Progress on the covariance evaluation approach at CNDC

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Contents

Covariance has been proposed to evaluate the quality of nuclear data since 1970's;

In principle, the *REAL* value of physics observables should not beyond the uncertainty boundary centering around the recommended nuclear data. (*Personally, this is not easy to satisfy cause REAL value is hard to be generated rigorously except MEAN value*)

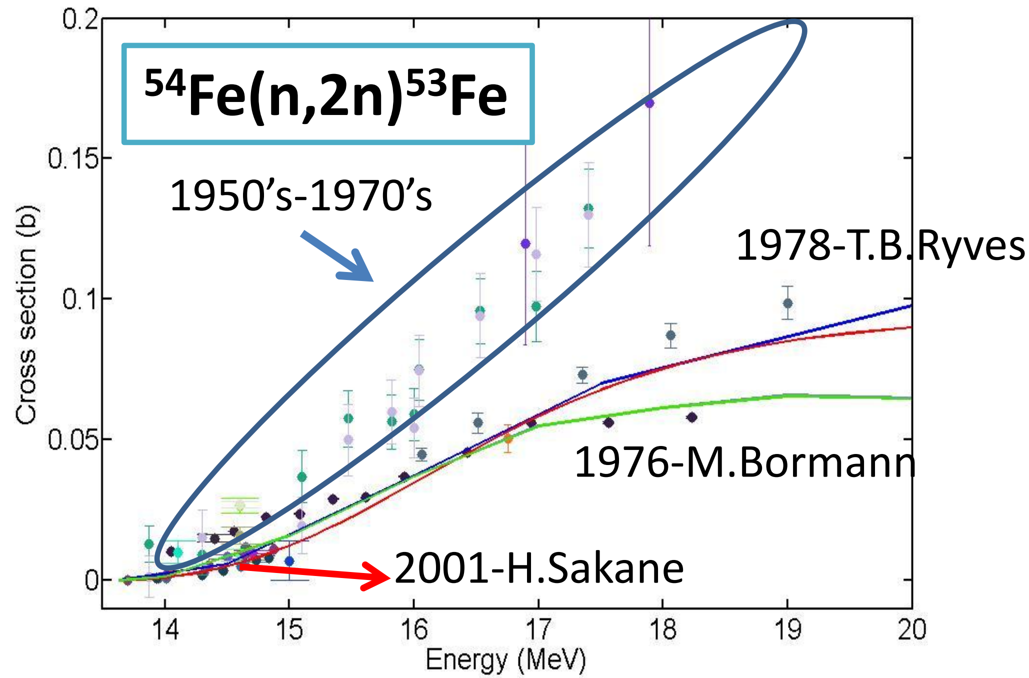
'REAL' value

≈

'MEAN' value

↓

Limited by current understandings of nuclear theory and experiment



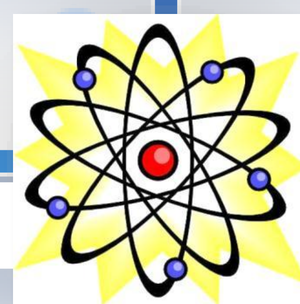
Our main purpose to evaluate COV is to ‘honestly’ propagate any related uncertainty in nuclear data recommendation process to COV in a scientific way, but not only the purpose to including REAL values within the boundary.

Nuclear Data Measurement

- Neutron flux
- Detectors
- Data of Monitor
- ……

Nuclear Model calculation

- Diversified theories
- Theoretical parameters
- Calculated chi2
- … …



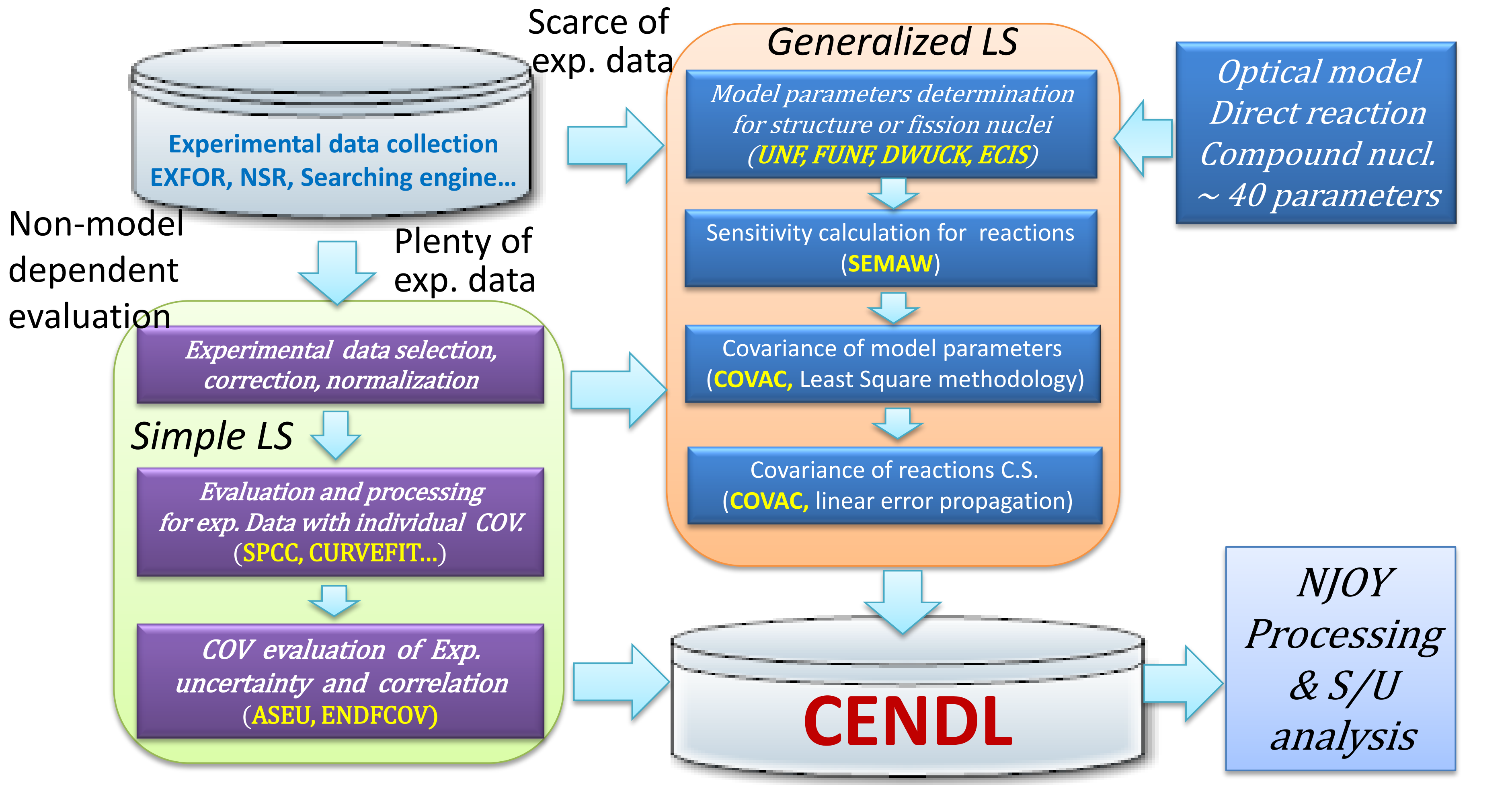
Evaluation of Exps.

