From nuclear model parameters to neutronic simulation with the CONRAD and LAST codes

DE LA RECHERCHE À L'INDUSTRIE

Consultancy Meeting on model code output & application nuclear data form structure
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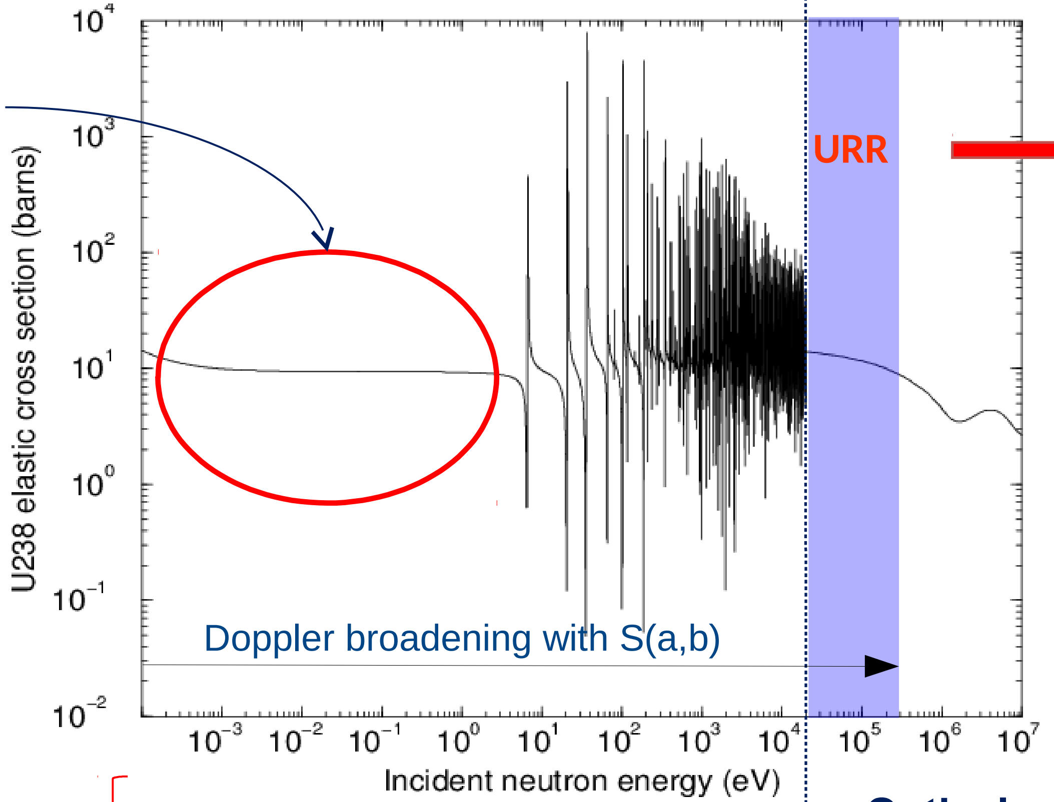
The Conrad tool box

RRR

« Continuum »

CINELmodel Thermal Scattering Law



Average resonance parameters calculated with the URR option of TALYS

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Probability Tables

+ for fission reaction
PFNS model
Neutron multiplicity model
(n,gf) model
Energy dependent penetration factor model
...

R-Matrix formalism

Optical model (ECIS, CCCP)

Statistical model (TALYS, CONRAD)

ESTIMA methos

SPRT method

The Library and Stochastic Transport (LAST) code is a Monte-Carlo neutron transport code developed at CEA Cadarache. It consists in C++ modules for intensive-computation functions, all led by a python wrapping. It handles Open-MPI parallel computation to improve calculation efficiency and reduce the calculation time. A few basic scores are available, such as k_{eff}, neutron flux and adjoint flux (sensitivity calculations, perturbation theory). The k_{eff} calculation accuracy has been numerically validated against the CEA reference code TRIPOLI-4

The LAST code is coupled with the nuclear data evaluation code CONRAD. Therefore, both standard ENDF-6 files and CONRAD theoretical files (containing nuclear model parameters and the associated covariance matrix) can be used to perform simulations. The coupling of CONRAD and LAST ensures the consistency among different nuclear data.

