IRSN
INSTITUT DE RADIOPROTECTION
ET DE SÛRETÉ NUCLÉAIRE

NUCLEAR DATA EVALUATION

ARIEL-H2020 INTERNATIONAL ON-LINE SCHOOL ON NUCLEAR DATA: THE PATH FROM THE DETECTOR TO THE REACTOR CALCULATION – NUDATAPAT

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Presentation Roadmap

- Nuclear Data: basic definitions

- Measurements and Evaluations: Where do they come from and what are they needed?

- Data processing for practical applications

  Data representation

  Data processing tools

  Data format for practical applications

- Examples

- Concluding Remarks

Institut de Radioprotection et de Sûreté Nucléaire* – IRSN

(Established on February 22, 2002 with a contingent workforce of about 1700 specialists)

MISSIONS:

- Provide support for the public authorities in nuclear safety and radiation protection for civil and defense activities, and safety of nuclear facilities and materials...
- Make available an emergency response center that can be called in at all times, together with field response teams…
- Define and implement national and international research and study programs…
- Contribute to radiological monitoring of the national territory and workers exposed to ionizing radiation...
- Contribute to providing the public with information in the field of radiological and nuclear risks…

*Institute for Radiological Protection and Nuclear Safety

Why data measurements and evaluation?

Speed of Light

O. C. Roemer (1676):	214,300,000 m/s
J. Bradley (1725):	299,042,000 m/s
A. H. L. Fizeau (1849):	315,300,000 ± 5,000,000 m/s
J. B. L. Foucault (1862):	298,000,000 ± 5,000,000 m/s
A. A. Michelson (1926):	299,796,000 ± 4,000 m/s
K. M. Evenson (1973):	299,792,458 ± 1.2 m/s

Most Recent Adopted Standard Light Speed Value is: 299,792,458 ± 1.2 m/s
(2014 CODATA* recommended values)
***Comité de données pour la science et la technologie**

Tokio Fukahori

Practical Application:

Time independent transport equation

$$\hat{\Omega}.\nabla\Phi + \Sigma_t\Phi = \int_{4\pi} d\hat{\Omega}' \int_0^{\infty} dE' \Sigma_s(E' \rightarrow E, \hat{\Omega}' \rightarrow \Omega)\Phi(E', \vec{r}', \hat{\Omega}) + S$$

Σ_t Macroscopic total cross section

$$S_t = S_s + S_f + S_g + S_{n,n'} + S_{n,2n} + \ldots$$

Σ_s Macroscopic scattering cross section

Source:

a) External
b) Internal $(\nu\Sigma_f\Phi)$

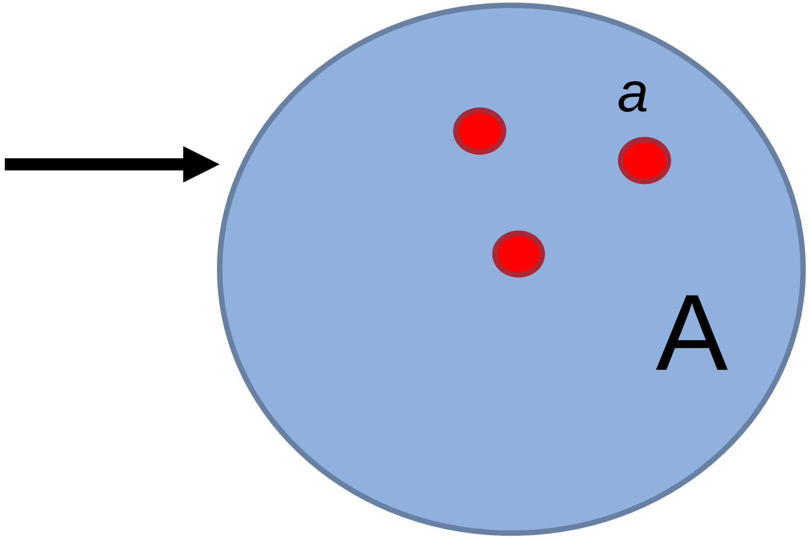
Accurate solution of the transport equation is the key for any problem. Hence the importance of the nuclear data is evident !!

Cross-Section Generation: The Big Picture for Practical Applications

How are these quantities determined:

(a) Measured by the time-of-flight technique, measured at reactors;
(b) Evaluated by using nuclear physics code describing the neutron-nucleus interaction;
(c) Generated using nuclear physics codes. This is not a good decision. It is seen as the last resort;

Simple Model of Particle Interactions



1. Probability that one arrow thrown at the small circle red of area a within A and reach a

$$\frac{a}{A}$$

2. If within A there are N a's then the probability is

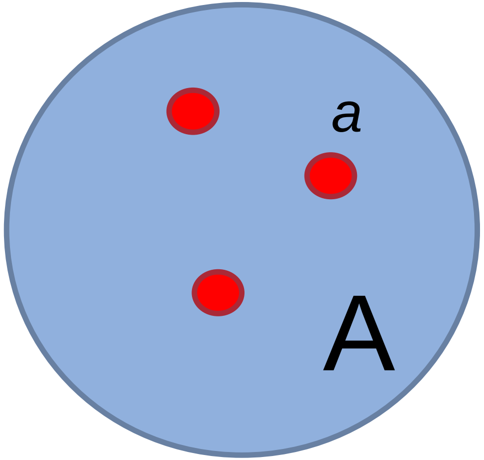
$$\frac{Na}{A}$$

3. However, if n arrows are thrown the probability becomes

$$\frac{\boldsymbol{Na}}{\boldsymbol{A}}n$$

This represents the expected numbers of hits

Simple Model of Particle Interactions



Numbers of hits with success:

$$\frac{Na}{A}n$$

1. If the arrows are incident particles (neutrons, protons, etc) it is not appropriate to think of individual particles. The ratio $^{n}/_{A}$ (number of particles n that arrives on A) is called the particle fluence. This quantity depends on the energy of the incident particle and is denoted by $\varphi(E) = {}^{n}/_{A}$

2. If each of the constituent of A is a nucleus with area a (a is called the cross section of that nucleus). It is a common practice to represent that area with the Greek letter σ

3. The number of hits is referred to as the reaction rate R. It is a measurable quantity

$$R = N\sigma\,\varphi(E)$$

4. The cross section can then be measured as

$$\sigma(E) = \frac{\left\{ {}^{R(E)}/_{N} \right\}}{\varphi(E)}$$

Simple Model of Particle Interactions

Some observations

$$\sigma(E) = \frac{\left\{ R(E) / N \right\}}{\varphi(E)}$$

1. Since the cross section $\boldsymbol{\sigma(E)}$ represents an area its unit is in cm^2

2. In the "atomic world" the unit barn is frequently used, that is,

   1 barn = 10^{-24} cm^2

3. Hence a nucleus with 1 barn cross section its nuclear radius is estimated to be about, from $\boldsymbol{\pi R^2}$, $\boldsymbol{R \sim 5.6 \times 10^{-13}}$ cm or 1 fm = $\boldsymbol{10^{-13}}$ cm

   Ex: ^{238}U $\boldsymbol{R} \sim 9.48$ fm then $\boldsymbol{\sigma_s} \sim 11.29$ barns

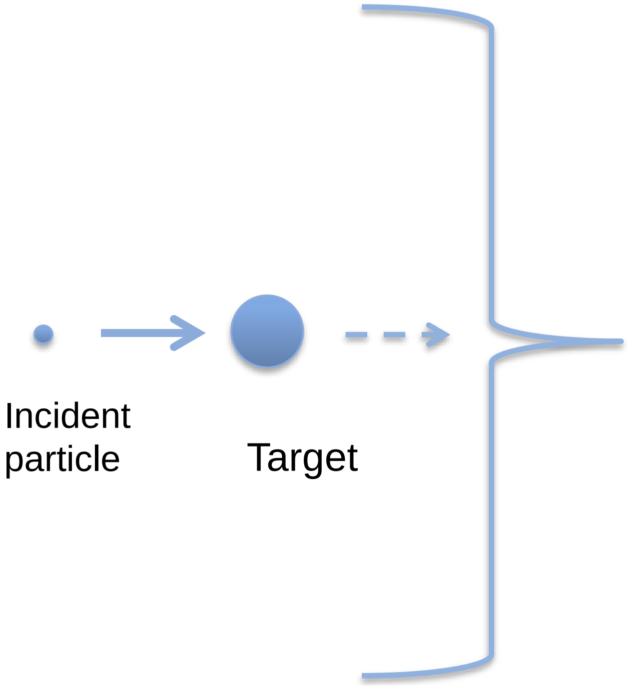
4. It is interesting to see that the unit for the quantity $\boldsymbol{N\sigma}$ is cm^{-1}

In Summary:

$\sigma(E)$ is known as the microscopic cross section.
It is an universal quantity which describes a particular nuclide. For instance, the ^{235}U fission cross section.

$\Sigma(E) = N\,\sigma(E)$ $\Sigma(E)$ is known as the macroscopic cross section. It is a problem dependent quantity.

