Appendix 4 – 4.

Method to Evaluate Covariance Data for the Thorium-Uranium Fuel Cycle;

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Method to Evaluate Covariance Data for the Thorium-Uranium Fuel Cycle

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Strategy of Evaluation

C.S. evaluated based on the experimental data

- Estimate a covariance by a Least-squares fitting to those measurements with GMA or SOK.
- Covariance of experimental data were re-constructed by evaluators.
- Examples — σ_t, σ_f, σ_{2n}, $\overline{\nu}$, *etc.*

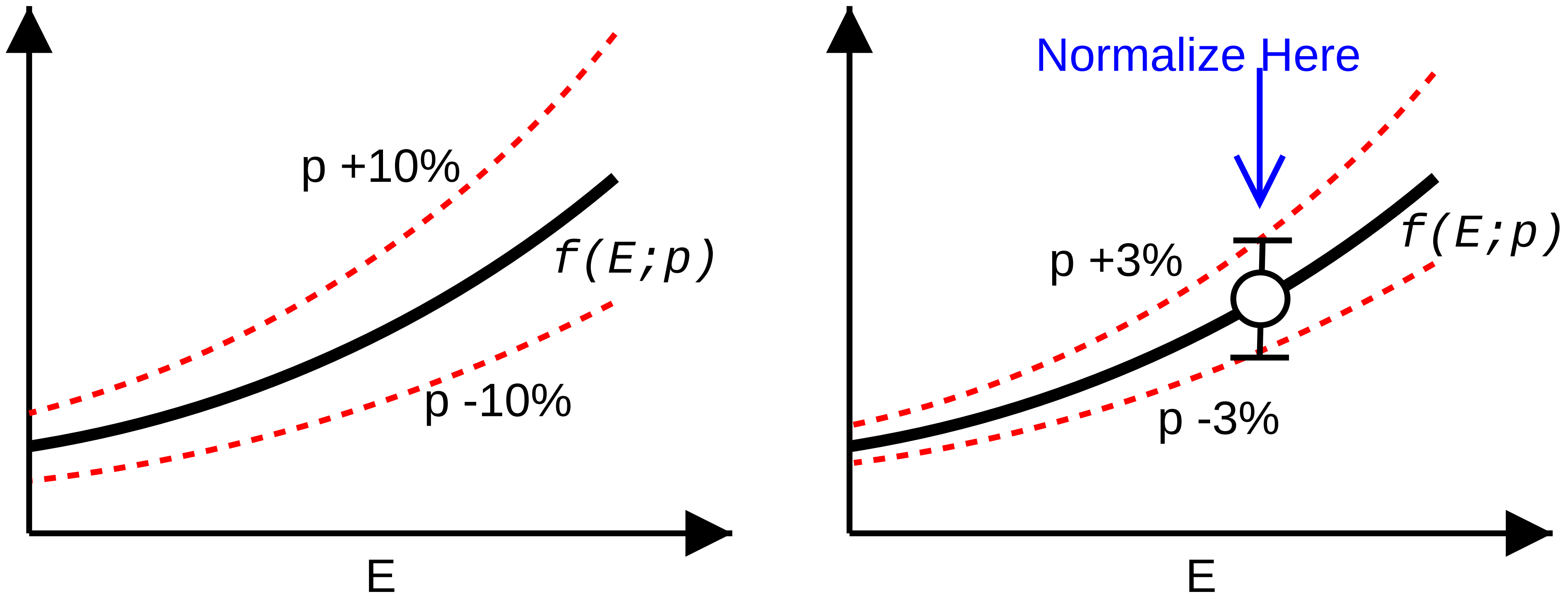
C.S. evaluated with a nuclear model

- Estimate the covariance with the KALMAN code.
- KALMAN calculates an error propagation from experimental data to the evaluated quantities though the covariance of model parameters.
- Examples: — σ_t (if OM used), σ_{inel}, χ, Legendre-coeff., resolved/unresolved resonance parameters.

Basic Idea

Inter/Extraporation of experimental uncertainties

- Calculate sensitivities of model parameters
- Estimate uncertainties in the parameters by experimental data
- Calculate uncertainties in the cross sections by the parameter uncertainties



for undergraduate students

Uncertainty reduction by a number of data-point

- If we have only one data point
  - Experimental data, $Y = y \pm z$ at $X = x$
  - We believe that the evaluated datum $\overline{y}$ has an uncertainty of z at $X = x$, and unknown for $X \neq x$.
- If we have many data points
  - It is often said that the uncertainty of evaluated data becomes small.
  - This is only true if those data are independent.
  - Statistical error becomes very small if you have many data points,
  - however, systematic error remains.