+ in the case where some evaluated data are preferred rather than the CONRAD theoretical calculation, LAST can merge the desired ENDF data with the CONRAD calculation.

Unresolved Resonance Range (URR) : limitation due to the width fluctuation correction in NJOY

Thermal Scattering Law (TSL) : how to handle huge S(alpha,beta) covariance matrix ?

Scattering Angular Distribution (SAD) : correlations between SAD and neutron cross sections

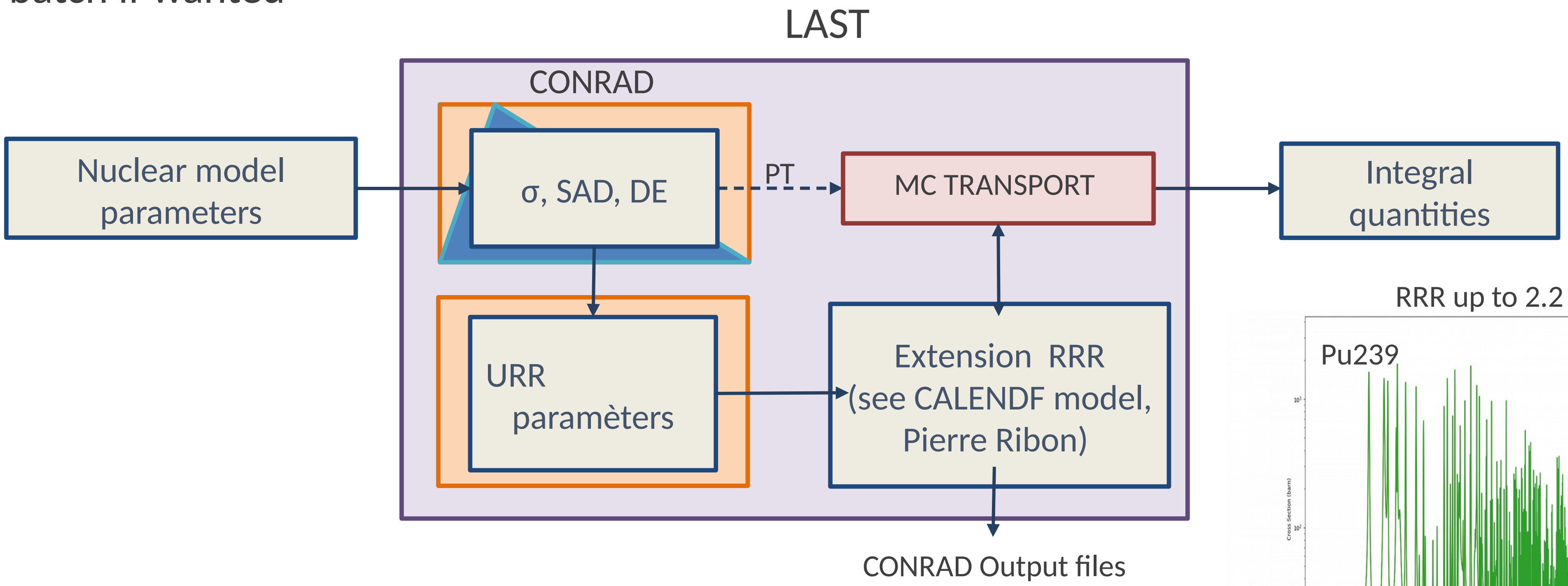
Fission models : progress in the resonance range with (n,gf) reaction, Class-II states, $P_f(E)$