Types of Microscopic Cross Sections



Resulting Reactions:

- (n,n) Elastic Scattering
- (n,n') Inelastic Scattering
- (n,γ) Radiative Capture
- (n,f) Fission
- (n,p), (n,α), (n,d) charge particle
- Etc

Some words of clarification

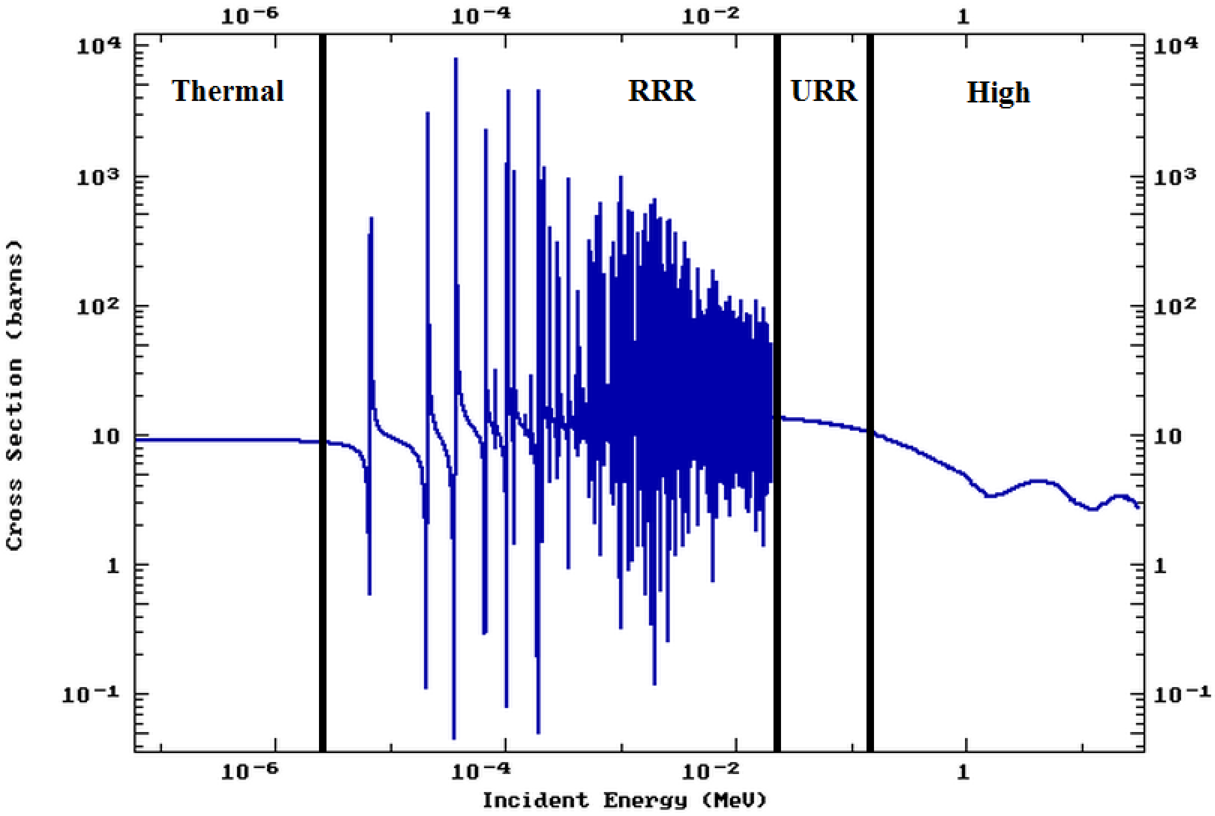
a) Thermal region: neutron energy is comparable to the chemical binding energy of the atoms in the molecule. Neutrons can gain or loose energy in the interaction process. Cross sections are a smooth function of energy;

b) Resolved and unresolved resonance region (RR and UR): compound nucleus formation leading to a very intricate shape of the cross section (resonances). Direct reactions are also possible. Cross sections are no longer a smooth function of the energy. High resolution time-of-flight machines are need to better see the resonances;

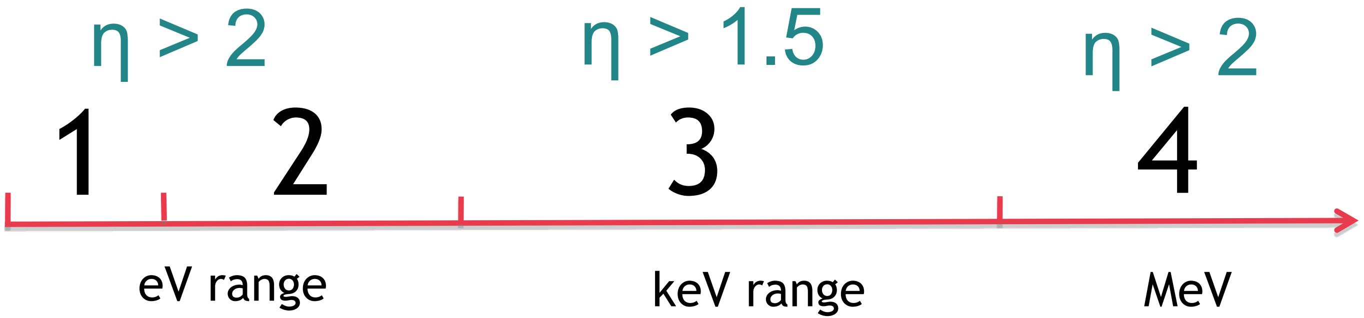
c) High energy: compound nucleus formation and direct reactions occurs: Resonance structures can no longer be noticeable. Cross sections are a smooth function of energy;

In all energy regions there are always SCATTERING and REACTION

^{238}U Elastic Scattering Cross Section at 0K



Energy Regions of Interest for Applications



- 1-2: Thermal Reactors (Thermal Scattering, smooth cross sections) – Neutron soft-spectrum;

- 3: Resonance region (highly oscillating data, resonance self shielding effects, etc.);

- 4: Fast region (Smooth cross section data)

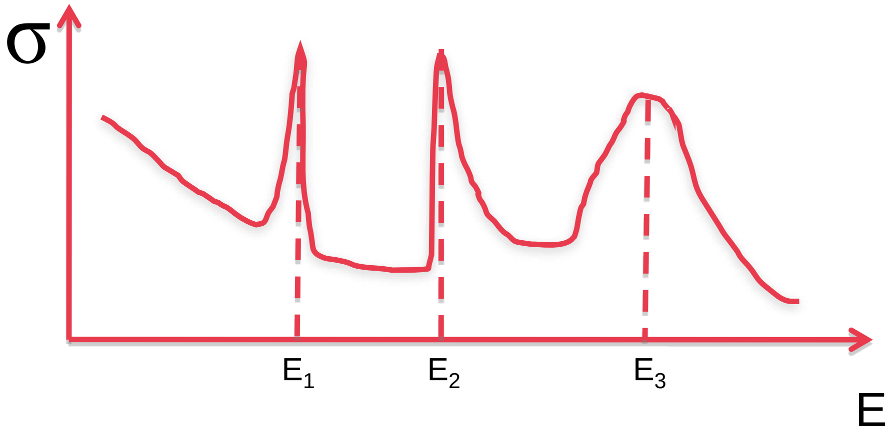
$$k_{eff} \propto \boldsymbol{\eta}$$

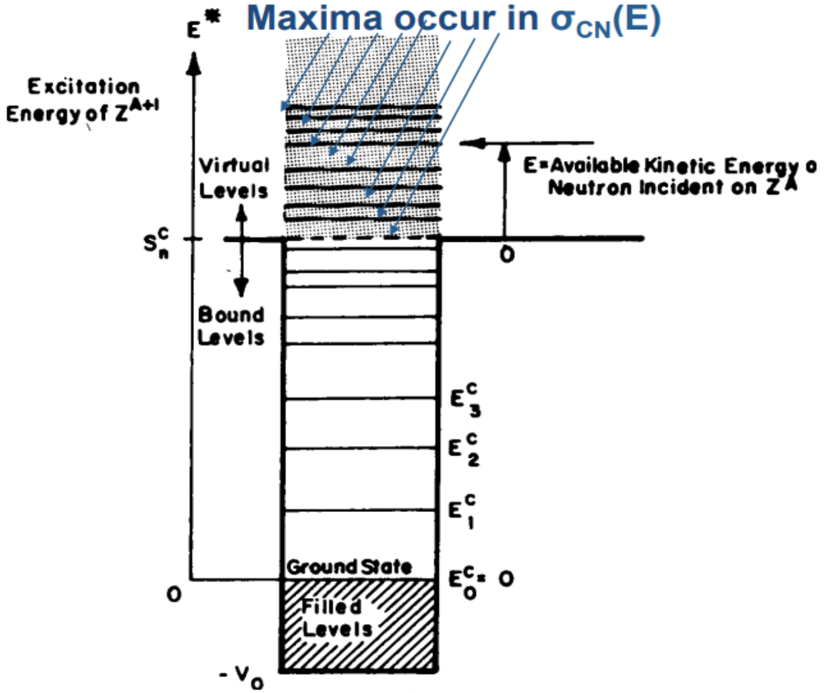
$$\boldsymbol{\eta} = \frac{\boldsymbol{\nu\sigma}_f}{\boldsymbol{\sigma}_a}$$

Resolved Energy Region:

Experimental resolution is smaller than the width of the resonances; resonances can be distinguished (“seen”). Cross section representation can be made by resonance parameters.

Compound Nucleus Energy Levels: resonances occurs





R-Matrix Formalisms

R-Matrix

- **Single-Level Breit-Wigner** **(Wigner-Eisenbud)**
- **Multi-Level Breit-Wigner** **(Wigner-Eisenbud)**
- **Adler-Adler** **(Kapur-Peierls)**
- **Reich-Moore** **(Wigner-Eisenbud)**
- **Multipole** **(Kapur-Peierls)**
- **R-Matrix Limited**

Unresolved Energy Region:

Cross section fluctuations still exist but experimental resolution is not enough to distinguish multiplets. Cross section representation made by average resonance parameters.