- Data filter
- Data correction
- Data normalization
- … …

Others

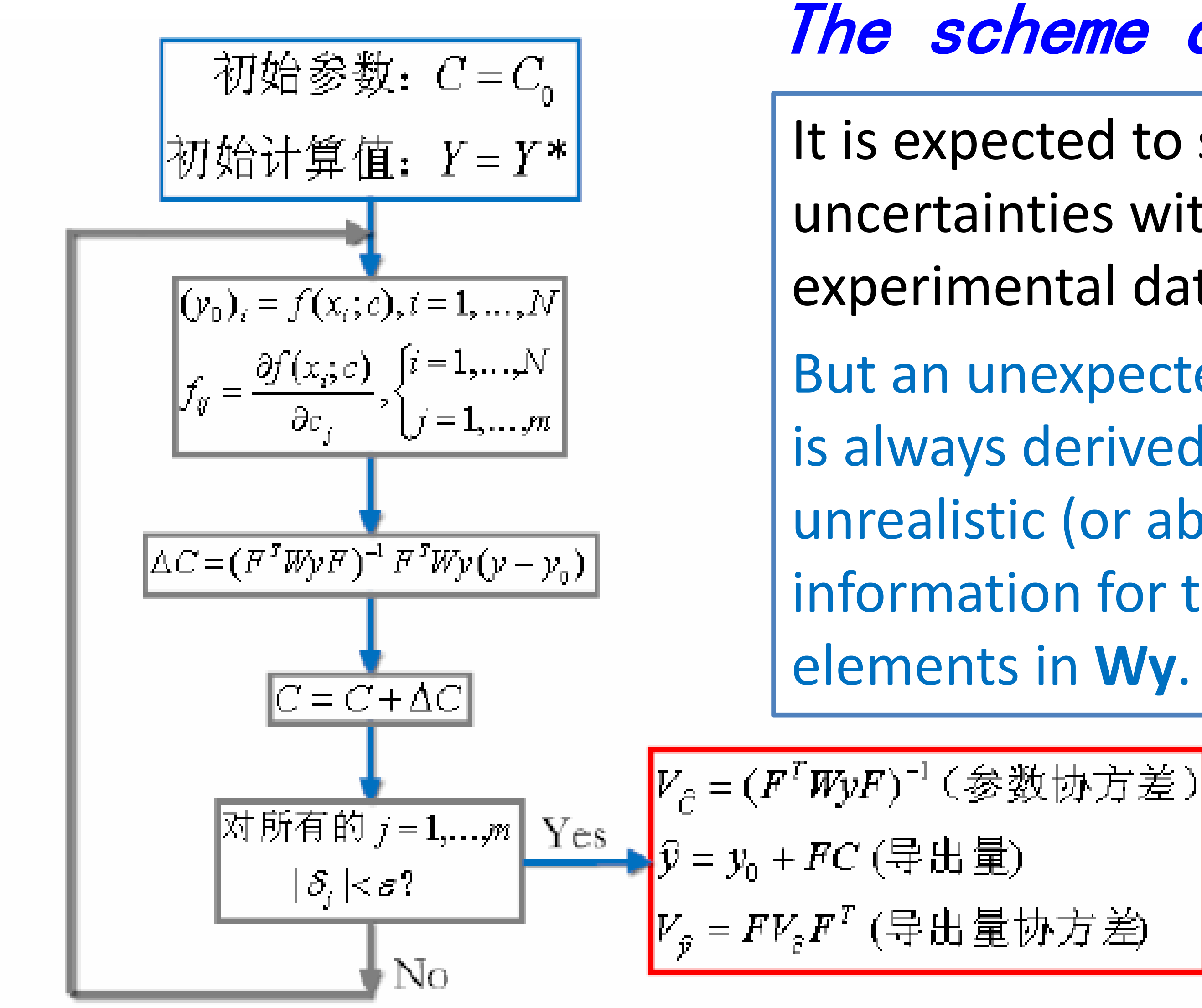
- Deviation from ***REAL***
- Neglected uncertainty
- … …

Deterministic approach: Data recommendation together with COV



Correlations among single (or multiple) set(s) of experimental data are vital elements to get an 'honest' covariance. But it is almost inaccessible in the real evaluation.

The scheme of general LS



It is expected to see the decreased uncertainties with the increased experimental data involved in LS.

But an unexpected low uncertainties is always derived due to the unrealistic (or absent) correlation information for the off-diagonal elements in **Wy**.

Contents

Covariance of uncertainties in measurement

Analysis of the sources of experimental uncertainties (ASEU)

Physics quantity y is derived based on N sets of experimental observables X following function F:

$$y = f(x_1, x_2, \cdots, x_N)$$

The experimental observables are independent of each other.

Taylor expansion around <X>, and the high order items are ignored:

$$y = f(\langle x \rangle) + \sum_{i=1}^{N} \left(\frac{\partial f}{\partial x_i}\right)\Big|_{x=\langle x \rangle} \times (x_i - \langle x_i \rangle) + \frac{1}{2!} \sum_{i=1, j=1}^{N} \left(\frac{\partial^2 f}{\partial x_i \partial x_j}\right)\Big|_{x=\langle x \rangle} \times (x_i - \langle x_i \rangle)(x_j - \langle x_j \rangle) + \cdots,$$