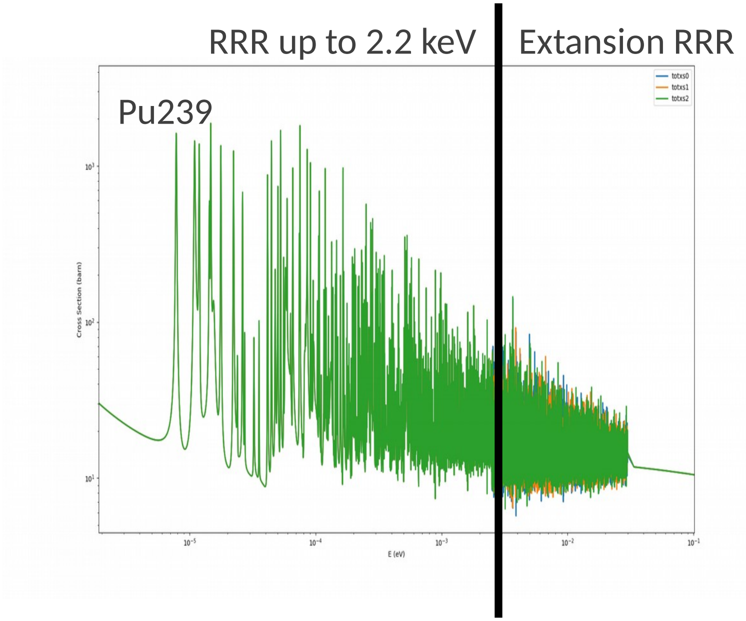
Direct capture in the RRR : imaginary part of the infinite radius as in REFIT (not yet implemented in CONRAD, not discussed here)

...

URR treatment

Random extension of the RRR by using URR parameters (+average parameter statistical laws) at each batch if wanted





- No URR format limitation
- No RRR/URR cross correlation issues
- No Probability Tables (PT)

Thermal Scattering Laws (H2O)

Molecular Dynamic parameters and covariance matrix

Table 5. Relative uncertainties and correlation matrix between the CAB model parameters after the marginalization.

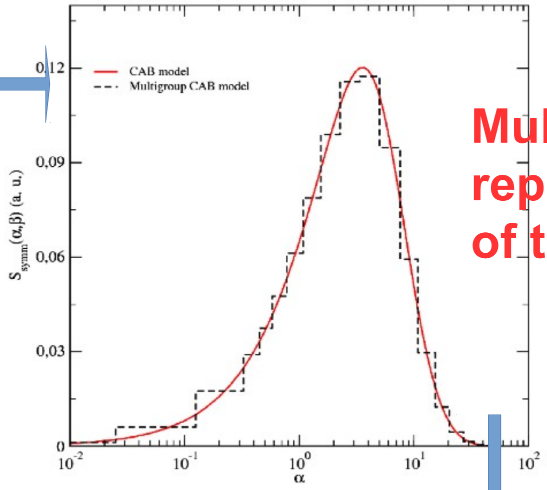
Parameter	Value	Relative uncertainties	Correlation matrix								
σ_0 (nm)	0.31644	2.3%	100	−77	93	69	33	−18	−64	83	−14
ϵ (kJ/mol)	0.7749	14.6%		100	−71	−98	−85	53	97	−54	−32
q_H (e⁻)	0.5564	3.2%			100	59	28	−2	−60	81	−18
d_{OH} (nm)	0.09419	6.3%				100	89	−63	−96	44	38
D_r (kJ/mol)	432.581	6.2%					100	−63	−88	6	57
β_{OH} (1/nm)	22.87	4.2%						100	51	−11	−28
θ_{OH} (°)	107.4	6.4%							100	−45	−9
k_θ (kJ/mol/rad^2)	367.81	3.8%								100	−14
d_{OM} (nm)	0.13288	2.7%									100

10 direct calculations only

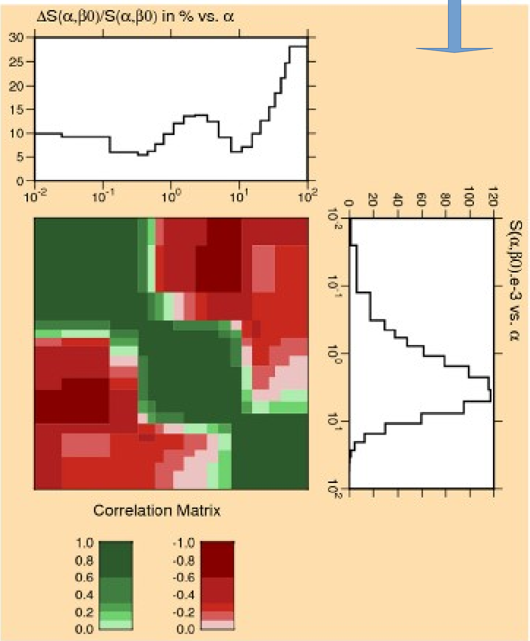
Table 7. Example of uncertainties on the reactivity (MOX configuration at room temperature) in pcm due to the nuclear data. The contribution of ^{1}H in H_2O comes from the present work. The other contributions were calculated with the covariance data base COMAC [32] developed at the CEA of Cadarache.

