71	-98	-85	53	97	-54	-32
q_H [e]	0.5564	3.2%			100	59	28	-2	-60	81	-18
d_{OH} [nm]	0.09419	6.3%				100	89	-63	-96	44	38
D_{OH} [KJ/mol]	432.58	6.2%					100	-63	-88	6	57
b_{OH} [1/nm]	22.87	4.2%						100	51	-11	-28
θ_0 [°]	107.4	6.4%							100	-45	-49
k_θ [KJ/mol/rad²]	367.81	3.8%								100	-14
a [nm]	0.13288	2.7%									100

- The relative uncertainties oscillate between 2% to 15%
- The water physics might change due to such large uncertainties !
- Solution $\Rightarrow$ produce covariances by including in the analysis **physical properties of water** and not only experimental neutron cross sections $\Rightarrow$ not yet done !

Propagation of the LEAPR parameter uncertainties

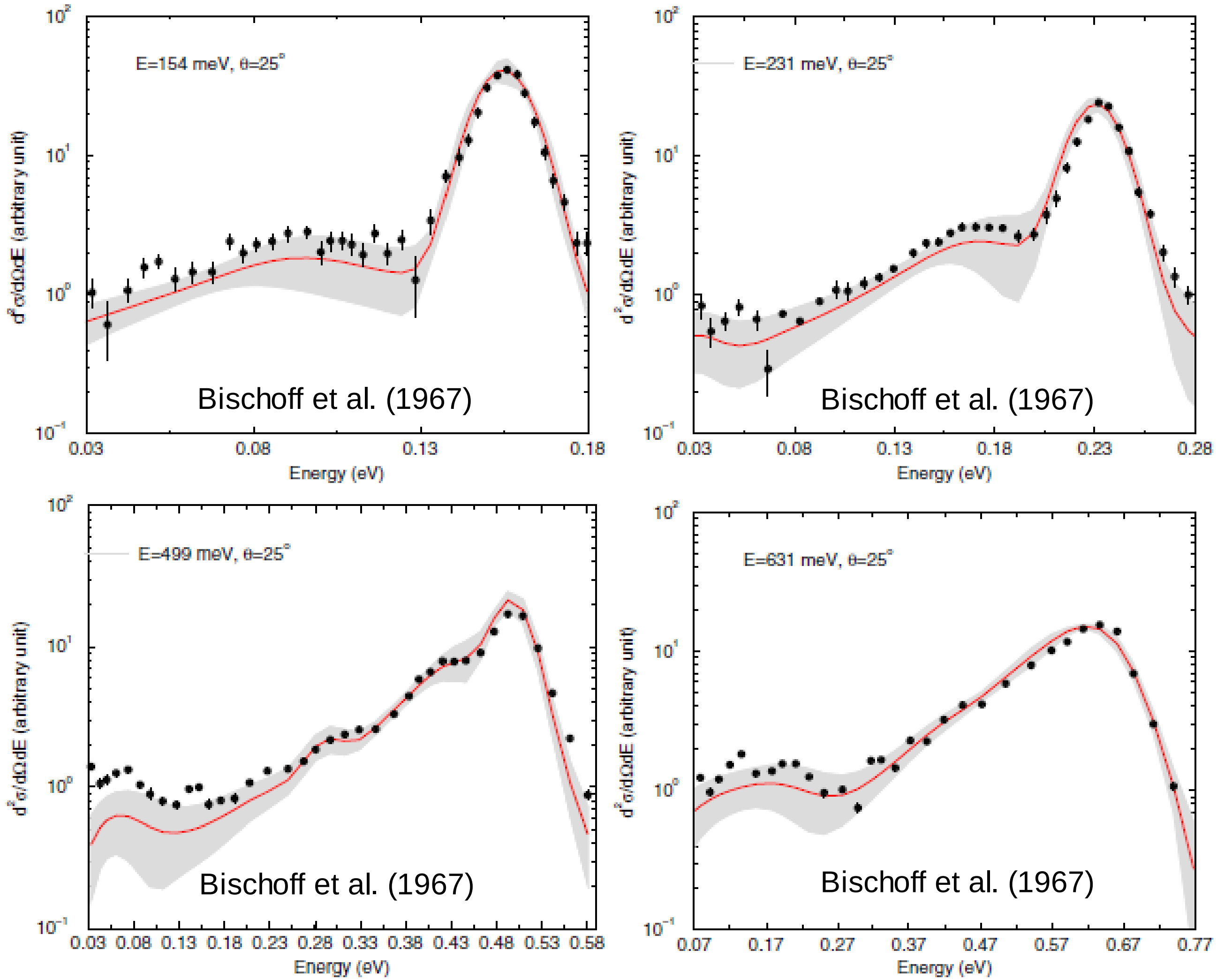


Covariance matrix for $S(\alpha,\beta_0)$



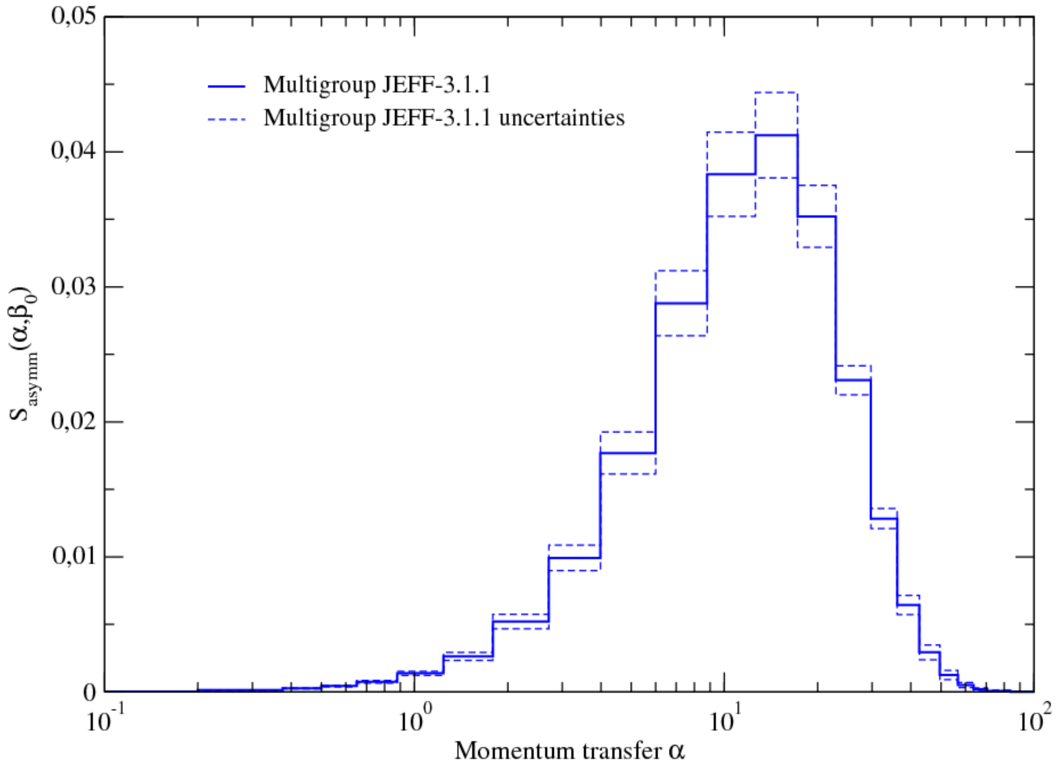
Propagation of the LEAPR parameter uncertainties