Uncertainty reduction by interpolation

- When a covariance evaluation is carried out, an interpolation method plays an important role.
  - If the 0-th order Spline is used,
    the quantity within the average-interval is assumed to be constant.
  - If the 1-st order Spline is used,
    the quantity behave just like a linear function within the interval .
  - If some appropriate function is used,
    it is automatically assumed that the function describes the data tendency perfectly.
- The covariance matrix of evaluated quantity is a consequence of error propagation from experimental data, however those are “corrupted” data by the fitting function adopted.

Covariance Data obtained by Fitting

Generalized Least-squares Fitting

- Estimate uncertainties at each energy-gird and correlations among them.
  - GMA : moves an experimental energy point to the nearest energy-grid.
  - SOK : assumes that $\sigma(E)$ varies linearly or it is constant between two energy-grids.
- No correlation if experimental data are uncorrelated.

Model Parameter Fitting

- Interpolation is made with some physical background.
- We believe that the mode is “true.”
- Correlation exists even if experimental data are uncorrelated.

KALMAN Calculation (I)

Covariance Evaluation with the KALMAN code

- includes
  - Statistical / systematic errors in the experimental data.
    - correlation from the systematic errors
  - Constraint by a physical model employed.
    - correlation from a model which is used for interpolation
- has advantages:
  - Inter/extra-polation of uncertainties to the region where no experimental data are available.
  - Deduction of uncertainties those can be obtained by calculations.

KALMAN Calculation (II)

Error propagation from experimental data to model parameters

$$\mathbf{P} = (\mathbf{C}^t \mathbf{V}^{-1} \mathbf{C})^{-1} \quad (1)$$

propagation from the parameters to calculated values

$$\mathbf{M} = \mathbf{C}\mathbf{P}\mathbf{C}^t \quad (2)$$

where **V**, **P**, **M** are the covariance matrices of experimental data, model parameter, and calculated values, **C** is the sensitivity matrix whose elements are $\partial f / \partial x$.

The most time-consumptive part is to construct the matrix **C**.

KALMAN Calculation (III)

Bayesian Method

$$
\begin{aligned}
\boldsymbol{x}_1 &= \boldsymbol{x}_0 + \mathbf{P}\mathbf{C}^t\mathbf{V}^{-1}\left(\boldsymbol{y} - \boldsymbol{f}(\boldsymbol{x}_0)\right) \\
&= \boldsymbol{x}_0 + \mathbf{X}\mathbf{C}^t\left(\mathbf{C}\mathbf{X}\mathbf{C}^t + \mathbf{V}\right)^{-1}\left(\boldsymbol{y} - \boldsymbol{f}(\boldsymbol{x}_0)\right) \qquad (3)
\end{aligned}
$$

$$
\begin{aligned}
\mathbf{P} &= \left(\mathbf{X}^{-1} + \mathbf{C}^t\mathbf{V}^{-1}\mathbf{C}\right)^{-1} \\
&= \mathbf{X} - \mathbf{X}\mathbf{C}^t\left(\mathbf{C}\mathbf{X}\mathbf{C}^t + \mathbf{V}\right)^{-1}\mathbf{C}\mathbf{X} \qquad (4)
\end{aligned}
$$

where $\boldsymbol{x}_0$ and $\boldsymbol{x}_1$ are prior / posterior vectors of the parameter, $\boldsymbol{y}$ is the experimental data vector.

$\boldsymbol{f}(\boldsymbol{x})$ is the vector which includes calculated values with the parameter $\boldsymbol{x}$, and usually this is a non-linear function. It can be linearized by the Taylor-series expansion near $\boldsymbol{x}_0$:

$$
\boldsymbol{y} = \boldsymbol{f}(\boldsymbol{x}) \simeq \boldsymbol{f}(\boldsymbol{x}_0) + \mathbf{C}(\boldsymbol{x} - \boldsymbol{x}_0) \qquad (5)
$$

KALMAN Code

The Program

- Non-linear least-squares fitting code
- The original code was developed by Y. Uenohara in Kyushu Univ.
- Renewed and extended by T. Kawano,
  collaboration with JAERI Nuclear Data Center
- Calculation of the Bayes equations
  - KALMAN itself does not calculate a nuclear model
  - One has to prepare an appropriate model