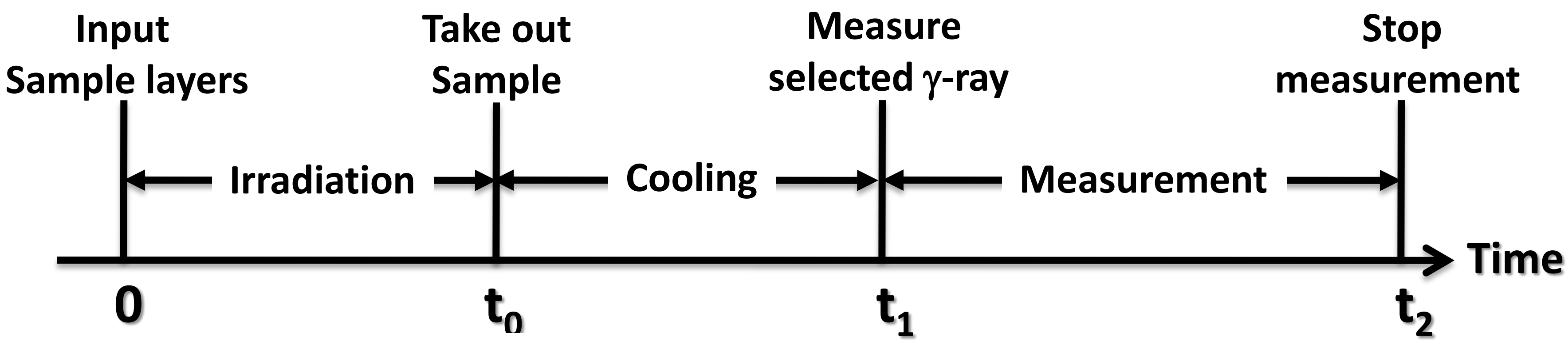
$$y = f(\langle x \rangle) + \sum_{i=1}^{N} \left(\frac{\partial f}{\partial x_i}\right)\Big|_{x=\langle x \rangle} \times (x_i - \langle x_i \rangle)$$

Covariance is derived based on the uncertainties of diversified experimental observables X, which the experimental uncertainty sources.

$$\sigma^2(y) \approx \sum_{i=1}^{N} \left(\frac{\partial f}{\partial x_i}\right)^2\Big|_{x=\langle x \rangle} \sigma_i^2 + \sum_{i \neq j}^{N} \left(\frac{\partial f}{\partial x_i} \cdot \frac{\partial f}{\partial x_j}\right)\Big|_{x=\langle x \rangle} Cov(x_i, x_j)$$

$$\begin{aligned}
Cov(y_i, y_j) &= \left< \left(\sum_{k=1}^{N} \frac{\partial f}{\partial x_k}\Big|_i \Delta x_{ki}\right)\left(\sum_{k=1}^{N} \frac{\partial f}{\partial x_k}\Big|_j \Delta x_{kj}\right) \right> \\
&= \sum_{kk'=1}^{N} \frac{\partial f}{\partial x_k}\Big|_i \frac{\partial f}{\partial x_{k'}}\Big|_j < \Delta x_{ki} \Delta x_{k'j} > \\
&= \sum_{kk'=1}^{N} \frac{\partial f}{\partial x_k}\Big|_i \frac{\partial f}{\partial x_{k'}}\Big|_j \rho_{ij}^{kk'} \sigma_{ik} \sigma_{k'j} \\
&= \sum_{kk'=1}^{N} \rho_{ij}^{kk'} \left(\frac{\partial f}{\partial x_k}\Big|_i \sigma_{ik}\right)\left(\frac{\partial f}{\partial x_{k'}}\Big|_j \sigma_{k'j}\right) \\
&= \sum_{kk'=1}^{N} \rho_{ij}^{kk'} \Delta y_{ki} \Delta y_{k'j}
\end{aligned}$$

Experimental Scheme of Activation



$$\sigma = \frac{\lambda AFC}{MN_A \eta \Phi S D \varepsilon I_\gamma K}$$

Observables in activation measurement:

λ: Decay constant

A: Atomic weights for sample

F: Correction factor in total γ activation

C: Counts of full energy peak

M: Mass of sample

η: isotope abundance in sample

Φ: neutron flux

S: Saturation factor

ε: Efficiency of detector

I_γ: Full energy peak efficiency

K: Fluctuation factor of neutron flux

$$D = e^{-\lambda(t_1 - t_0)} - e^{-\lambda(t_2 - t_0)}$$

$^{90}Zr(n, 2n)^{89}Zr$

39 sets of experimental data measured with activation

序号 IND	EXFOR 编号	年代	作者	能量(MeV)	点数	INSTITUTE	设备	中子源	测量方法	探测器	MONITOR
1	10022018	1969	R.C.Barrall+	1.46e7~	1	1USASTF	HENRE	D-T	ACTIV	NAICR	13-AL-27(N,A)11-NA-24,,SIG
2	10431039	1971	A.Bari	1.48e7~	1	1USAARK	CCW	D-T	ACTIV	GELI	26-FE-56(N,P)25-MN-56,,SIG
3	10477009	1975	R.A.Sigg+	1.48e7~	1	1USAARK	CCW	D-T	ACTIV	GELI SCIN	13-AL-27(N,P)12-MG-27,,SIG 13-AL-27(N,A)11-NA-24,,SIG
4	10536015	1975	B.P.Bayhurst+	1.41e7~2.45e7	7	1USALAS	CCW VDG	P-T D-TD-T D-D	ACTIV	PROPC	13-AL-27(N,A)11-NA-24,,SIG
5	10536016			1.62e7~2.80e7	4	同上	VDG	D-D D-T	ACTIV	PROPC	1-H-1(N,EL)1-H-1,,DA
6	10751002	1978	S.L.Sothras+	1.48e7~	1	1USASMU	VDG	D-T	ACTIV	GELI	13-AL-27(N,P)12-MG-27,,SIG 82-PB-208(N,2N)82-PB-207-M,,SIG 26-FE-56(N,P)25-MN-56,,SIG
7	11645014	1961	R.J.Prestwood +	1.21e7~1.98e7	15	1USALAS		D-T	ACTIV		92-U-238(N,F),,SIG
8	11896005	1960	C.H.Reed	1.41e7~	1	1USALAS			ACTIV		
9	12956006	1975	R.Spangler+	1.41e7~	1	1USATEX		D-T	ACTIV	NAICR	13-AL-27(N,A)11-NA-24,,SIG
10	20033009	1965	R.Rieder+	1.40e7~1.47e7	3	2AUSIRK	CCW	D-T	ACTIV	NAICR	13-AL-27(N,A)11-NA-24,,SIG 13-AL-27(N,A)11-NA-24,,SIG
11	20033010			1.47e7~	2	同上	同上	同上	同上	同上	同上
12	20513009	1974	S.M.Qaim+	1.47e7~	1	2GERJUL	DYNAGEN	D-T	ACTIV	GELI	13-AL-27(N,A)11-NA-24,,SIG
13	20891014	1968	B.Minetti+	1.47e7~	1	2ITYTUR	CCW	D-T	ACTIV		
14	21807002	1982	A.Pavlik+	1.23e7~1.95e7	13	2AUSIRK 2ZZZGEL	CCW 2AUSIRK VDG 2ZZZGEL	D-T	ACTIV	NAICR	13-AL-27(N,A)11-NA-24,,SIG 1-H-1(N,EL)1-H-1,,SIG
15	21807003			1.34e7~1.48e7	17	同上	同上	同上	同上	同上	同上