Double differential scattering cross section



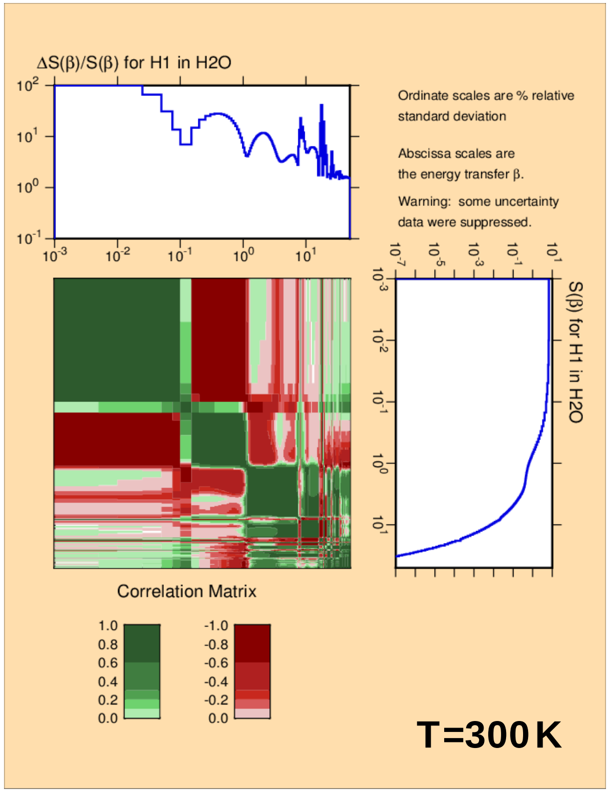
Generation of covariance matrix between $S(\alpha_g,\beta)$

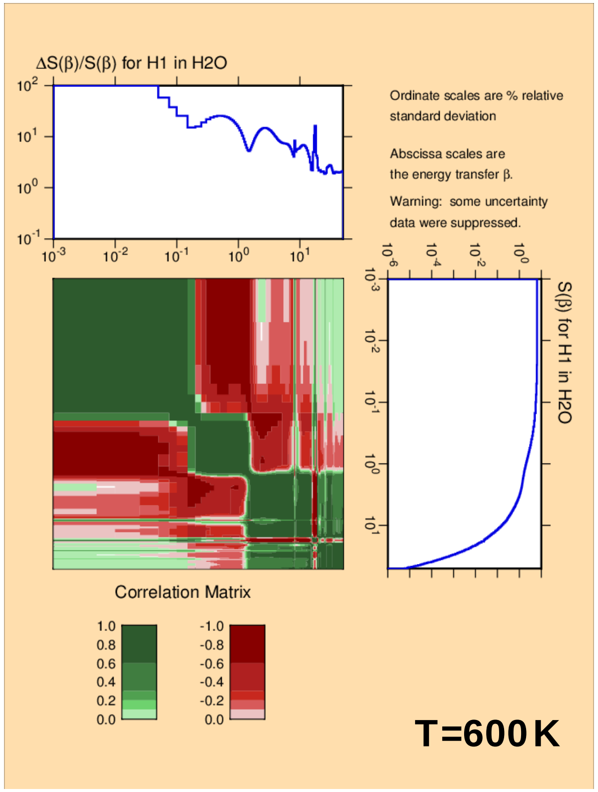
Because of the size of the $S(\alpha,\beta)$ matrix, it is not possible to create a full covariance matrix between the $S(\alpha,\beta)$ ⇒ **we use a multigroup representation $S(\alpha_g\beta)$**



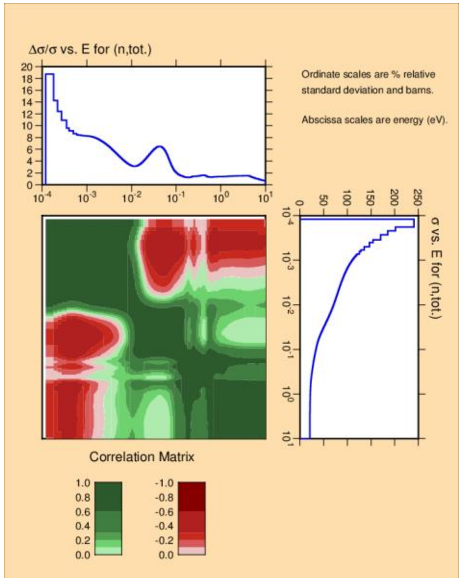
Generation of covariance matrix between $S(\langle\alpha\rangle,\beta)$