Some examples

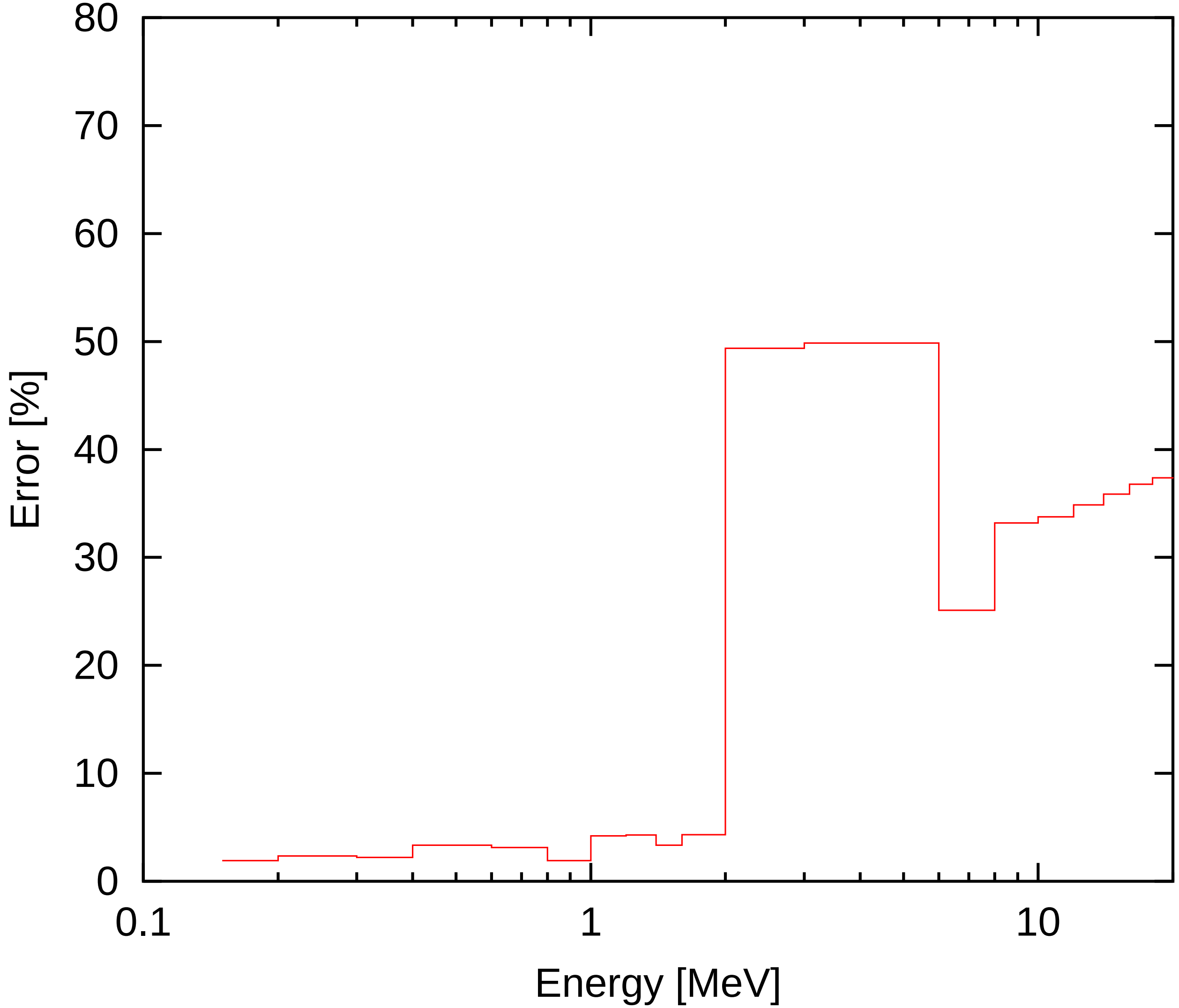
- ^{56}Fe covariance, presented at Gatlinburg (1994)
- JENDL-3.2 Covariance File
- JENDL Dosimetry File
- JENDL-3.3

KALMAN System

- Optical model
  - ELIESE-3 (Igarasi)
  - ECIS-88 (Raynal)
- Hauser-Feshbach and Exciton models
  - GNASH (Arthur and Young)
  - CASTHY (Igarasi)
- Prompt-neutron fission spectrum, based on the Madland-Nix model
  - FISPEKL-2 (Ohsawa)
- Direct/Semidirect capture model
  - DSD (Kawano)
- Resolved resonance parameters
  - GFR (Kawano)
- Unresolved resonance parameters
  - ASREP (Kikuchi)