Cross section formalism:
Statistical models such as the Hauser-Feshbach model combined with Optical model; level density models based on Bethe theory or Gilbert and Cameron theory, etc.; fission widths model based on Hill-Wheeler fission barrier penetration theory; giant dipole mode for gamma capture widths, etc.

High Energy Region:

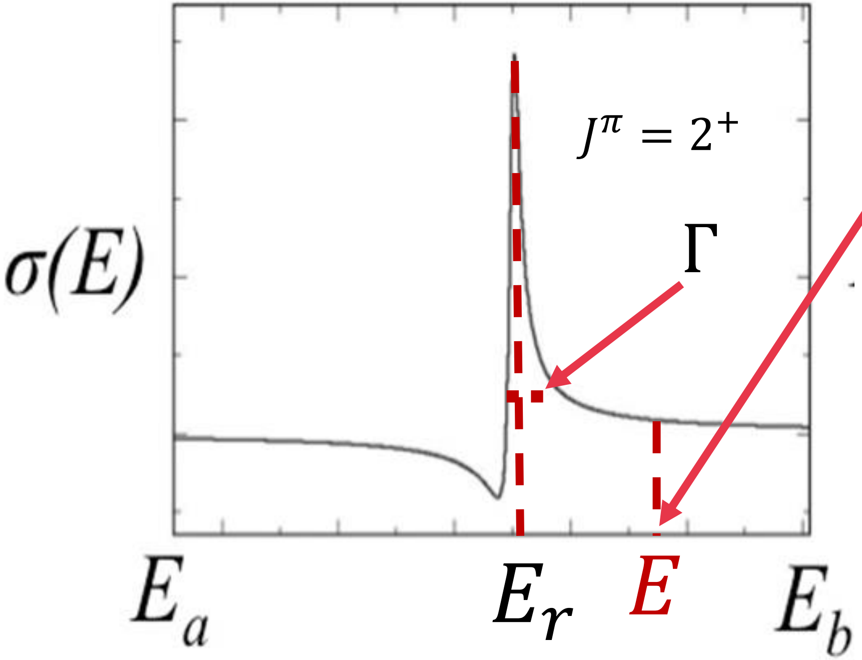
No cross section fluctuations exist. Cross sections are represented by smooth curves.

Cross section formalism:

Statistical models such as the Hauser-Feshbach model; intra-nuclear Cascade model; pre-equilibrium model; evaporation model, etc.

Cross Section Resonance Formalism

Example: resonances described by six parameters $E_r, \Gamma_\gamma, \Gamma_n, \Gamma_{f1}, \Gamma_{f2}, J^\pi$
(evaluated parameters)



$$\sigma(E) \approx g(j) \frac{\Gamma_n \Gamma_\gamma / \Gamma}{(E - E_r)^2 + \frac{\Gamma^2}{4}}$$

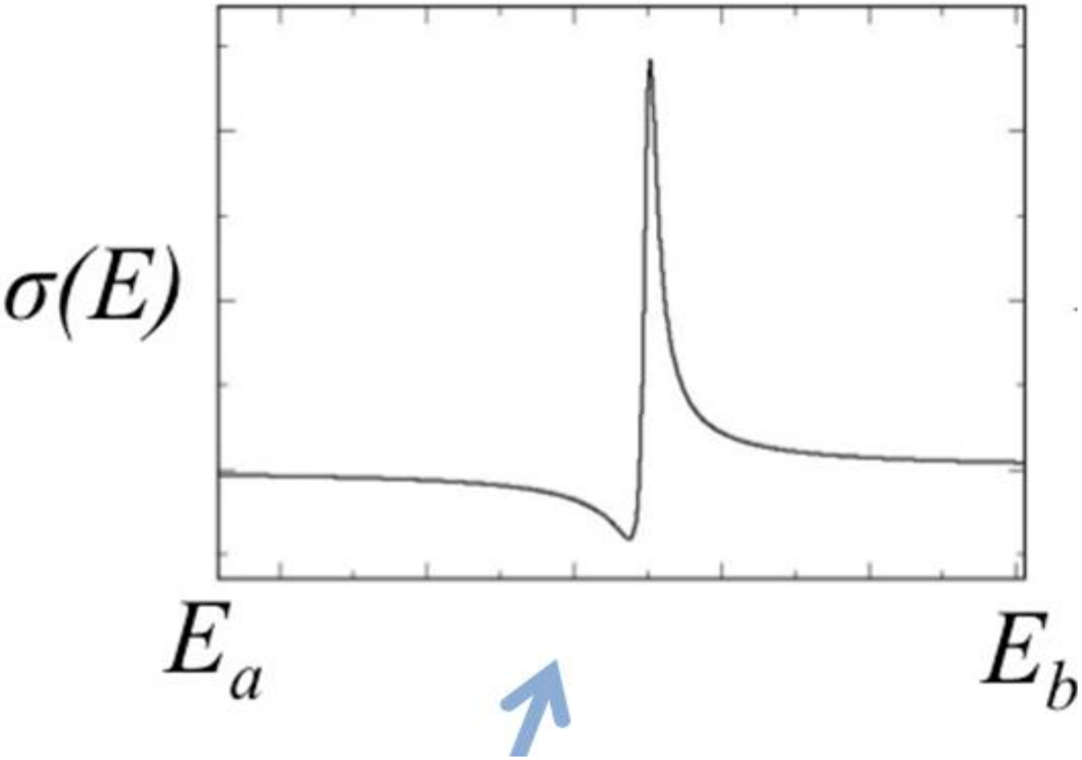
Differential and Integral Data

Differential Data:

Experimental differential data are found in data storages such as EXFOR (EXperimental FORmat) data base

Integral Data:

(a) Integral Criticality Safety Benchmark Experiment Project (ICSBEP). Include critical and subcritical benchmark experiment data;
(b) International Reactor Physics Benchmark Experiments (IRPhE) Project;
(c) Shielding Integral Benchmark Archive and Database (SINBAD)

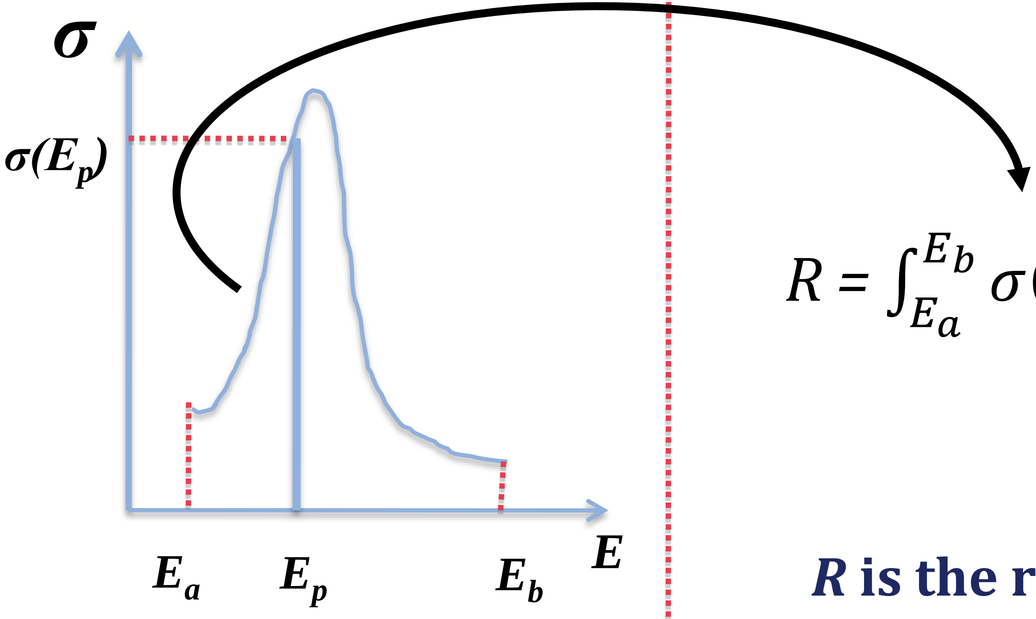


Differential data $\sigma(E) \pm \delta\sigma$

$$R = \int_{E_a}^{E_b} \sigma(E)\varphi(E)dE$$

Integral data $R \pm \delta R$

Differential and Integral



σ(E) as a function of energy

$$R = \int_{E_a}^{E_b} \sigma(E)\varphi(E)dE$$

R **is the reaction rate (measured quantity)**

Differential

Integral

Neutron Cross-Section Measurement Facilities

- Key facilities for neutron cross-section differential data by the time-of-flight (TOF)
  - RPI Gaerttner LINAC (US)
  - ORNL ORELA (US) – shutdown but has archives of data that are still used
  - IRMM GELINA in Belgium (Europe)
- Additional facilities for nuclear data measurements
  - LANL LANSCE (US)
  - ORNL SNS (US) – thermal moderator data measurements
  - CERN n_TOF (Europe)
  - J-PARC (Japan)

Integral Data

Ultimate Goal is to Check and Validate Evaluated Nuclear Data and Methods

- Neutron birth inducing event is unknown
- Can only obtain data integrated over neutron energy
- Sub-critical and critical assembly measurements: reaction rates, number of neutrons per fission, reactivity worth
- Decay constants for radioactive actinides and fission products for use in spent fuel reactivity analysis
- Provide excellent grounds for testing the differential data
- Integral quantities average over energy, space and angle