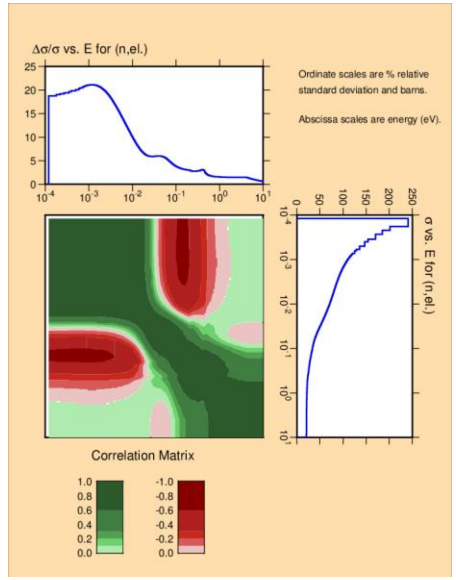
The extreme multigroup representation is to average the $S(\alpha,\beta)$ over the α grid $\Rightarrow$ **one-group description $S(\langle\alpha\rangle,\beta)$**

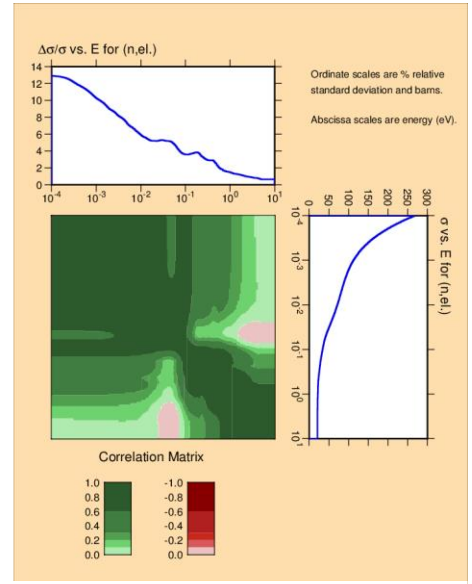




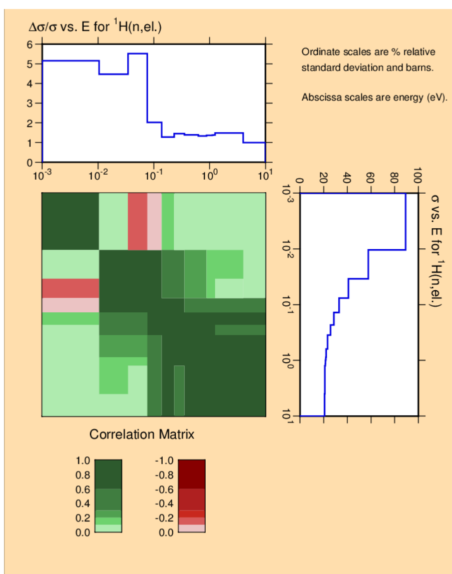
Covariance matrix for the elastic cross section