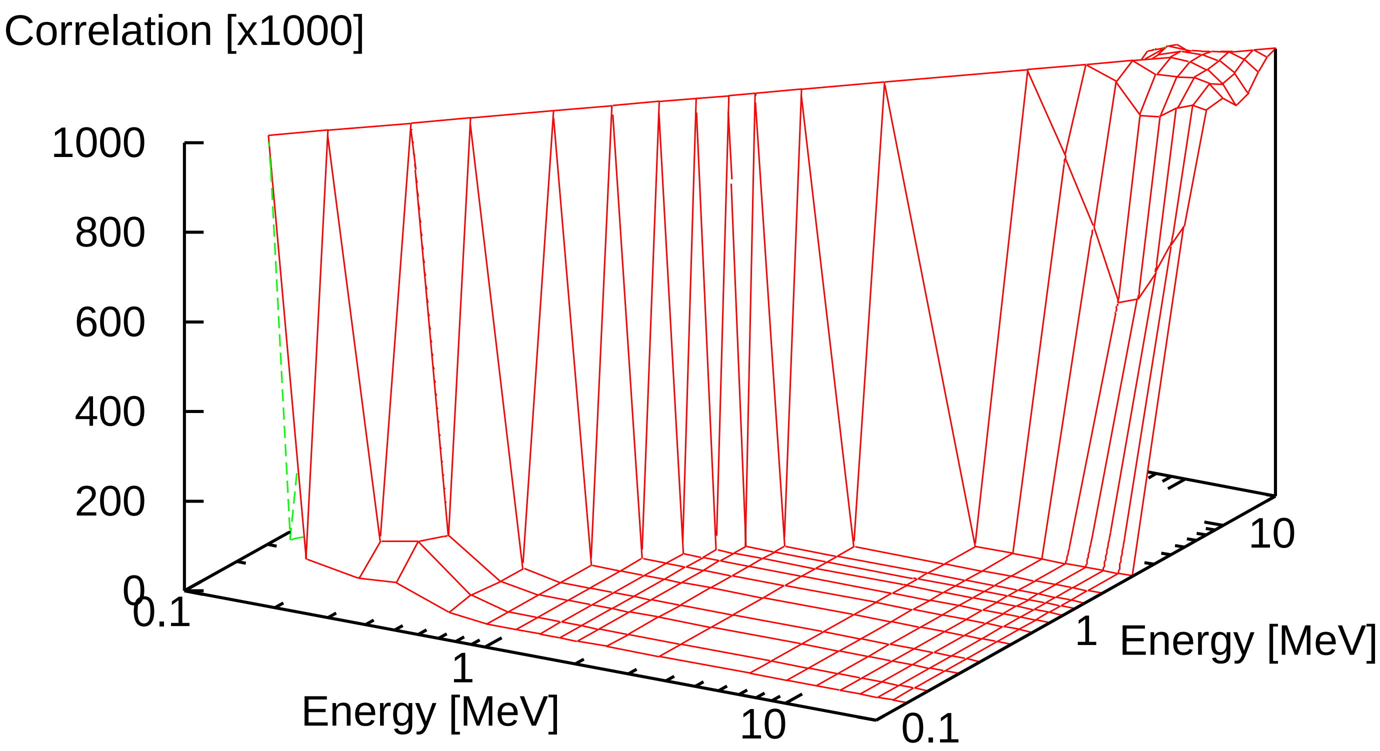
Example (I)