Isotopes	(n,f)	Capture	(n,n)	(n,n')	(n,xn)	ν_{tot}	χ_{fast}	χ_{th}	Total
^{1}H in H_2O		46	110						119
^{10}B		8							8
^{16}O		114	24	4					117
^{90}Zr		11	24	7					27
^{91}Zr		13	16	4					21
^{92}Zr		8	22	4					24
^{94}Zr		2	59	3					59
^{96}Zr		2	13	1					14
^{235}U	2	6	3	1		5		4	9
^{238}U	114	88	80	−60	25	35	12		160
^{238}Pu	1	70	−20	1		9	1		67
^{239}Pu	278	371	26	5		57	0	126	484
^{240}Pu	42	178	−16	−5	1	2	9		182
^{241}Pu	108	96	8			88	58		179
^{242}Pu	3	131	10	2		2	1		131
^{241}Am	−3	47	2	29		1			47
Total	322	475	156	−59	25	111	60	126	619

Uncertainty in pcm on keff (UOX fuel)



Multigroup representation of the S(alpha,beta)



Multigroup S(alpha,beta) covariance matrix

Problems to get positive definite matrix

Scattering Angle Distribution

Optical Model Parameters and covariance matrix

Table 1. Model parameters and the corresponding uncertainty (1σ) and the correlation matrix for n+^{56}Fe reaction*

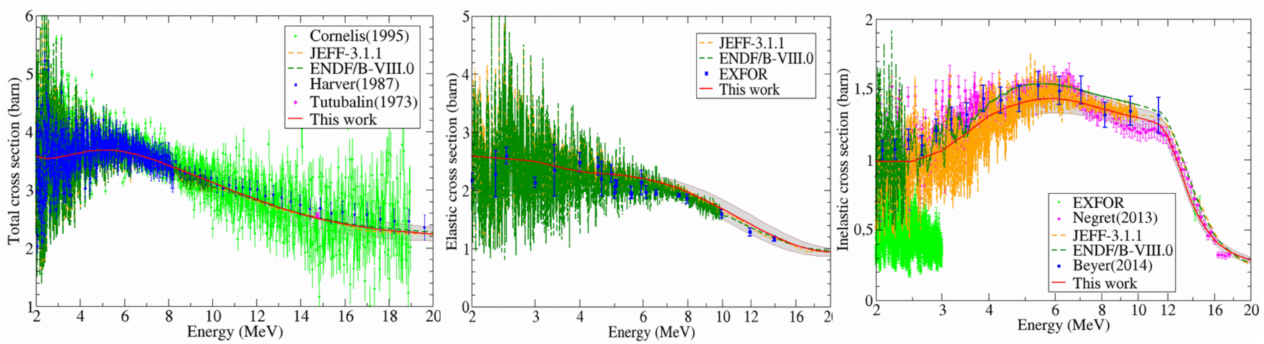
Parameter	A_{SO} (MeV)	V_{HF} (MeV)	a_0 (fm)	r_0 (fm)	$T(^{56}Fe)$ (MeV)
Value	15.126	92.627	0.6032	1.224	1.352
Uncertainty	1.966	9.554	0.0551	0.019	0.118
Correlation matrix	1.000				
	-0.486	1.000			
	-0.851	0.312	1.000		
	0.325	-0.808	-0.307	1.000	
	0.487	0.104	-0.575	-0.414	1.000