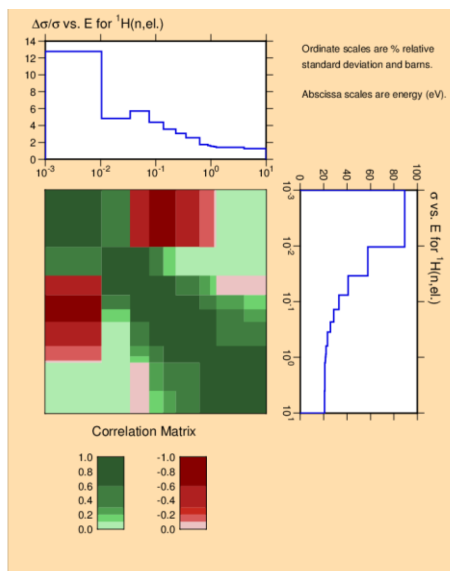


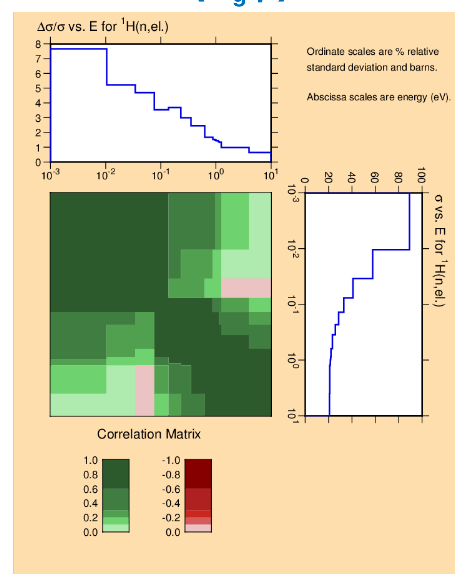




From LEAPR parameters **From S(⟨α⟩,β) matrix** **From $S(\alpha_g,\beta)$ matrix**