Uncertainties in ^{238}U Capture Cross Sections



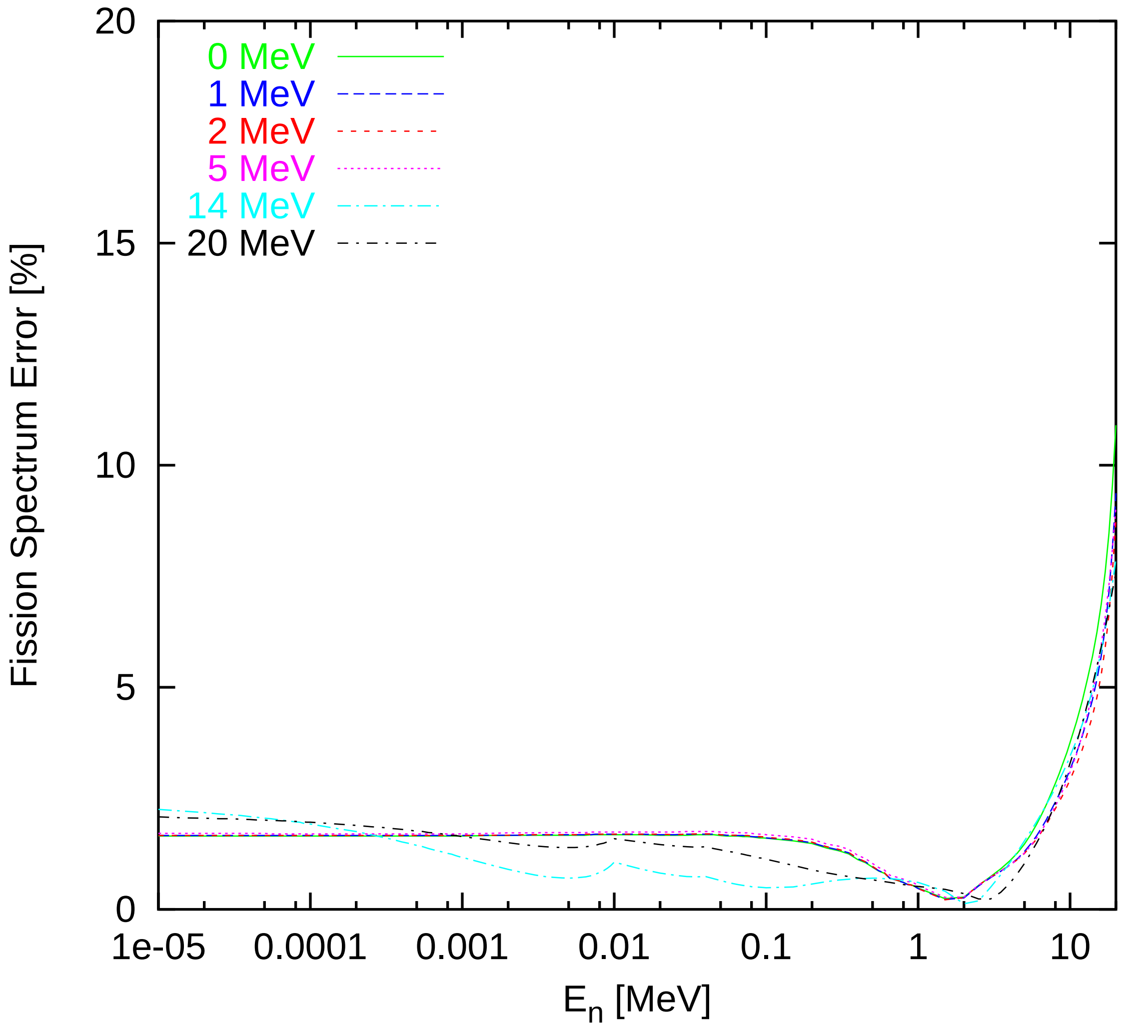
Example (I), cont.

Correlation of ^{238}U Capture Cross Sections



Example (II)