Simultaneous differential and integral data analysis and evaluation are necessary to remove bias on the data

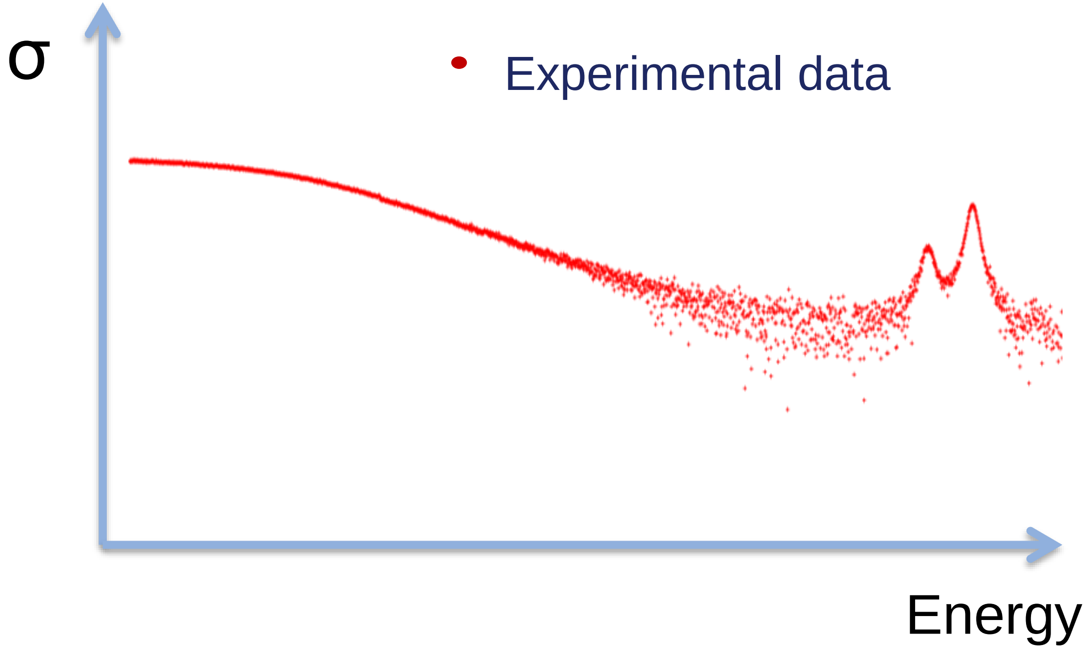
Nuclear Data Evaluation Tools

Nuclear data evaluation codes are used to evaluate the experimental data in a form suitable for application. The evaluated data are converted in the ENDF format and adopted in the nuclear data libraries such as JEFF, ENDF, JENDL, etc.

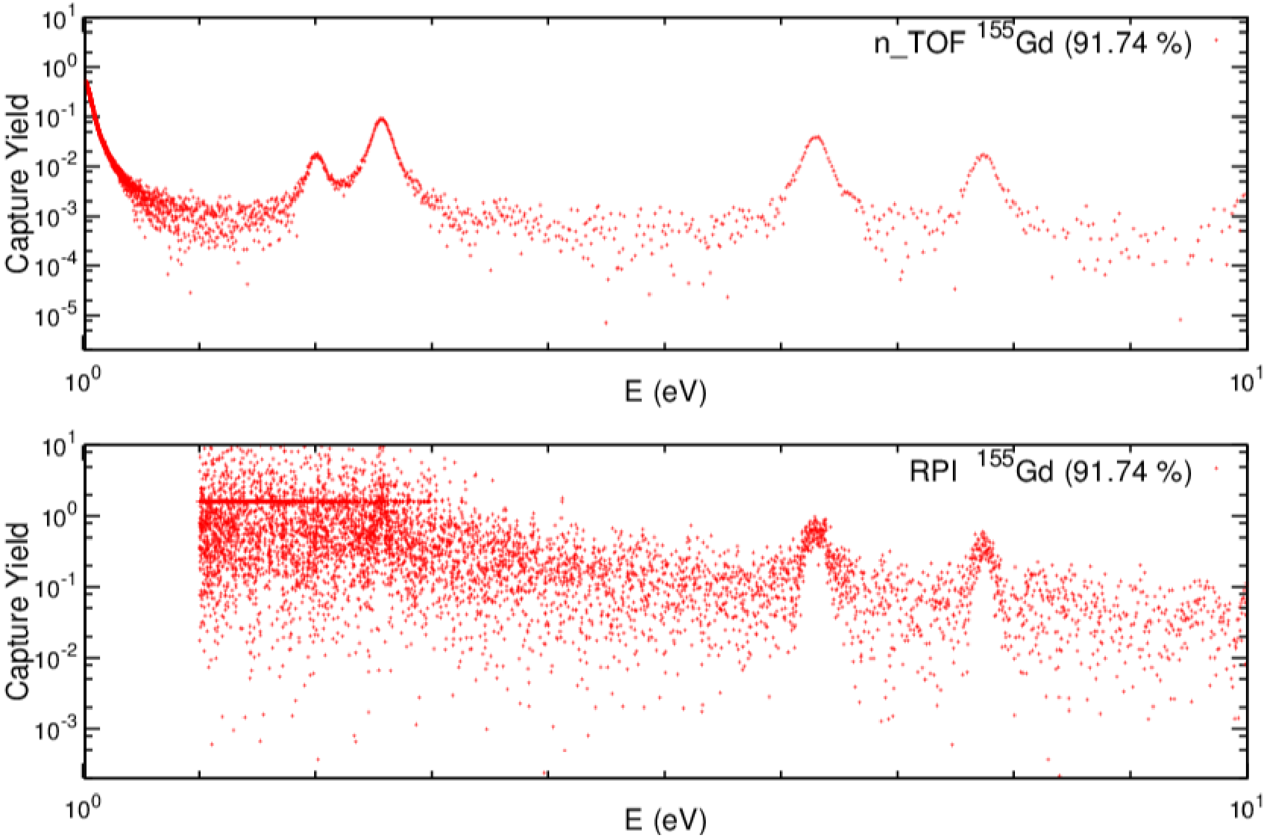
Few existing evaluation tools are:

- SAMMY: developed and maintained at ORNL (US). Used for resonance analysis and evaluation;
- CONRAD: developed and maintained at CEA (France). Used for resonance analysis and evaluation;
- TALYS: available from IAEA. Mainly used for high energy evaluation;

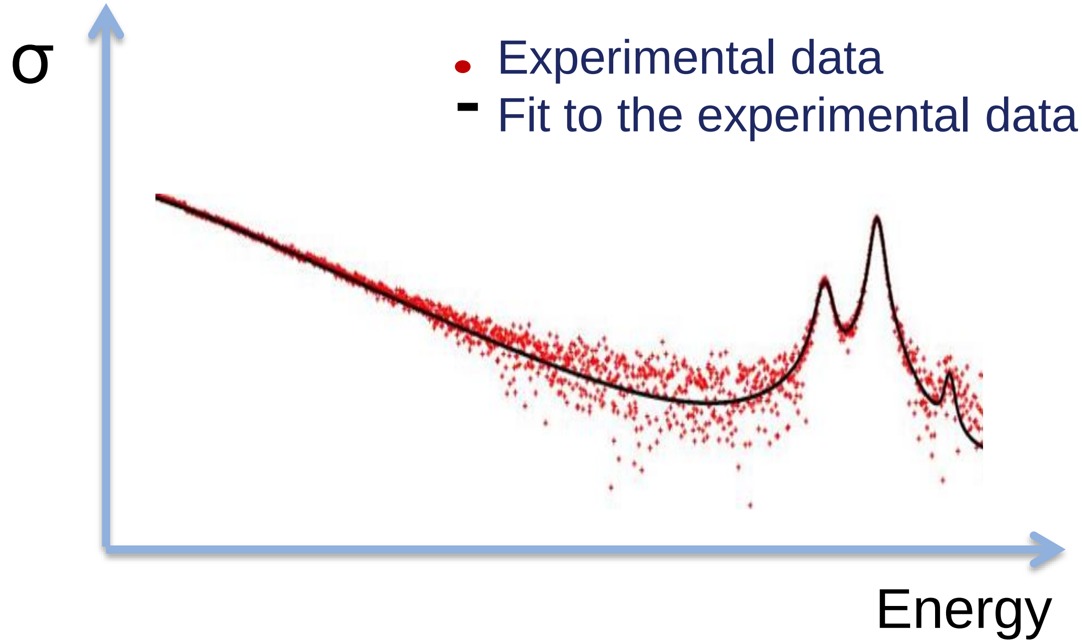
What is a nuclear data evaluation ? Why is it needed for ?



Experimental data



Experimental data



Answer: Best representation of the experimental data with a nuclear model !!