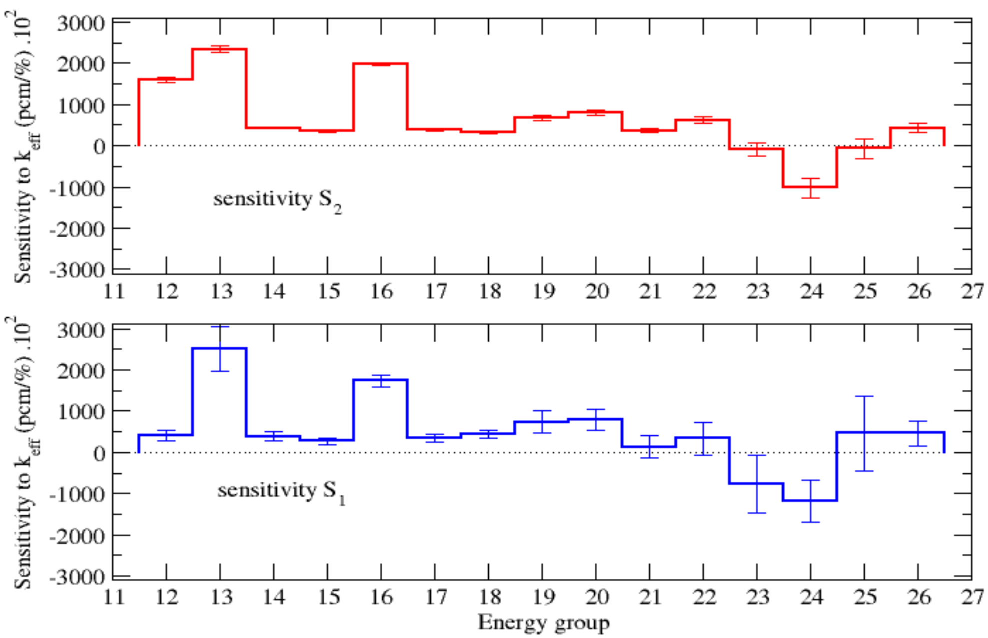


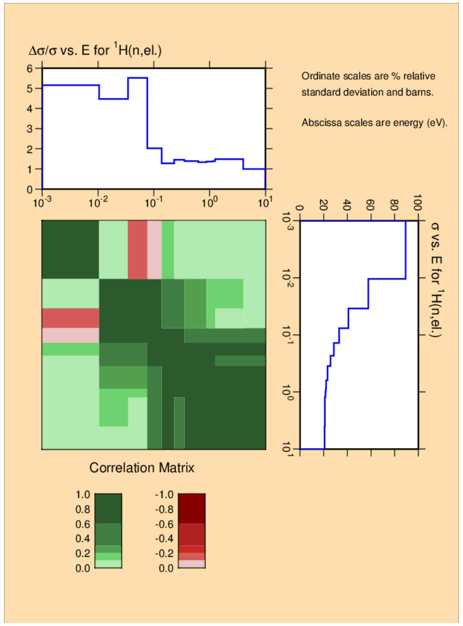
Propagation of the uncertainties : IFP method

In theory, the IFP method implemented in the Monte-Carlo code TRIPOLI4 can be used to calculate the sensitivity to the elastic cross section and to the $S(\alpha_{g,}\beta)$ or $S(\langle\alpha\rangle,\beta)$ elements

In practice, we are limited by the convergence of the IFP method for the $S(\alpha_{g,}\beta)$ or $S(\langle\alpha\rangle,\beta)$ elements

$\Rightarrow$ For the moment, the IFP method of TRIPOLI4 can only be applied to the elastic cross section





Propagation of the uncertainties : IFP method – PST001.1

In theory, the IFP method implemented in the Monte-Carlo code TRIPOLI4 can be used to calculate the sensitivity to the elastic cross section and to the $S(\alpha_{g,}\beta)$ or $S(\langle\alpha\rangle,\beta)$ elements

In practice, we are limited by the convergence of the IFP method for the $S(\alpha_{g,}\beta)$ or $S(\langle\alpha\rangle,\beta)$ elements

$\Rightarrow$ For the moment, the IFP method of TRIPOLI4 can only be applied to the elastic cross section

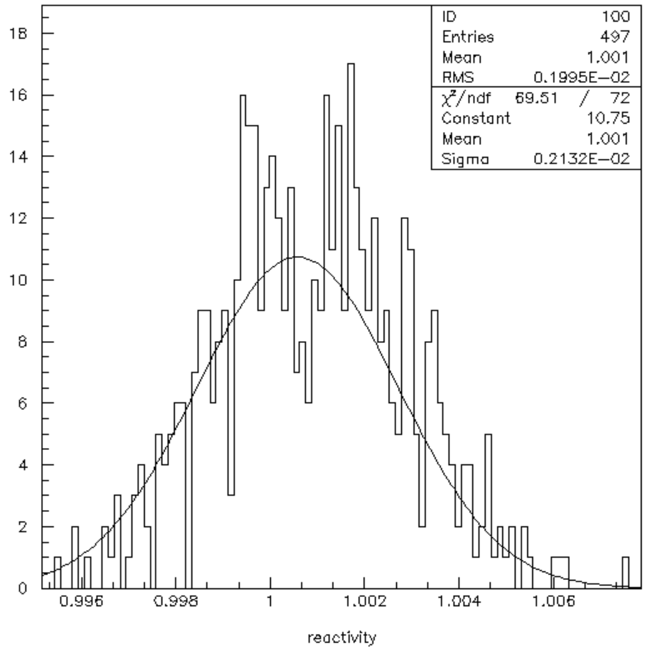
IFP sensitivity	IFP uncertainty	Origin of the covariance matrix		
		LEAPR parameters	$S(\langle\alpha\rangle,\beta)$	$S(\alpha_g,\beta)$
sensitivity $S_1(\sigma_n)$	$\pm$70 pcm	114 pcm	159 pcm	125 pcm
sensitivity $S_2(\sigma_n)$	$\pm$ 10 pcm	130 pcm	161 pcm	132 pcm