Uncertainties in ^{235}U Fission Spectrum

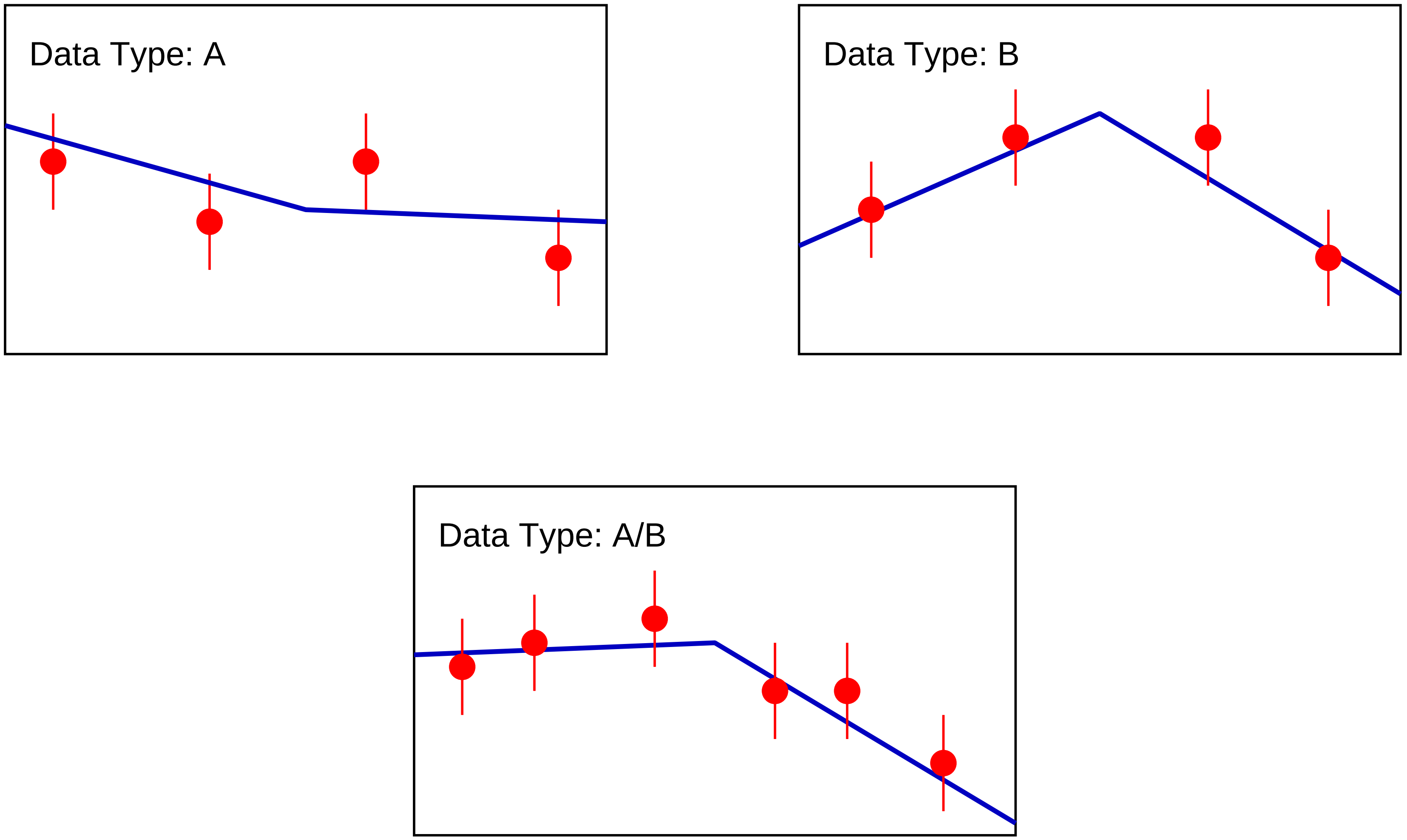


Generalized Least-Squares Fitting Code

- Fission cross section is still hard to predict by theories within a few percent uncertainties.
- However the fission cross section data are often high quality, and this procedure allows us to try to resolve discrepancies in measured values to determine the best value.
- Based on the Bayesian statistics.
- Simultaneous fitting to different kinds of measurements.
- Involves statistical, systematical uncertainties & correlation.
- Provides mean values as well as a covariance matrix.