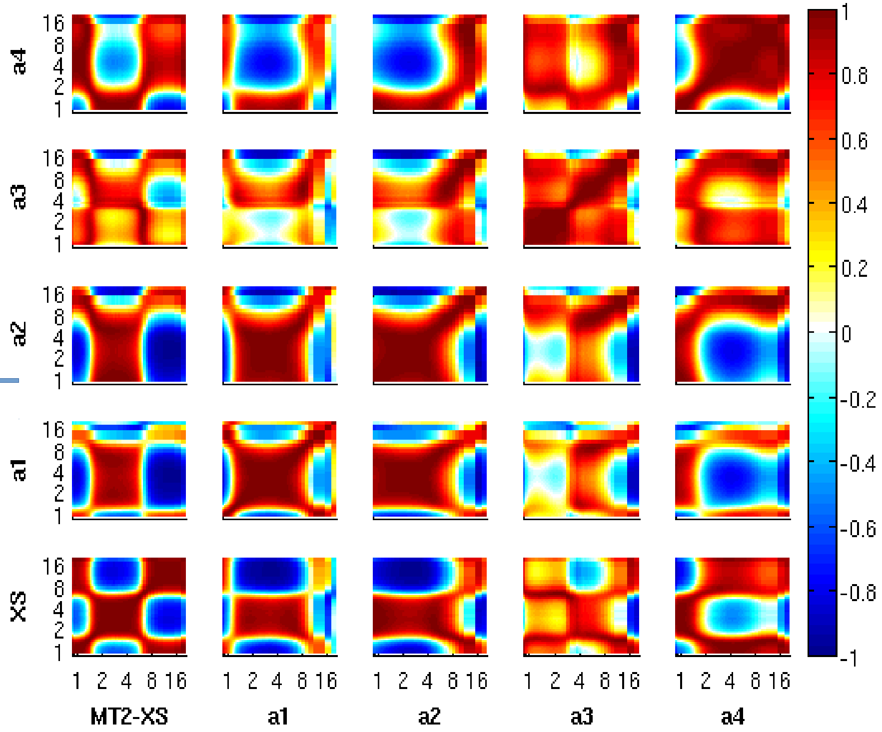
Use perturbation formalism

Table 5. Uncertainty (in pcm) concerning k_{eff} from the OMP parameters and the correlation between AD and XS deduced from k_{eff}.

Benchmark	Perturbation	Δk_{eff}	$\Delta k_{eff}/k_{eff}$	$\Delta\rho$
Thermal	AD	46.8±2.0	49.0±2.1	51.2±2.2
	XS	70.8±1.7	74.1±1.8	77.5±1.9
	AD&XS	67.9±1.7	71.0±1.7	74.3±1.8
	Correlation		-0.3924±0.0454	
Fast	AD	95.7±2.0	94.1±2.0	92.5±2.0
	XS	172.7±1.9	169.9±1.9	167.1±1.9
	AD&XS	71.7±2.2	70.5±2.2	69.3±2.2
	Correlation		-1.0243±0.0165*	

Keff uncertainties (thermal and fast benchmarks) and correlations between SAD and XS