The three covariance matrices provide nealy equivalent results close to 140 pcm

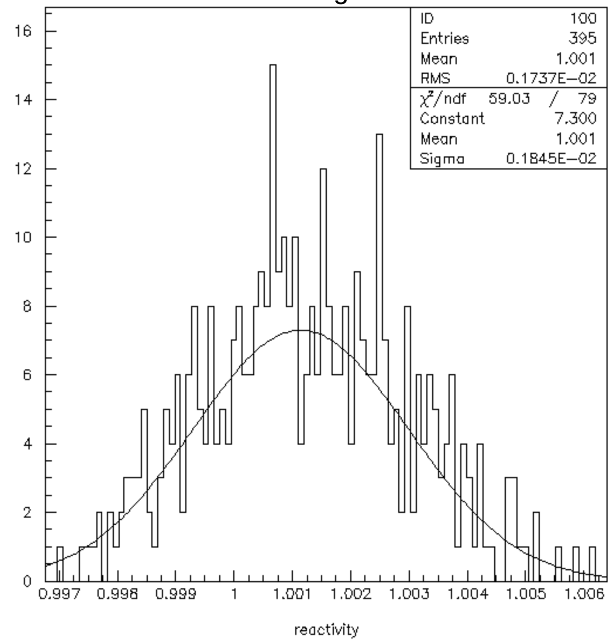
Propagation of the uncertainties : TMC method – PST001.1

Méthode de propagation	Origin of the covariance matrix	
	$S(\langle\alpha\rangle,\beta)$	$S(\alpha_g,\beta)$
Sensibilité IFP $S_2(\sigma_n)$	161 pcm	132 pcm
Total Monte Carlo	213 pcm	184 pcm

From $S(\langle\alpha\rangle,\beta)$ matrix



From $S(\alpha_g,\beta)$ matrix



IFP and TMC provide nearly equivalent results ⇒ difference of 50 pcm

IFP method - Application to UOX cell

Decomposition of the keff uncertainty **without the S(α,β) contribution**

Isotope	FISSION	CAPTURE	ELASTIC	INELASTIC	NXN	NU	DISTRIBUTION	DISTRIBUTION_TH	TOTAL
H1		150	17						**151**
B10		26							**26**
O16		97	14	2					**98**
Zr90		11	72	4					**72**
Zr91		27	30	2					**40**
Zr92		27	20	2					**33**
Zr94		2	8	2					**8**
Zr96		2	6						**6**
U234	1	6	2						**6**
U235	104	174	13			276		142	**371**
U236		1							**1**
U238	29	165	83	38	18	32	9		**195**
TOTAL	**108**	**303**	**118**	**39**	**18**	**277**	**9**	**142**	**465**

IFP method - Application to UOX cell

Decomposition of the keff uncertainty **with the S(α,β) contribution**

Isotope	FISSION	CAPTURE	ELASTIC	INELASTIC	NXN	NU	DISTRIBUTION	DISTRIBUTION_TH	TOTAL
H1_H2O		150	105						**183**
B10		26							**26**
O16		97	14	2					**98**
Zr90		11	72	4					**72**
Zr91		27	30	2					**40**
Zr92		27	20	2					**33**
Zr94		2	8	2					**8**
Zr96		2	6						**6**
U234	1	6	2						**6**
U235	104	174	13			276		142	**371**
U236		1							**1**
U238	29	165	83	38	18	32	9		**195**
TOTAL	**108**	**303**	**158**	**39**	**18**	**277**	**9**	**142**	**477**

⇒ Low impact on the final uncertainty

Conclusions

What is needed for the propagation of the TSL uncertainties ?

Define a simple format to store the covariance matrix between the LEAPR parameters

- Easy to use for TMC calculations and deterministic sensitivity calculations
- If possible, covariance matrix between the MD parameters should be converted in covariance matrix between the LEAPR parameters

Define a multi-group format to store the covariance matrix between $S(\alpha_g,\beta)$

- Such a format is needed if TSL file is not created via LEAPR
- Can be used for TMC calculations
- Deterministic sensitivity calculation issues not yet solved
- Difficult to ensure that the matrix is still definite positive when it is stored in the file