Simultaneous Evaluation

Evaluation of σ_f based on the Absolute/Relative Measurements



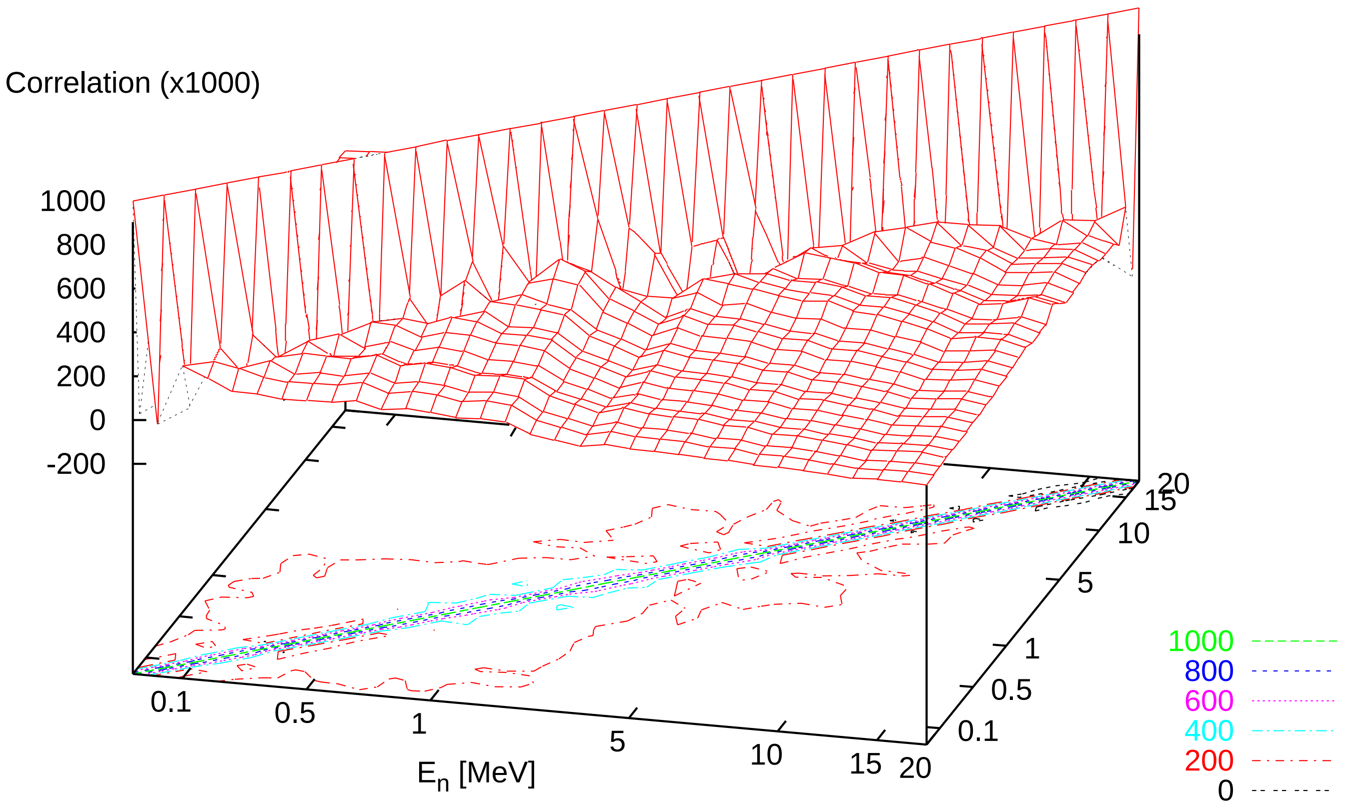
Evaluation of Fission Cross Sections

Simultaneous Evaluation for JENDL-3.3

- Absolute Measurements
  - ^{233}U, ^{235}U, ^{238}U, ^{239}Pu, ^{240}Pu, and ^{241}Pu
- Relative Measurements
  - ^{233}U/^{235}U, ^{238}U/^{235}U, ^{238}U/^{233}U, ^{239}Pu/^{235}U, ^{240}Pu/^{235}U, ^{241}Pu/^{235}U, and ^{240}Pu/^{239}Pu
- 4661 Data Points
- 211 Spline Knots

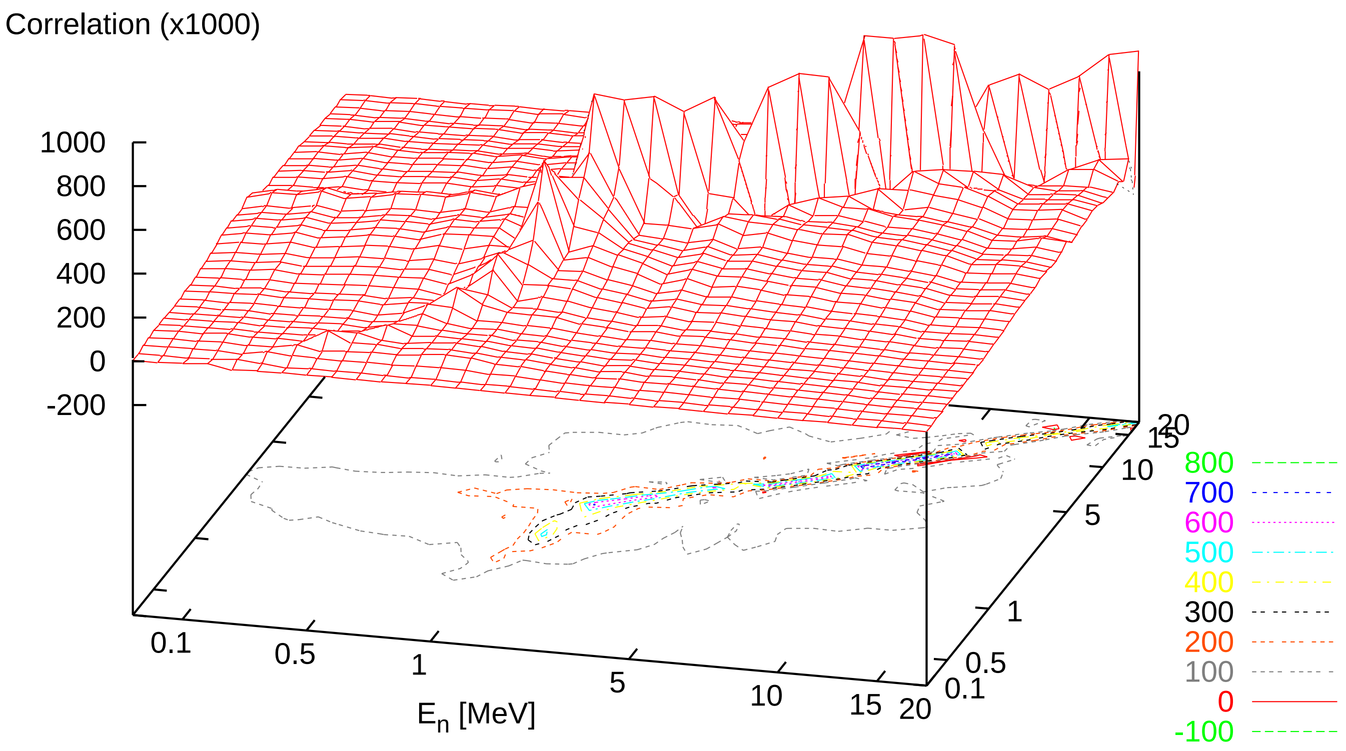
Results (I)