Evaluated Nuclear Data Library

- Include information pertinent to practical applications;
- Information such as cross section, resonance parameters, angular distributions, fission spectrum, thermal scattering data, data covariance, etc.;
- There are quite a few known evaluated nuclear data libraries such as the ENDF, JEFF, JENDL, CENDL, TENDL, etc.;
- Evaluations are tested before their inclusion in the evaluated nuclear data library;

ENDF Data Format (contents)

File	Description	File	Description
1	General Information	10	Cross Sections for the Production of Radioactive Nuclides
2	Resonance Parameters	11	General Comments of Photon Production
3	Neutron Cross Sections	12	Photon Production and Multiplicities and Transition Probability Arrays
4	Angular Distribution of Secondary Particles	13	Photon Production Cross Sections
5	Energy Distribution of Secondary Particles	14	Photon Angular Distribution
6	Coupled Energy-Angle Distribution of Secondary Particles	15	Continuous Photon Energy Spectra
7	$S(\alpha, \beta)$ Scattering Law Data	23	Photon Interaction Cross Section
8	Radioactive Decay and Fission Product Data	27	Atomic From Factors or Scattering Functions
9	Multiplicities for Production of Radioactive Nuclides	30 - 40	Data Covariance Files

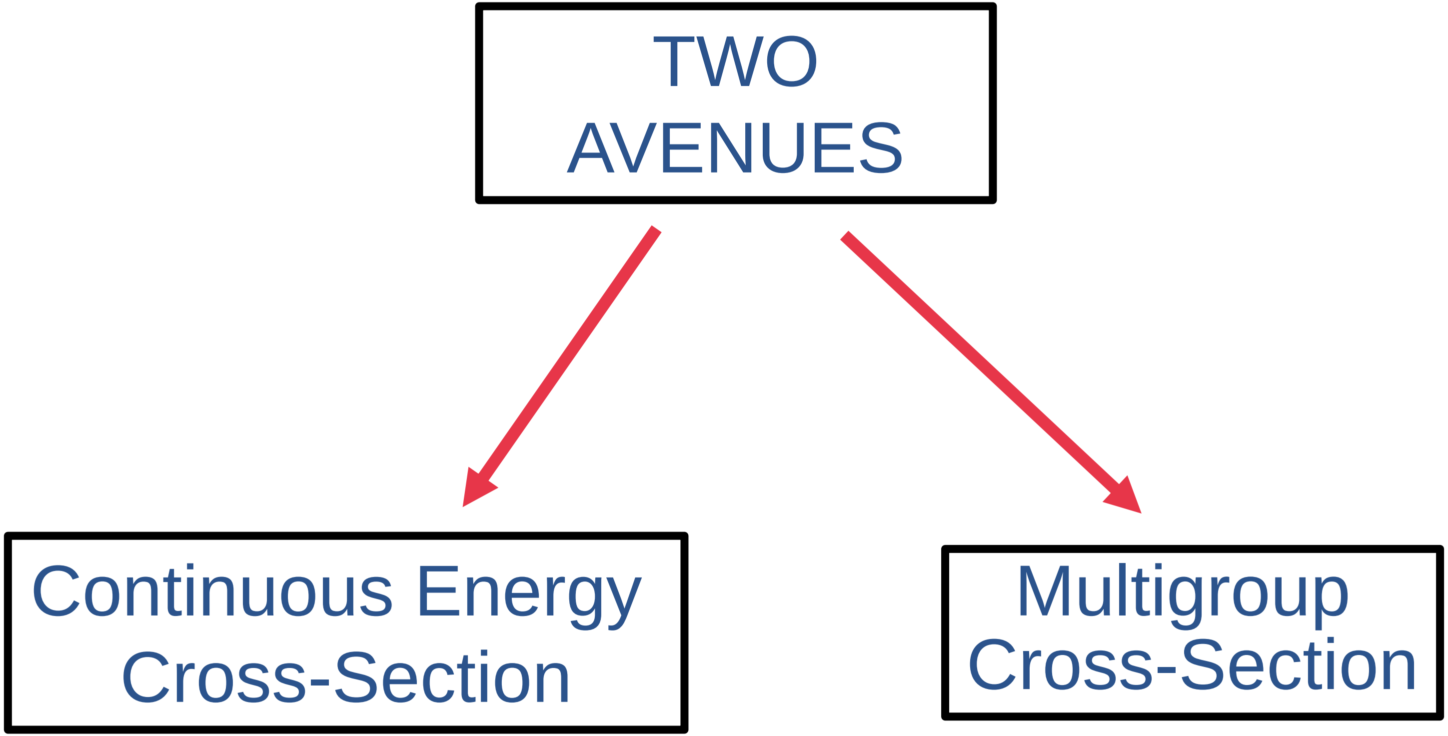
Nuclear Data Processing Tools

Nuclear data processing codes convert ENDF data to continuous energy (CE) or multigroup (MG) libraries for transport and criticality codes.

Few existing tools are:

- AMPX: developed and maintained at ORNL (US)
- NJOY: developed and maintained at LANL(US)
- FRENDY: developed and maintained at JAEA (Japan)
- GALILEE: developed and maintained at CEA (France)
- GAIA: developed and maintained at IRSN (France)

Nuclear Data Processing Tools



Nuclear Data Processing Tools

1. Continuous Energy Library(MC) – Monte Carlo (MC) applications

a) Read ENDF data and convert to linearized «point data»:

$$\{(\sigma(E_i), E_i); i = 1, \ldots, Number\ Points\}$$

b) Calculate energy-angle distribution: $\sigma(E_i \rightarrow E_j; \theta)$

c) Convert point data to probability distribution for MC calculations. Example, probability table generation:

$$\{\sigma_i, p(\sigma_i), i = 1, \ldots, N_{table\ entries}\}$$

Nuclear Data Processing Tools

2. Multigroup Applications (MG) – MG library generation

a) Define an energy group-structure $\{E_1, E_2, \ldots, E_{G+1}\}$. There will be G energy groups ΔE, such as $\Delta E_g = E_{g+1} - E_g$

b) Average data over the specified energy group-structure with a flux weighting spectrum

The 1 D group averaged cross section is

$$\sigma_g = \frac{\int_{E_g}^{E_{g+1}} \varphi(E)\sigma(E)dE}{\int_{E_g}^{E_{g+1}} \varphi(E)dE}$$

c) Compute resonance self-shielding data (Very important step!!)

Covariance

Basic Definitions

For a random variable x such as that $x \in \{x_1, \dots, x_N\}$

$$\bar{x} = \frac{1}{N}\sum_{i=1}^{N} x_i$$

$$\boldsymbol{S}_x^{\boldsymbol{2}} = \frac{1}{N - \boldsymbol{1}}\sum_{i=1}^{N}(x_i - \bar{x})^{\boldsymbol{2}}$$

Basic Definitions

Extension to physical quantities (not of random nature). However, probability distribution provides a feeling of what are the possible values:

$$\bar{x} = \int_a^b x\, f(x) dx$$

$$\int_a^b f(x) dx = 1$$

Normalized $f(x)$

Central values and uncertainties

Experimental values are commonly described by a mean value and an uncertainty (standard deviation)

$$\bar{x} \pm \Delta x$$

$$(\Delta x)^{2} = \langle (x - \bar{x})^{2} \rangle$$

$(\Delta x)^{2}$ is the variance and corresponding standard deviation is $\sqrt{(\Delta x)^{2}} = \Delta x$

Covariance

Measures the degree of variability of two random variables:

1. Covariance

$$\mathrm{cov}(x_i, x_j) = \langle \delta x_i \delta x_j \rangle = \langle (x_i - \bar{x}_i)(x_j - \bar{x}_j) \rangle$$

2. Correlation Matrix

$$\mathrm{R}(x_i, x_j) = \frac{\mathrm{cov}(x_i, x_j)}{\sqrt{\mathrm{cov}(x_i, x_i)\mathrm{cov}(x_j, x_j)}} = \frac{\langle \delta x_i \delta x_j \rangle}{\Delta x_i \Delta x_j}$$

3. Relative Covariance Matrix

$$\mathrm{rcov}(x_i, x_j) = \frac{\mathrm{cov}(x_i, x_j)}{\bar{x}_i \bar{x}_j} = \mathrm{R}(x_i, x_j) \frac{\Delta x_i \Delta x_j}{\bar{x}_i \bar{x}_j}$$

Uncertainty Propagation

Assumption: just linear portion taking into account

For a quantity y as a function of n variables $(x_1, \ldots, x_n)$, that is, $y = f(x_1, \ldots, x_n)$ where $\bar{x}$ is the mean value, one can write:

$$\delta y = \left(\frac{\partial y}{\partial x_i}\right)_{x=\bar{x}} \delta x_i + \ldots$$

The variance of y (after some casual algebra) is:

$$\text{var}(y) = \sum_{ij} \frac{\partial y}{\partial x_i} < \delta x_i \delta x_j > \frac{\partial y}{\partial x_j}$$

Uncertainty Propagation

One should bear in mind that no high order terms have been considered, that is, the equation is on valid for a linear variation of y as a function of n variables $(x_1, \ldots, x_n)$. The matrix form is:

$$\mathrm{var}(y) = S\,C\,S^t$$ where

C is the covariance of x, that is, $< \delta x_i \delta x_j >$

S is the sensitivity of y to x, that is, $\frac{\partial y}{\partial x}$

S^t is the transpose of S

ENDF Covariance Representation

File	Description
30 - 40	Data Covariance File Contents
30	Sensitivities
31	COVARIANCES OF THE AVERAGE NUMBER OF NEUTRONS PER FISSION
32	COVARIANCES OF RESONANCE PARAMETERS
33	COVARIANCES OF NEUTRON CROSS SECTIONS
34	COVARIANCES FOR ANGULAR DISTRIBUTIONS OF SECONDARY PARTICLES
35	COVARIANCES FOR ENERGY DISTRIBUTIONS OF SECONDARY PARTICLES
40	COVARIANCES FOR PRODUCTION OF RADIOACTIVE NUCLEI