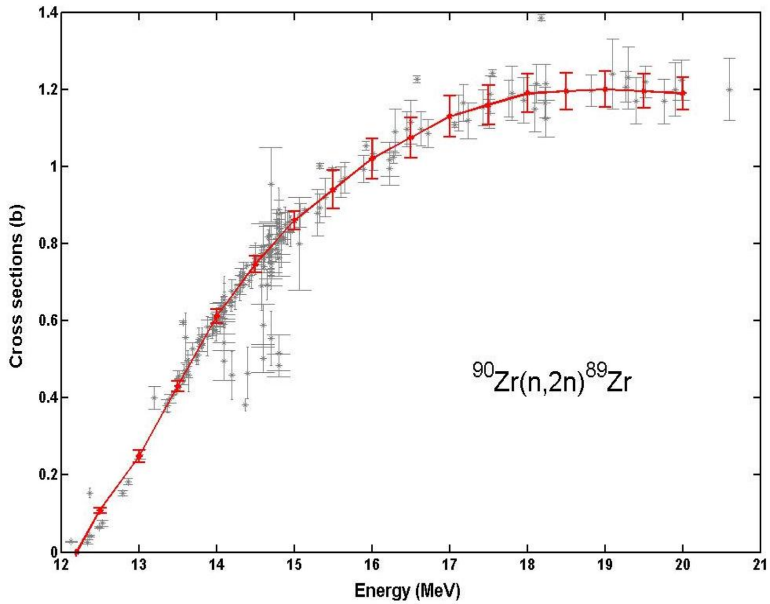
$^{90}Zr(n, 2n)^{89}Zr$

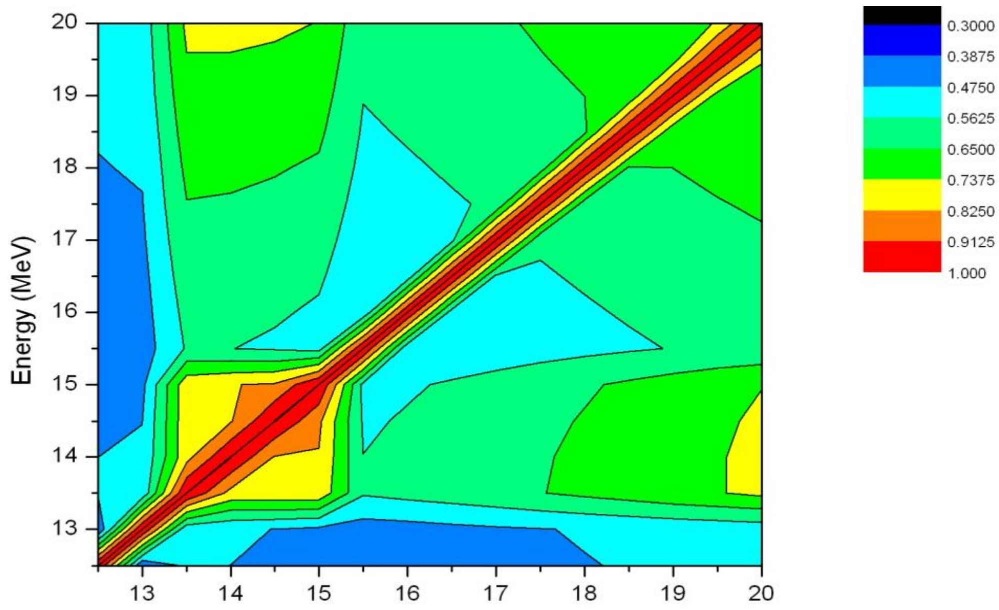
Mainly supported by Hanlin Lu(CNDC)

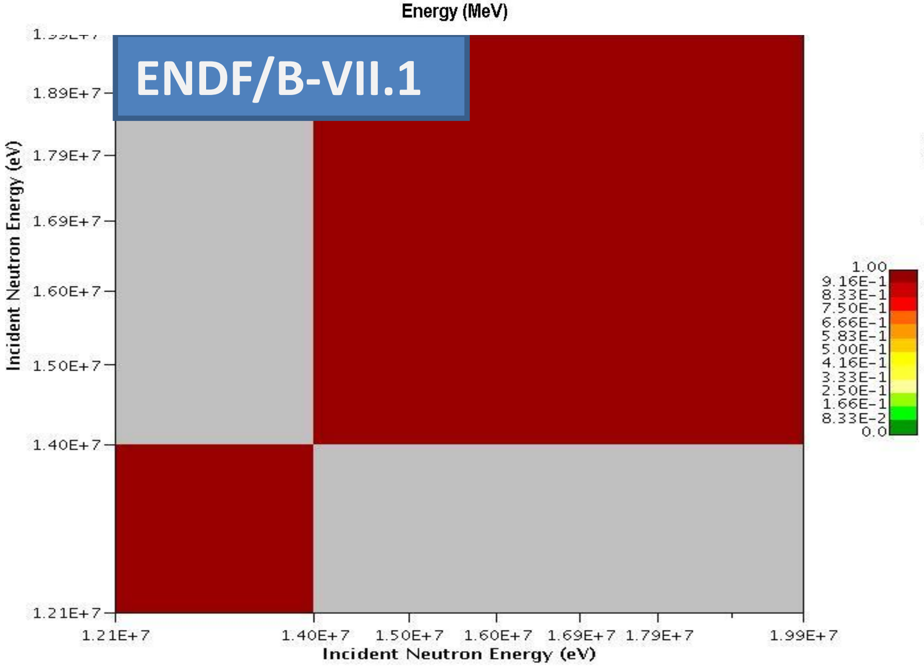
To an extend, ASEU is trying to express the current skill level of experiment.