Correlation of ^{235}U Fission Cross Sections



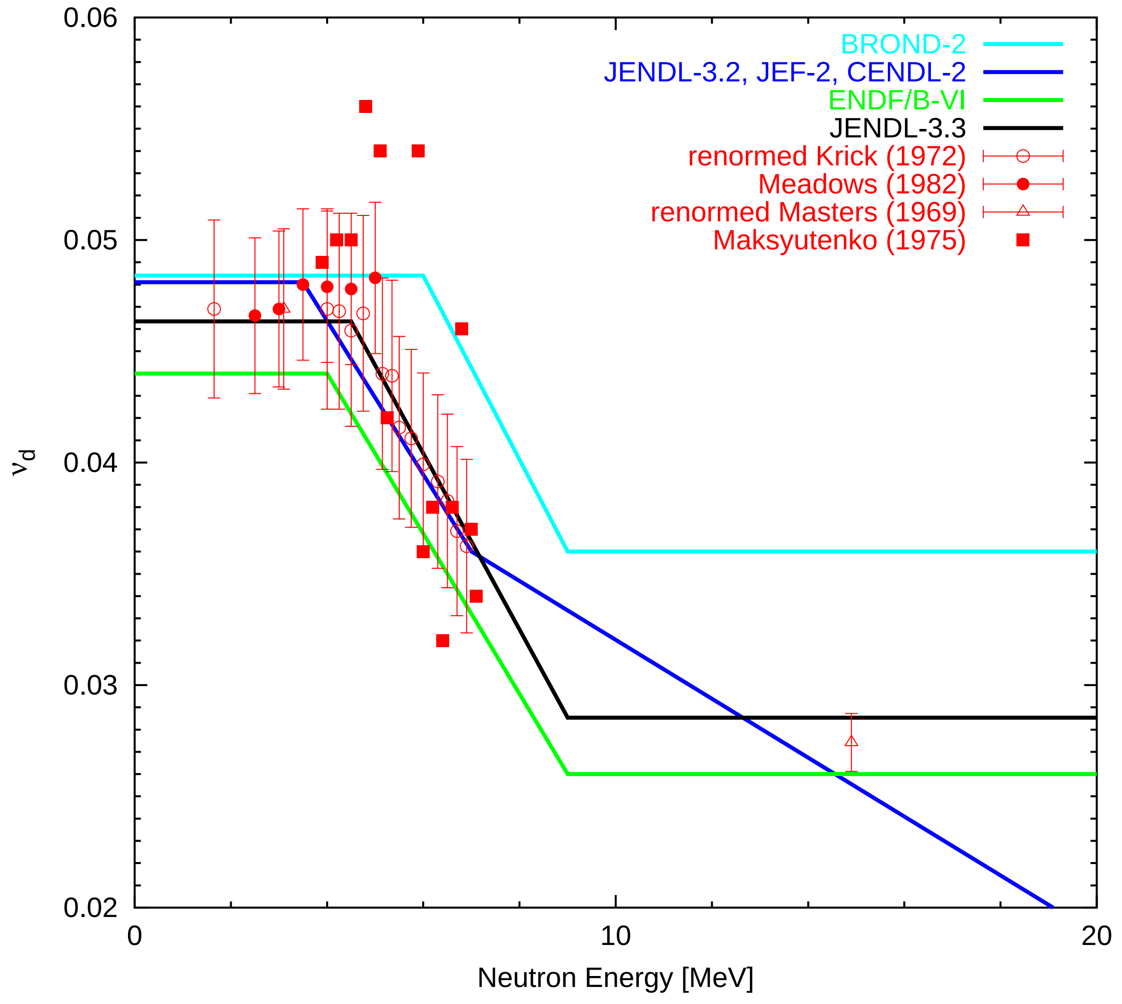
Results (II)

Correlation between ^{235}U and ^{238}U



Results (III)

Evaluated ν_d for ^{238}U



Results (III), cont.

Covariance of ν_d for ^{238}U

Node (MeV)	ν_d	Error (%)	Correlation ($\times 1000$)			
0.0	0.04634	3.409	1000			
4.5	0.04634	3.409	1000	1000		
9.0	0.02853	3.873	537	537	1000	
20.0	0.02853	3.873	537	537	1000	1000

Concluding Remarks

- Covariance evaluation tools have been developed
- Kyushu University and JAERI Nuclear Data Center
- Two important codes and some utilities
  - KALMAN — Bayesian parameter estimation
  - SOK — Least-squares fitting
- Two important results those can be processed with NJOY
  - JENDL-3.2 covariance file
  - JENDL-3.3
- Its principle is very simple
  - Error propagation from exerimental data to evaluated values