ENDF Covariance Resonance Representation

FILE 32

For a set of resonance parameters $(p_1, \ldots, p_n)$ (FILE 2) with resonance parameter covariance $< \delta p_i \delta p_j >$ (FILE 32) the group cross section covariance $< \delta\bar{\sigma}_{xg} \delta\bar{\sigma}_{xg'} >$ can be obtained as:

$$< \delta\bar{\sigma}_{xg} \delta\bar{\sigma}_{xg'} > = \sum_{ij} \frac{\partial\bar{\sigma}_{xg}}{\partial p_i} < \delta p_i \delta p_j > \frac{\partial\bar{\sigma}_{xg'}}{\partial p_j}$$

Calculated by nuclear data processing code

Provided in ENDF

ENDF Covariance Resonance Representation

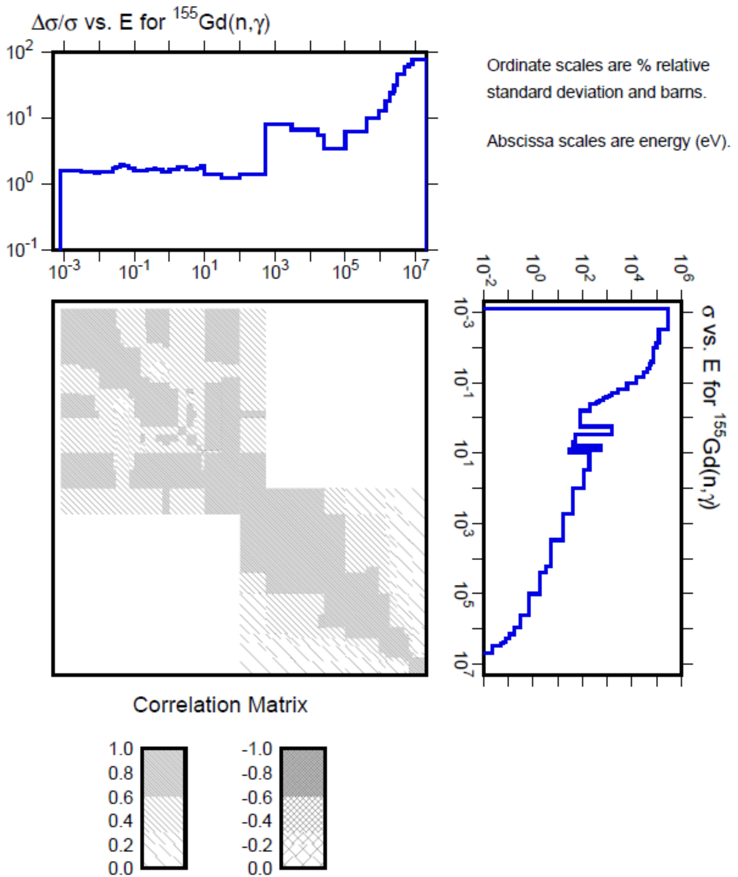
FILE 33

For a set of energy dependent reaction cross section (FILE 3) there will a corresponding covariance $cov(\sigma)$ in FILE 33. the group cross section covariance $<\delta\bar{\sigma}_{xg}\delta\bar{\sigma}_{xg'}>$ can be obtained as:

$$<\delta\bar{\sigma}_{xg}\delta\bar{\sigma}_{xg'}> = \frac{1}{\varphi_g\varphi_{g'}}\int_{E_g}^{E_{g+1}}\int_{E_{g'}}^{E_{g'+1}}\varphi(E)\varphi(E')\,cov(E)\,dE\,dE'$$

Provided in ENDF

Covariance for ^{155}Gd



^{155}Gd ENDF/B-VIII resonance parameter covariance processed with NJOY/ERRORR. Group covariance generated based on the 44-neutron group structure with a constant weighting spectrum

Practical Application

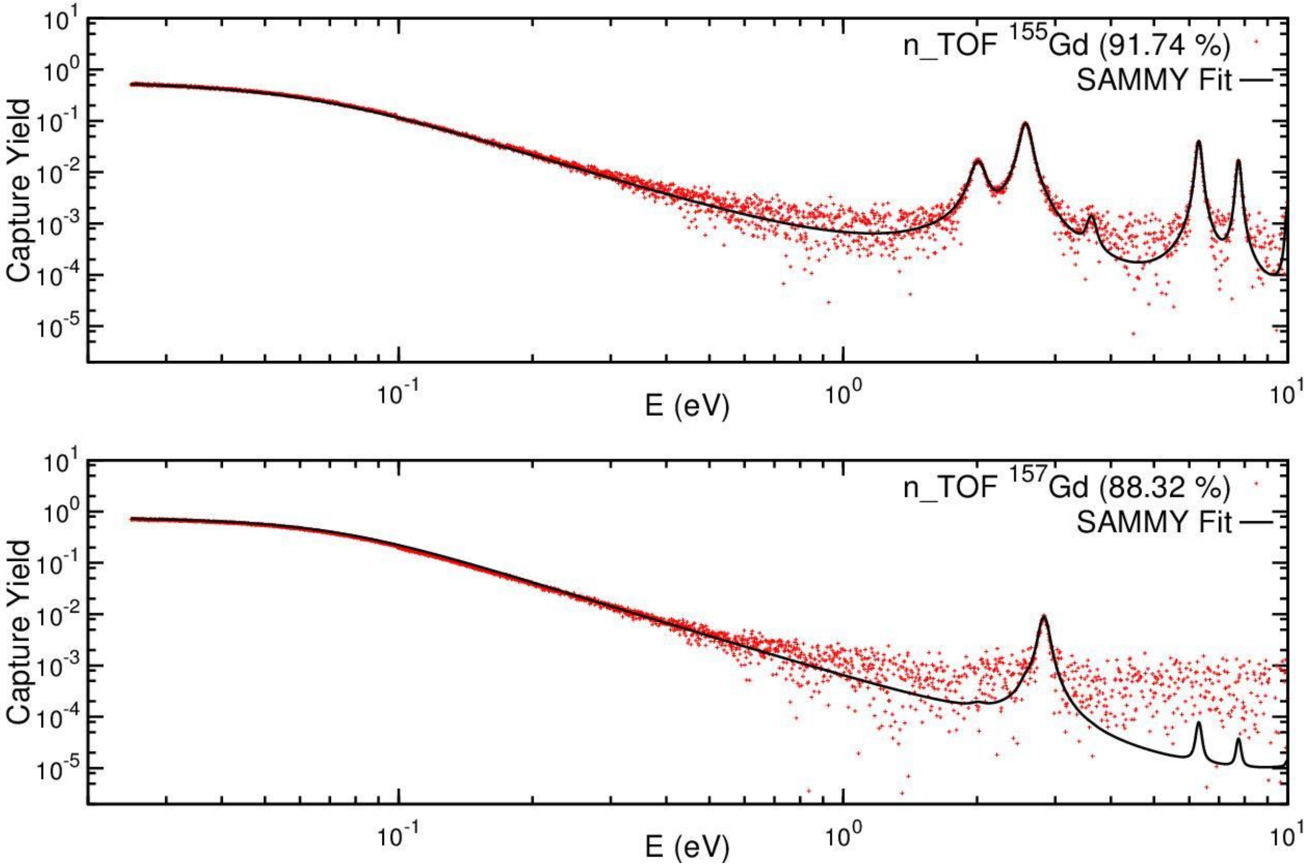
- The work consist of evaluating the Gd isotopes in the resonance region (^{155}Gd, ^{157}Gd)
- Use of several differential data measured at the RPI and n_TOF
- Evaluation performed using the computer code SAMMY
- Testing the new IRSN evaluation using integral benchmark from the ICSBEP data bank

Experimental Differential Data Base

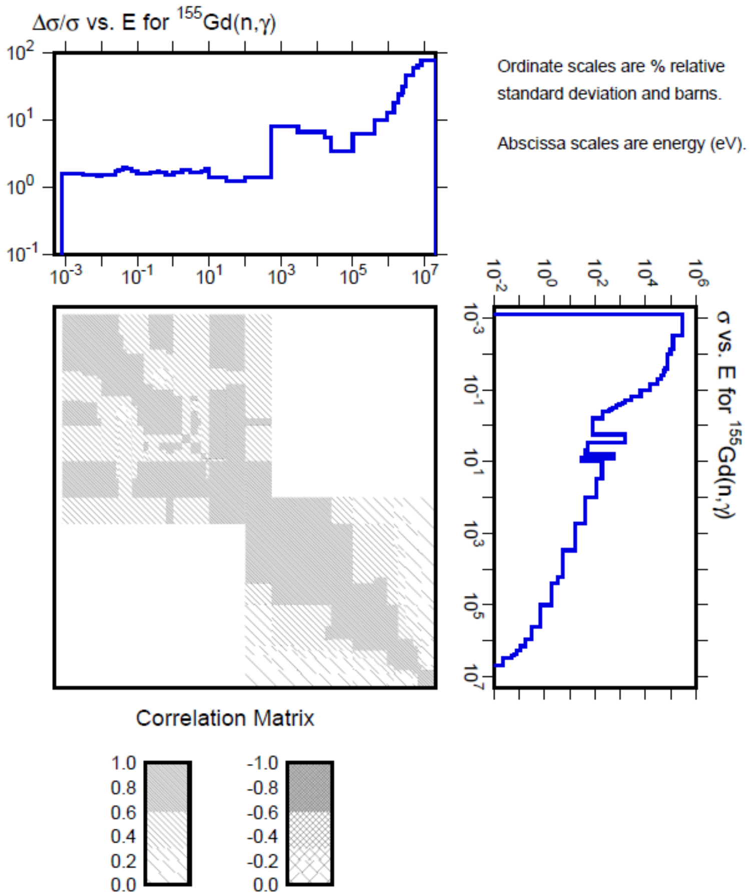
Experimental transmission and capture data