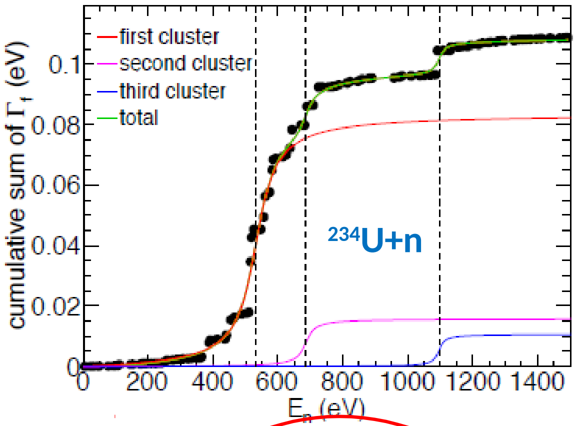


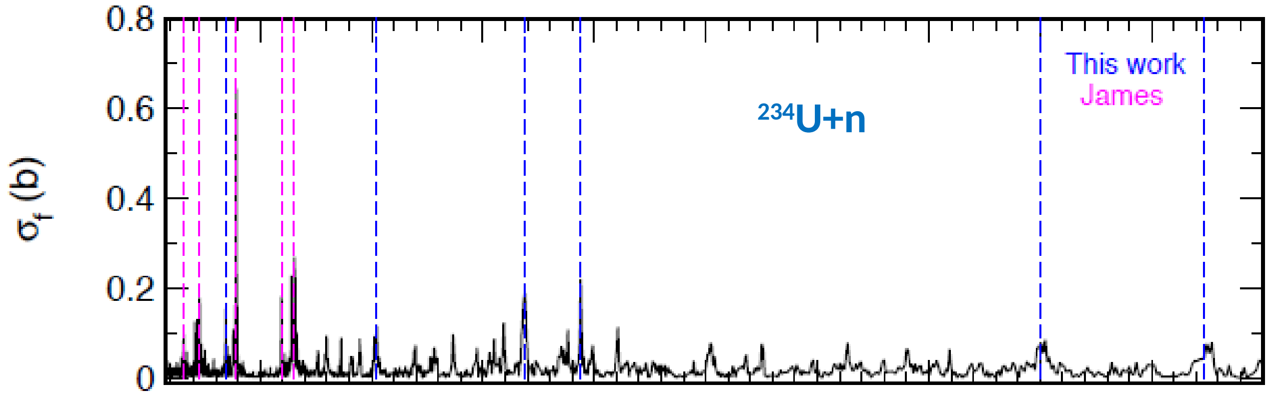


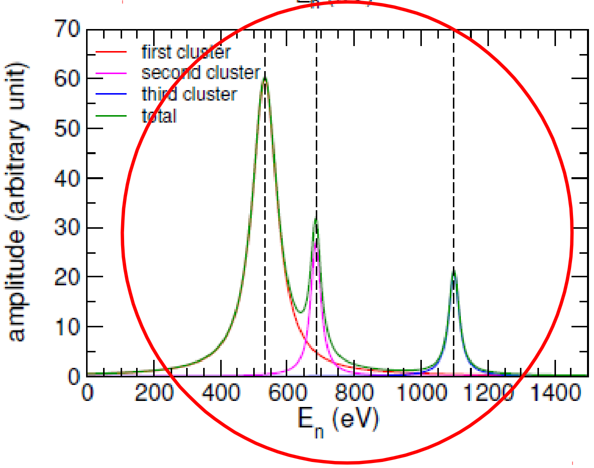
Correlation matrix between SAD and first-four orders Legendre coefficients

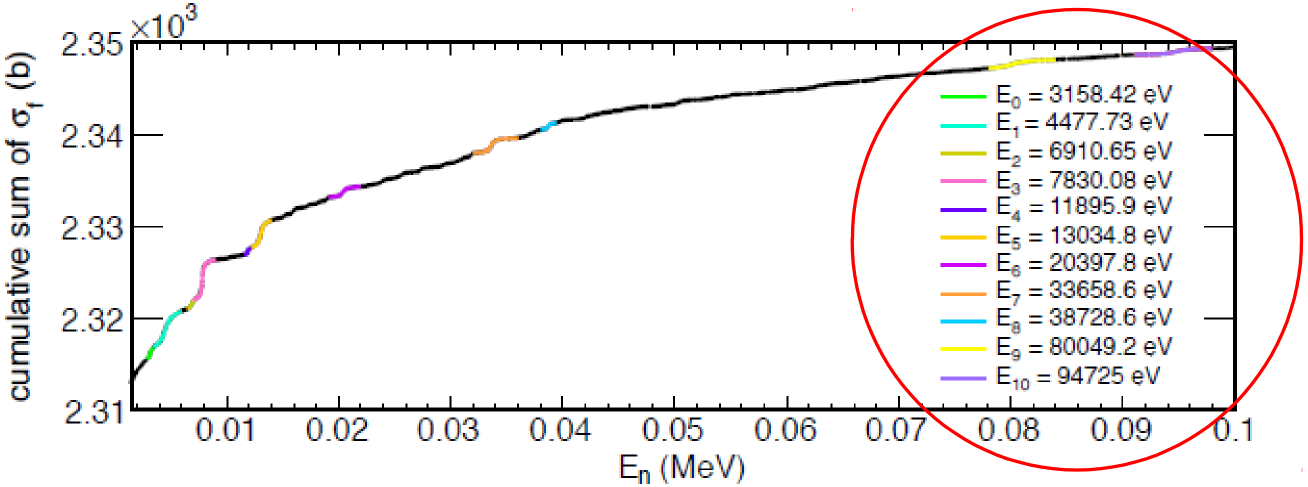
FISSION MODELS IN THE RRR: (n,gf) reaction, Class-II states, Pf(E), neutron multiplicity

$$\Gamma_{\lambda,f} = 2\gamma^2_{\lambda,f} P_f$$









Class-II states included in the RRR and URR analysis : **How to store this information in nuclear data files ?**

Merci de votre attention