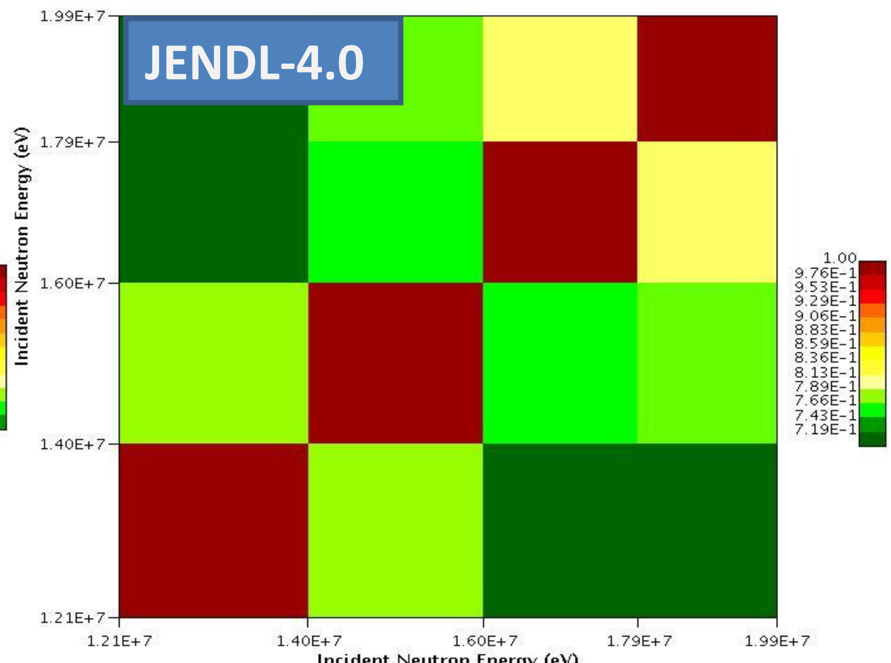
Observables in measurement		Uncertainties of $^{90}Zr(n,2n)\,^{89}Zr$		Correlations (averaged value)
	Error source	12-20MeV	13.5-15MeV	
Statistics	Count	4.0-0.6%	0.3-0.6%	0.0
Neutron flux	● Differential C.S. T(d,n)^{4}He ● Background correction from D-D and other nuclei ● correction for neutron scattering	3-1% 1% 1.5-0.6%	1% 0.5% 0.5%	0.3 1.0 0.0
Sample	● Sample weighting ● Isotopic abundance ● γ self-absorption	0.5% 0.2% 0.5%	Same Same Same	1.0 1.0 1.0
Monitor err. $^{27}Al(n,\alpha)^{24}Na$	Cross section error of Monitor	4-2%	1.3-0. 5%	0.6
Detector err.	Efficiency of detector	2%	Same	1.0
Activation	Decay data	1%	Same	1.0
others	Time of irradiation	0.1%	Same	1.0