Data Set	Enrichment (%)	Energy Range (eV)	Flight Path (m)	Density (at/b)
Natural Gadolinium				
Transmission (RPI)	-	0.2 - 300.0	25.585	7.806×10^{-4}
Transmission (RPI)	-	0.3 – 500.0	25.597	1.566×10^{-3}
Transmission (RPI)	-	0.3 – 1000.0	25.597	1.566×10^{-3}
Capture (RPI)		0.2 – 1000.0	25.585	7.806×10^{-4}
^{155}Gd				
Capture (RPI)	91.74	0.2 - 1000.0	25.567	3.083×10^{-4}
Capture (n_TOF)	91.74	0.025 - 50.0	183.90	1.236×10^{-6}
Capture (n_TOF)	91.74	1.0 - 1000.0	183.90	1.244×10^{-4}
^{157}Gd				
Capture (RPI)	90.96	0.2 - 1000.0	25.569	5.820×10^{-4}
Capture (n_TOF)	88.32	0.025 - 50.0	183.90	5.753×10^{-6}
Capture (n_TOF)	88.32	1.0 - 1000.0	183.90	2.340×10^{-4}

n_TOF data (SAMMY Fitting) for $^{155,157}Gd$



Covariance for ^{155}Gd



Integral Benchmark Testing (ICSBEP)

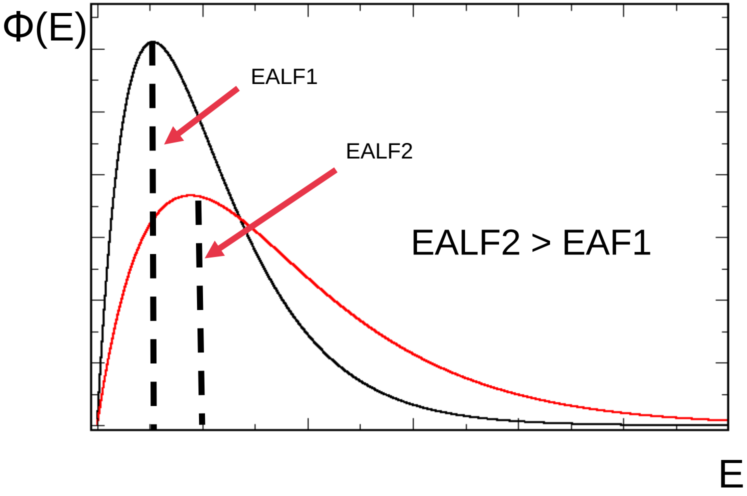
Benchmark ID	EALF (eV)	Gd concentration (ppm)
LEU-COMP-THERM-042-C02	0.178	-
LEU-COMP-THERM-006-C04	0.190	68
MIX-SOL-THERM-006.C04	0.190	359
PU-SOL-THERM-034.C04	0.240	1131
LEU-COMP-THERM-005-C04	0.281	480
PU-SOL-THERM-034.C06	0.292	1896
PU-SOL-THERM-034.C09	1.792	3692

Benchmark testing:

What is EALF ?(Energy of Average Lethargy of neutron causing Fission)

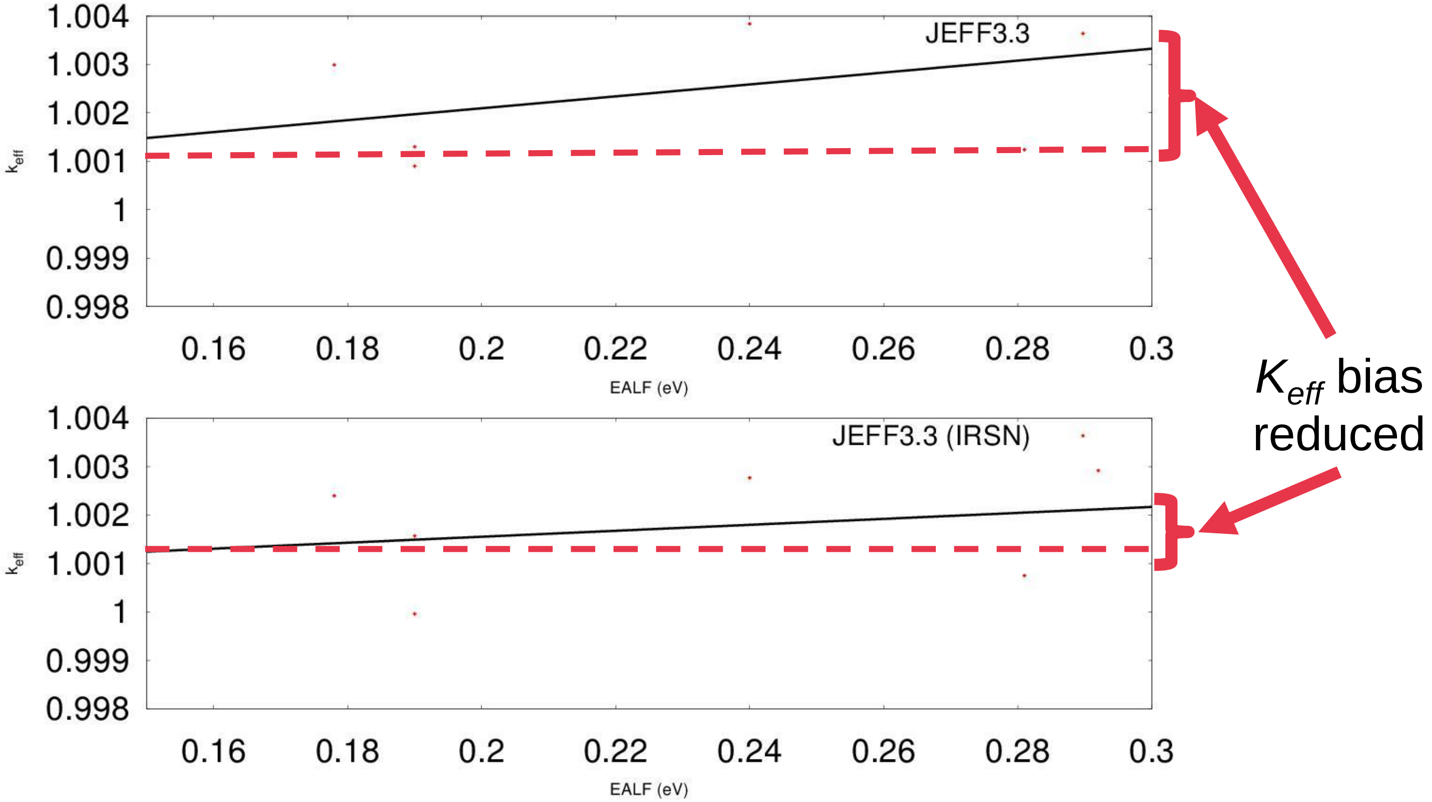
- Provide information on the energy region on the neutron spectrum Φ(E)

- It can be seen as the centroid of Φ(E)



$$\text{EALF} = \frac{\int E\Phi(E)dE}{\int \Phi(E)dE}$$

RESULTS



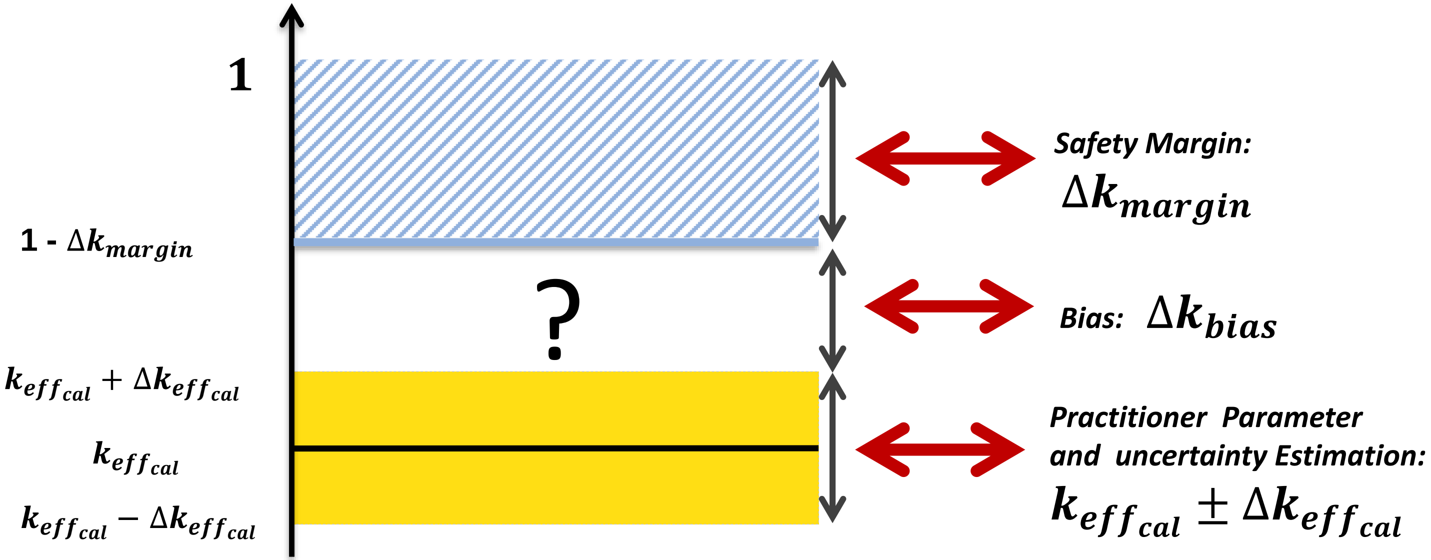
Criticality Safety Assessment IRSN (France)