$^{90}Zr(n, 2n)^{89}Zr$

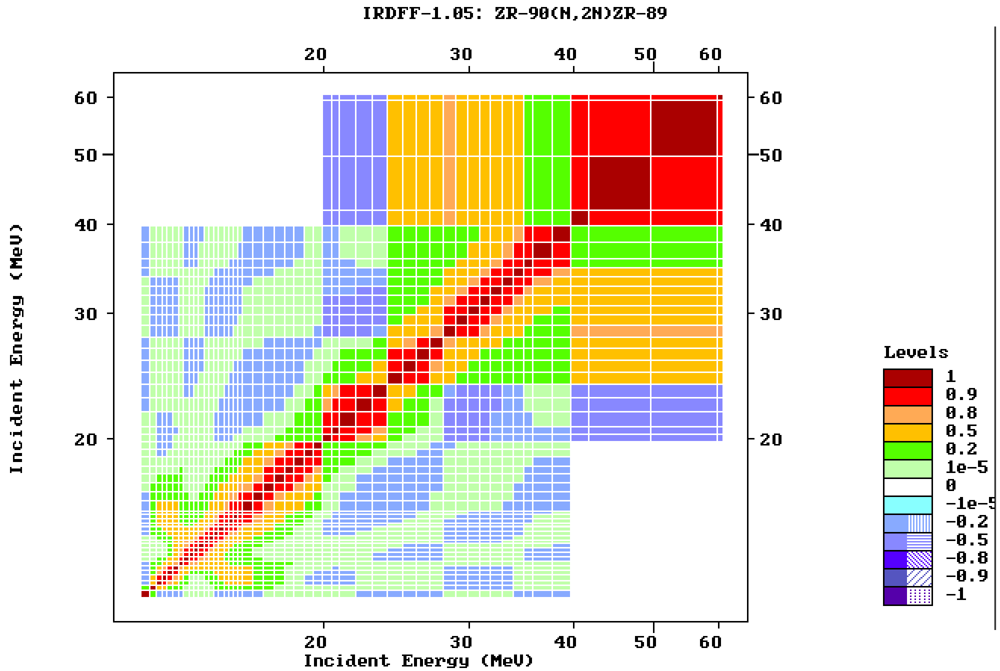


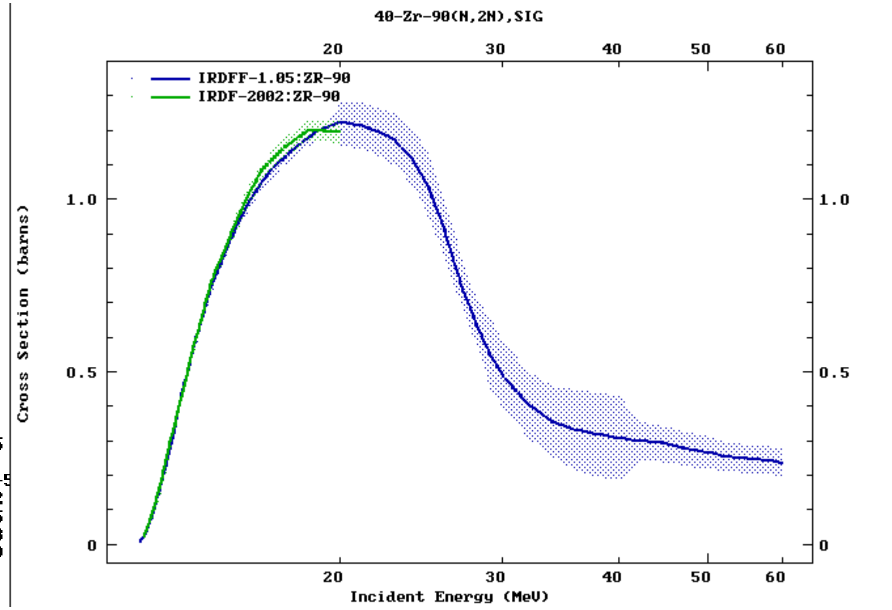






$^{90}Zr(n,2n)^{89}Zr$



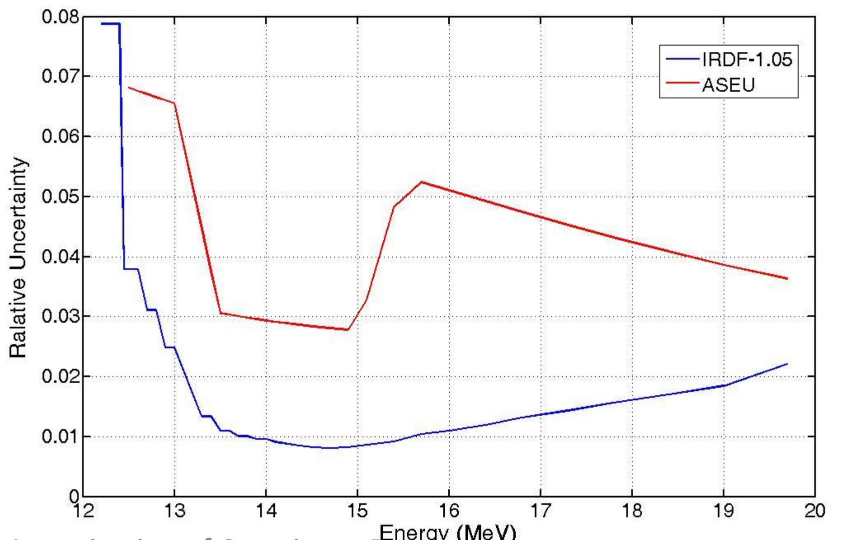


IRDF-1.05:

0-20MeV: K. I. Zolotarev

20-60MeV: Trkov

Produced by LS method



Contents

Model dependent COV

Para. Estimation by Bayesian statistics

$$p(\mathbf{p}|D) = L(D|\mathbf{p})p_a(\mathbf{p})/[\int L(D|\mathbf{p}')p_a(\mathbf{p}')d\mathbf{p}']$$

Para. COV

$$(V_p)_{kq} = \langle(p_k-\langle p_k\rangle)(p_q-\langle p_q\rangle)\rangle$$
$$= \int(p_k-\langle p_k\rangle)(p_q-\langle p_q\rangle)p(\mathbf{p}'|D)d\mathbf{p}'$$

$$p(\mathbf{p}|D) = C\exp\{(-1/2)[\mathbf{y}-\mathbf{f}(\mathbf{p})]^+\mathbf{V_y}^{-1}[\mathbf{y}-\mathbf{f}(\mathbf{p})]\}$$

$$p(\mathbf{p}|D) = C\exp\{(-1/2)[\mathbf{y}-\mathbf{f}(\mathbf{p})]^+\mathbf{V_y}^{-1}[\mathbf{y}-\mathbf{f}(\mathbf{p})]\}p_a(\mathbf{p})$$

$p_a(\mathbf{p}) = 1$ （等概率假设）

$$[\mathbf{y}-\mathbf{f}(\mathbf{p})]^+\mathbf{V_y}^{-1}[\mathbf{y}-\mathbf{f}(\mathbf{p})] = \text{minimum}$$

$$p(\mathbf{p}|D) = C\exp\{(-1/2)[\mathbf{y}-\mathbf{f}(\mathbf{p})]^+\mathbf{V_y}^{-1}[\mathbf{y}-\mathbf{f}(\mathbf{p})] + (-1/2)(\mathbf{p}-\mathbf{p_a})^+\mathbf{V_a}^{-1}(\mathbf{p}-\mathbf{p_a})\}.$$

$$[\mathbf{y}-\mathbf{f}(\mathbf{p})]^+\mathbf{V_y}^{-1}[\mathbf{y}-\mathbf{f}(\mathbf{p})] + (\mathbf{p}-\mathbf{p_a})^+\mathbf{V_a}^{-1}(\mathbf{p}-\mathbf{p_a}) = \text{minimum}$$

LS:

$$\Delta\hat{C} = (F^TV^{-1}F)^{-1}F^TV^{-1}(Y-Y_0)$$

$$\hat{V}_C = (F^TV^{-1}F)^{-1}$$

$$\hat{Y} = F\Delta\hat{C} + Y_0$$

$$\hat{V}_{\hat{Y}} = FV_cF^T$$

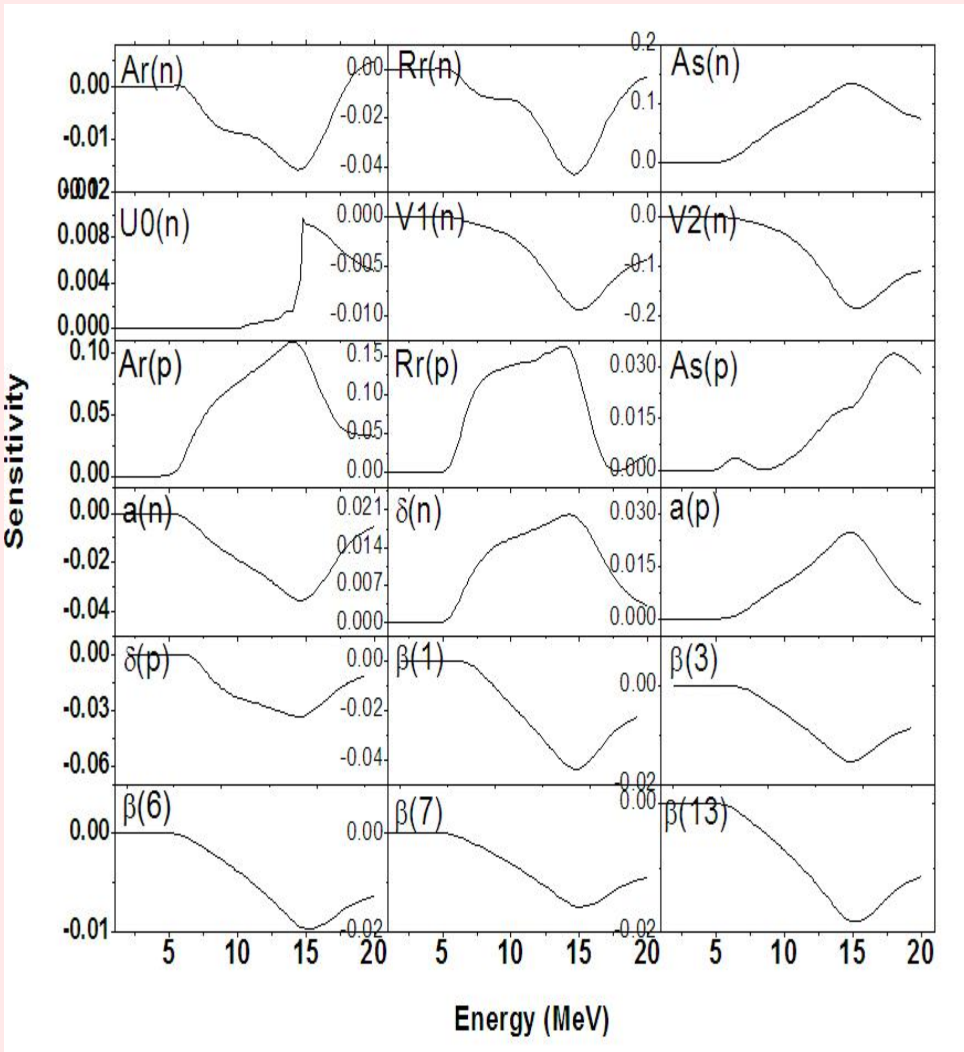
Central issues:

Sensitivity (F)

Exp. COV (V_Y)

灵敏度计算结果举例

Sensitivity of para. for $^{48}Ti(n,p)^{48}Sc$



34 theo. para.

- OMP for neutron：

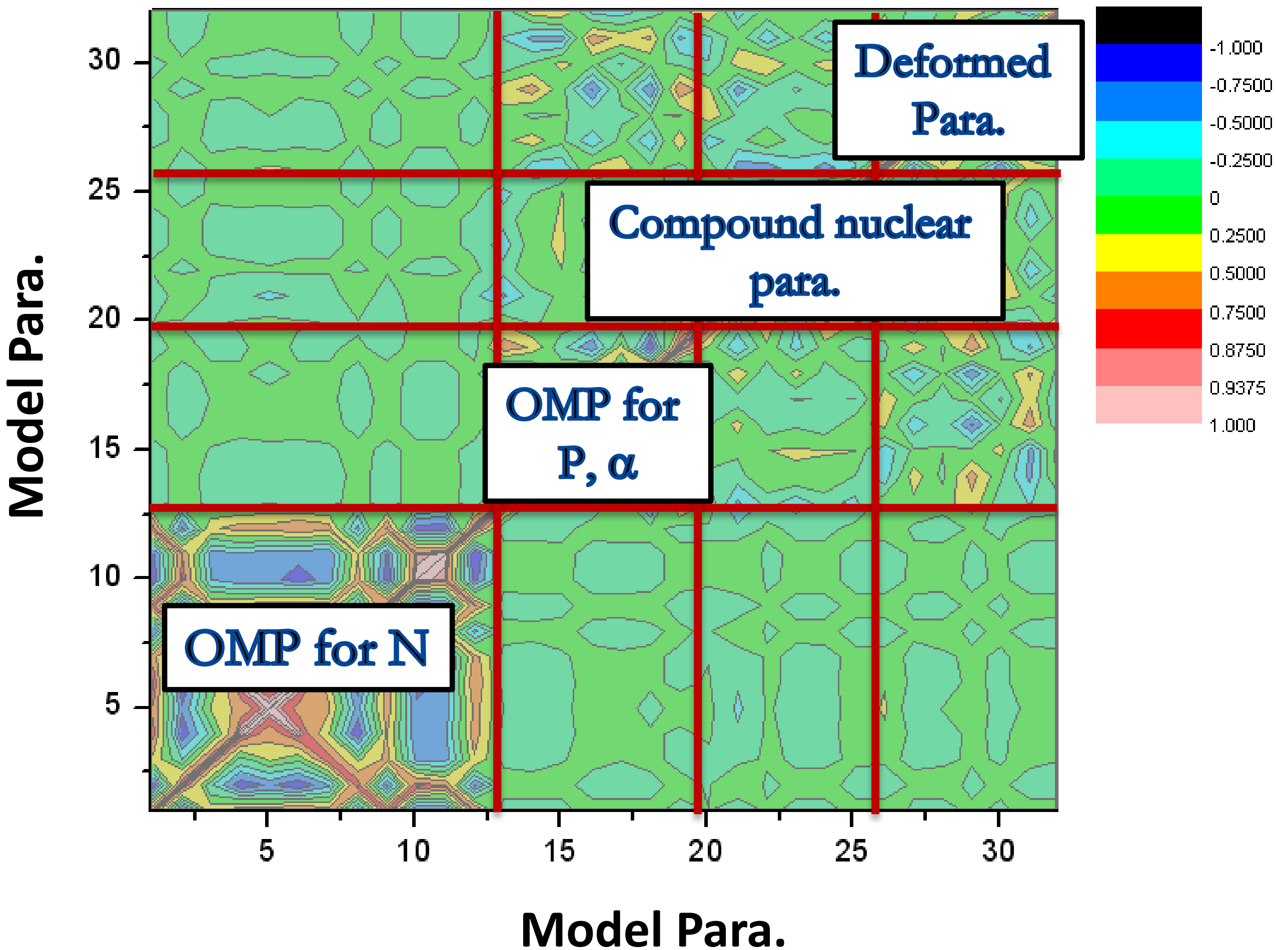
U0, V0, V1, V2, VSO, W0, Rr, Ar, As, Aso

- OMP for proton： V0, W0, Rr, Ar, As
- OMP for ^{4}He ： U0, Rr, Ar
- Level density, pair correction for

  (n,inl), (n,p), (n,^{4}He), (n,2n)
- XS by E1 GDR (n,inl), (n, γ)
- Kalbach factor： K
- Beta deformed values for 5 inelastic levels

→ Values > 10^{-3}

n+^{48}Ti Correlated coefficient matrix



Summary 究 RGY

The current covariance scheme is utilized in the evaluation of COV for structure nuclei and fission nuclei for CENDL.

Correlation is one of the most important components in the LS approach to experimental data evaluation. It is really impossible to ‘honestly’ derive all correlations between adopted multiple sets of . The fact promotes us to find a compensate way in nuclear data evaluation.