Safety Parameter:
k_{eff}

Subcritical Limit Threshold

$$1 - \Delta k_{margin} - \Delta k_{bias} > k_{eff\,cal} + \Delta k_{eff\,cal}$$

$$\Delta k_{bias} = \Delta k_{ND} + \Delta k_{calc\_schem}$$



Criticality Safety Assessment IRSN (France)

Parameters Values:

$\boldsymbol{a}$) $\Delta \boldsymbol{k_{margin}}$(common used values)

Normal configuration: 0.95 corresponding to 5000 pcm* (10^5 x 0.05)

Abnormal configuration: 0.97 – 0.98 corresponding to 3000 to 2000 pcm

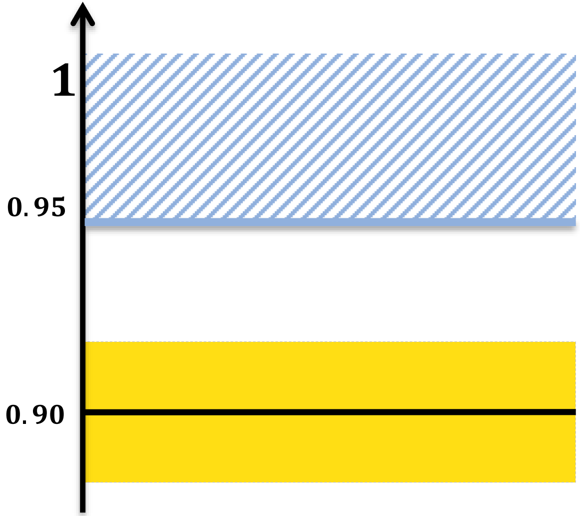
$\boldsymbol{b}$) $\Delta \boldsymbol{k_{eff_{cal}}}$(controlled quantity thru a Monte Carlo Calculation (MC)

n_Sigma standard deviation in a MC. Values used is n=3 (in France)

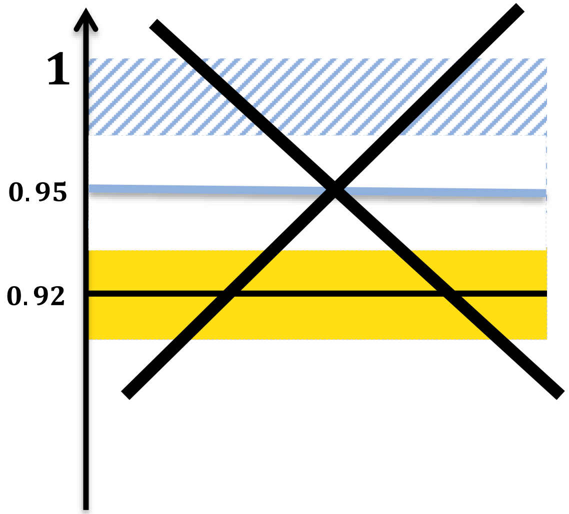
c) $\Delta \boldsymbol{k_{bias}}$ derived from differences of calculated $\boldsymbol{K_{eff}}$ and experimental $\boldsymbol{K_{eff}}$, that is (C–E). This is where data measurement, evaluation, validation, uncertainty quantification play an extremely important role !!!

*Where 1 pcm = percent mille (1 pcm = 10^5)

Criticality Safety Assessment

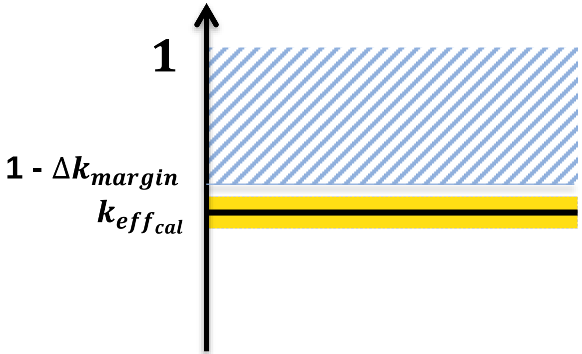


Acceptable but not very efficient



Not acceptable

Criticality Safety Assessment



In this scenario the application k_{eff} ($k_{eff_{cal}}$) is very close to the k_{eff} corresponding to the safety margin (1 - Δk_{margin}).

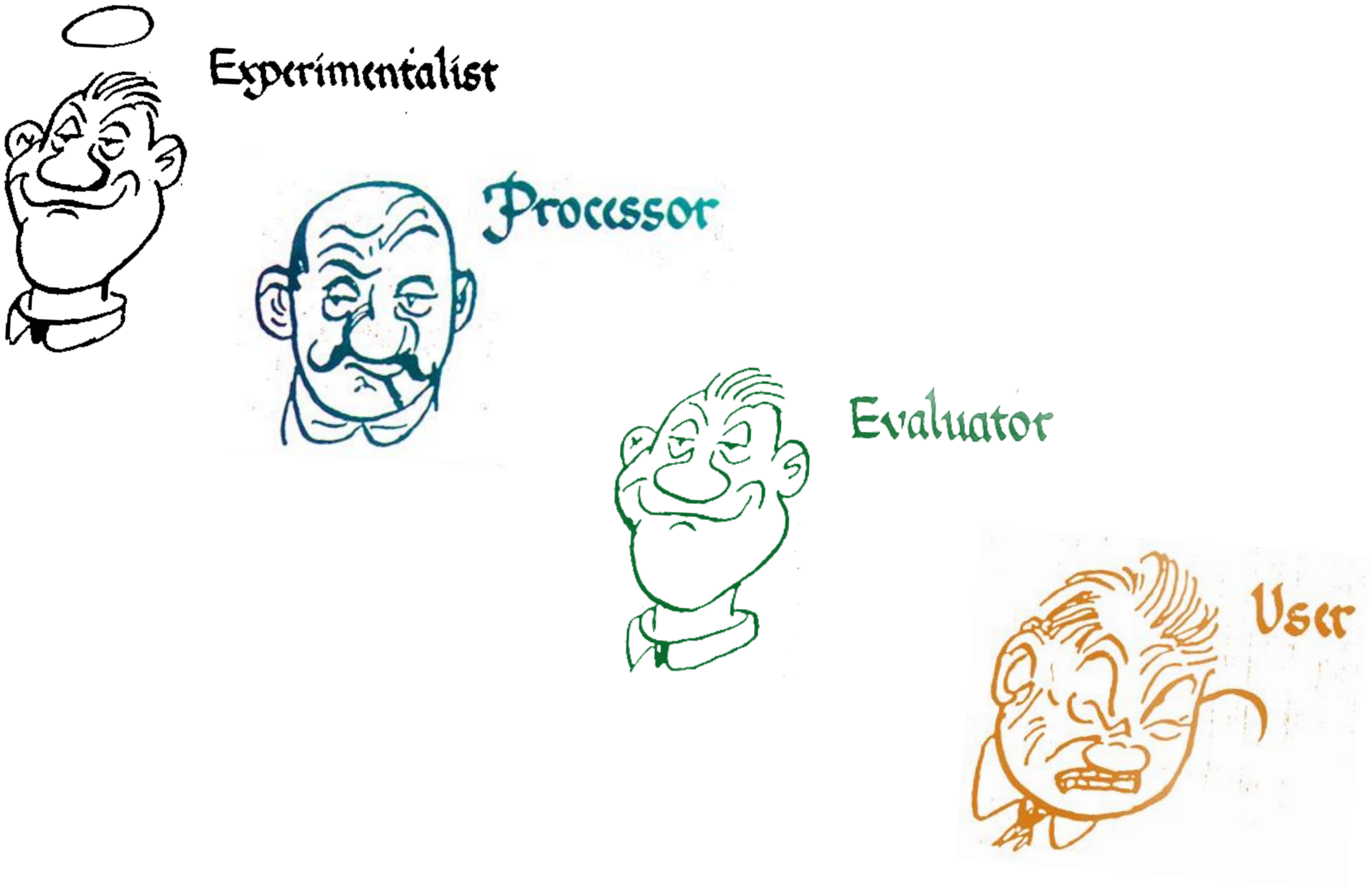
The nuclear data uncertainty will be such that:

$$1 - \Delta k_{margin} = k_{eff_{cal}} + \Delta k_{bias} + \Delta k_{eff_{cal}}$$

Concluding Remarks

- First principles (measurements, evaluation, etc) are and will be the backbone for nuclear science developments;
- Nuclear data evaluation and data uncertainties must rely upon experimental data,
- Methodologies for estimating biases and uncertainties is crucial to understand the nuclear system;
- Tight connections with experimental facilities around the world for has helped IRSN to address issues on ND and uncertainty
- Final evaluations include covariance information;
- IRSN has been performing benchmark experiments to help understanding and improving differential data evaluation;
- Any nuclear system design and evaluation will be as good as the data used;

"If one wants to build a nuclear system device (reactor, shipping cask, etc.), nuclear data accuracy must be taken into account, otherwise the project is a game" *Yasuyuki Kikuchi*


Experimentalist
Processor
Evaluator
User