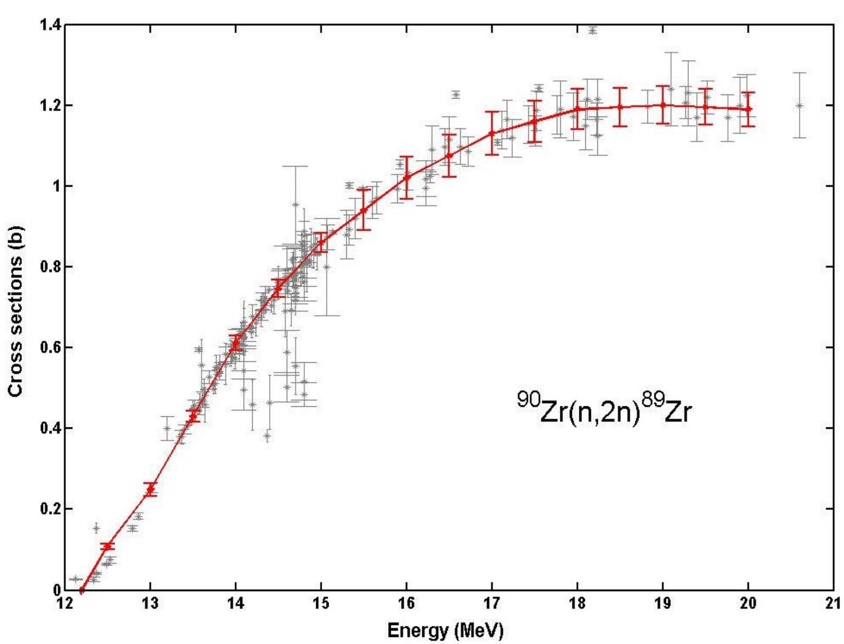
Besides LS approach, thoroughly *analyze the sources of experimental uncertainties (ASEU)* is helpful to provide an auxiliary way to construct covariance directly from adopted experimental data. It derives a covariance to express the current level of ability in experiments comprehensively, which is more acceptable by Experimental Physicist, Roberto recommends to use this Experimental covariance as the prior input of LS.

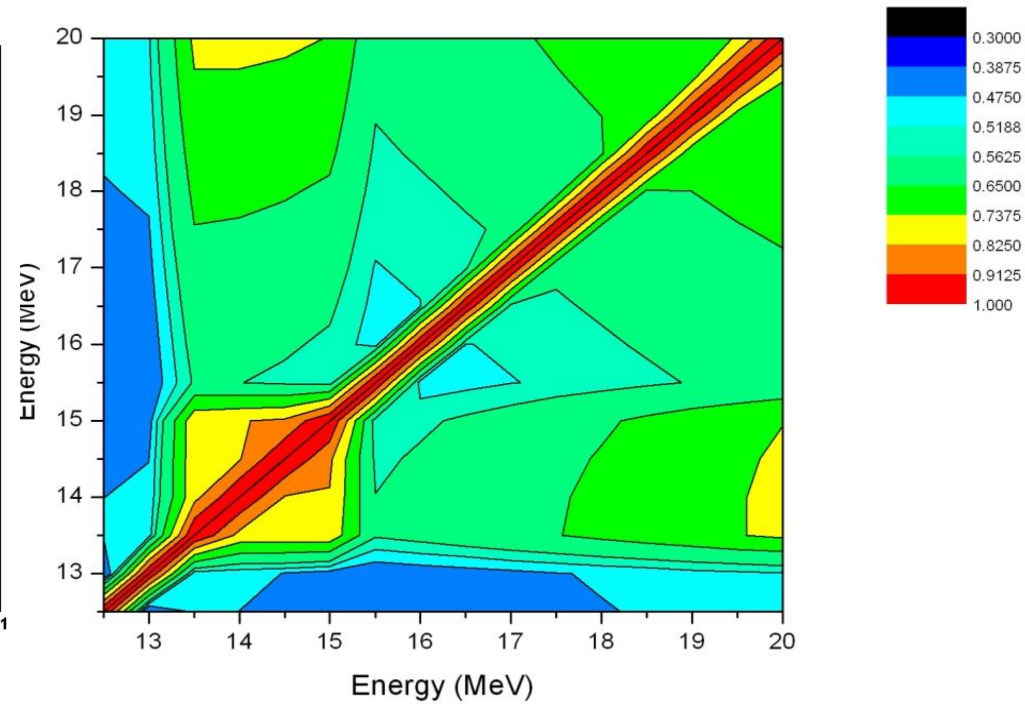
We are discussing the nonlinear impact on the COV of the model-dependent case recently.

Thank you!

$^{90}Zr(n,2n)^{89}Zr$

- This covariance is directly produced from experimental observable uncertainties in Table above but not LS.
- 39 set of experimental data, which are used in cross section fitting by LS, are adopted in the separated covariance evaluation.
- The linear energy dependence is taken both for uncertainty and correlation.
- *Correlated uncertainty will be decreased in future regarding multi-sets of data are available at same energy region.*



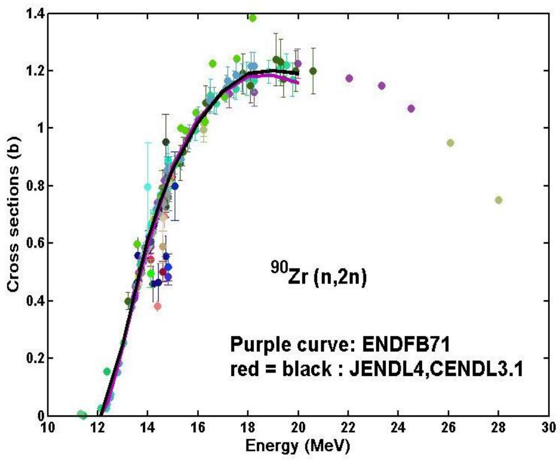


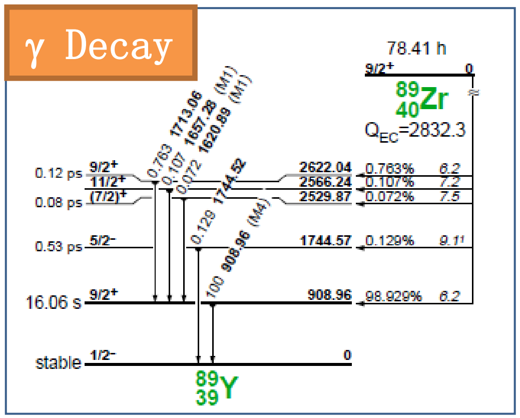
$^{90}Zr(n, 2n)^{89}Zr$

CHINA INSTITUTE OF ATOMIC ENERGY

ASEU for $^{90}Zr(n,2n)^{89}Zr$:

Experiment conditions in ASEE interests	
1	Time
2	Energy region
3	Num. of reported Energies
4	Institute
5	Accelerator
6	Neutron source
7	Method
8	Detector
9	Monitor cross sections





- E_{th} = 12.1MeV, relative higher, easy avoid the influence from neutrons at low energies;
- $T_{1/2}$ of ^{89}Zr = 78hour, sample is easy to be irradiated, cooled and detected;
- Few cascading in ^{89}Y decay, better to be detected.
- 39 measurements are available in EXFOR

Activation measurement is adopted for all experiments.
Most of γ energies are selected as 909keV from ^{89}Y