Nuclear Data Sensitivity and Uncertainty Analysis

Tutorial Lecture 2

I. Kodeli
IAEA representative at OECD/NEA Data Bank, Paris
on leave from Jožef Stefan Institute, Ljubljana
ivo.kodeli@oecd.org

Intercomparison on the Usage
of Computational Codes in Radiation Dosimetry

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Time-independent Boltzmann Transport Equation

\[ \vec{\Omega} \cdot \nabla \phi(\vec{r}, \vec{\Omega}', E') + \sum_T (\vec{r}, E) \phi(\vec{r}, \vec{\Omega}, E) \]

\[ = \int_{E_{\text{max}}}^{\infty} \int dE' d\Omega' \sum_s (\vec{r}, \vec{\Omega}', \vec{\Omega}, E' \to E) \phi(\vec{r}, \vec{\Omega}', E') = Q(\vec{r}, \vec{\Omega}, E) \]

where:

- \( \phi(\vec{r}, \vec{\Omega}, E) \): angular flux at location \( \vec{r} \) with energy \( E \), direction \( \vec{\Omega} \)
- \( \sum_T (\vec{r}, E) \): total macroscopic cross-section at energy \( E \)
- \( \sum_s (\vec{r}, \vec{\Omega}', \vec{\Omega}, E' \to E) \): scattering cross-section from \( E' \) to \( E \)
Particle transport methods

- **Monte Carlo**: MCNP, KENO, McBEND, TRIPOLI, MORSE, EGS4, PENELope, EGS4, MONK, ITS, FLUKA, LAHET
- **Deterministic discrete ordinates**: ANISN, DOORS, DANTSYS, PARTISN, TWOTRAN, CEPXS/ONELD
The only certainty concerning the scientific data, measured or calculated, is that they differ from their true values.

Reasons:
experimental errors, unperfect instruments, counting statistics, approximations used in modelisation (geometry, material composition), calculational methods and physical theory.

Predictions of measured data can be only based on weighted averages of all possible true values. Weights and averages represent probabilities and expectation values.
Outline

- **Sources of uncertainty** in particle transport
- **Probability theory** - mathematical introduction & definitions (uncertainties, covariance matrices, error propagation)
- **Cross section covariance matrices** (construction, available data)
- **Methods for sensitivity and uncertainty analysis**
- **Examples of cross section sensitivity/uncertainty code** system based on deterministic methods
Sources of Uncertainty in Transport Calculations

- **Mathematical methods and simplifications**
  e.g. M/C statistics, $S_N$ space/energy/angular discretization, anisotropic scattering order, convergence criteria

- **Nuclear data uncertainties**: transport cross-sections, dosimeter response functions, fission spectra ($U, Pu$)

- **Radiation source description** (space, energy distribution)

- **Geometry modelling, material compositions** (1D / 2D / 3D, $r-\theta$ to x-y conversion, dosimeter locations...)
Probability theory

Applied long time ago to repeated observations of random variables (coin tossing):

$$\langle x \rangle = \sum_i \frac{x_i}{N}$$

Extension to physical quantities which are not random variables: the probability distribution indicates how plausible various possible values are.

$$\langle x \rangle = \sum_i \langle f_i \rangle x_i$$  \hspace{1cm} f = probability distribution function

$$\langle x \rangle = \int x f(x) dx$$

$$\sum_i f_i = 1$$
Expressing uncertainties

In practice an experimental result is usually characterized by its mean value and standard deviation:

\[ \langle x \rangle \pm \Delta x \]

where

\[ (\Delta x)^2 = \langle (x - \langle x \rangle)^2 \rangle \]

...variance of x

Standard deviation (\(\Delta x\) or \(\sigma\))

*Normal (Gaussian)*: \(\pm 1\ \sigma \sim 68\%\) confidence level
  \(\pm 2\ \sigma \sim 95\%\) probability “

*Flat distribution*: \(\pm 1\ \sigma \sim 58\%\) probability “
Covariance matrices

More than single value involved $\Rightarrow$ Covariance matrices

$$\text{cov}(x_i, x_j) = \langle \delta x_i, \delta x_j \rangle = \left( (x_i - \langle x_i \rangle)(x_j - \langle x_j \rangle) \right)$$

Correlation matrix :

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

Relative covariance matrix :

$$r \text{cov}(x_i, x_j) = \frac{\text{cov}(x_i, x_j)}{\langle x_i \rangle \langle x_j \rangle} = R(x_i, x_j) \frac{\Delta x_i \Delta x_j}{\langle x_i \rangle \langle x_j \rangle}$$
Covariance matrices

Assumption: linear relationship between quantities is valid within few $\sigma$.

- Uncorrelated (statistical) errors
- Correlated (systematic) errors: calibration, standards...

Uncertainties are to some extent subjective. But construction of the matrices must follow mathematical reasoning, in particular matrices must be:

- **Symmetric**
- **Non-negative**, i.e. having positive or zero eigenvalues (zero mean redundant information)
Propagation of uncertainty

Often a quantity \( (y) \) is not measured directly but is obtained from other quantities \( (x_i) \). In first order linear approximation:

\[
\delta y = \frac{\partial y}{\partial x_i}\bigg|_{x=\langle x \rangle} \delta x_i + \ldots \\
\delta y = a \delta x + x \delta a + \delta a \delta x
\]

The derivatives are evaluated at the expectation values of these density functions. First order approximation assumes that the partial derivatives are constant over the interval of variation of the variable described by the uncertainty. Nonlinear dependence is linearised, i.e. second order derivatives are neglected.
Propagation of uncertainty

General case:  \( \bar{y} = (y_i), \bar{x} = (x_i) \)

\[ V(y) = P \cdot V(x) \cdot P^T \]

where

\( V = \) relative covariance matrix

\[ P_{ij} = \frac{x_j}{y_i} \frac{\partial y_i}{\partial x_j} = \text{relative sensitivity matrix} \]
Propagation of uncertainty

\[ V(y) = P \cdot V(x) \cdot P^T = \begin{vmatrix} x \frac{\partial y_1}{\partial x_1} & x \frac{\partial y_1}{\partial x_2} & y \frac{\partial y_1}{\partial x_1} & y \frac{\partial y_1}{\partial x_2} \\ x \frac{\partial y_2}{\partial x_1} & x \frac{\partial y_2}{\partial x_2} & y \frac{\partial y_2}{\partial x_1} & y \frac{\partial y_2}{\partial x_2} \end{vmatrix} \begin{vmatrix} \left( \frac{\partial x_1}{\partial x_1} \right)^2 & \frac{\partial x_1}{\partial x_1} \frac{\partial x_2}{\partial x_1} & \frac{\partial x_1}{\partial x_1} \frac{\partial x_2}{\partial x_2} \\ \frac{\partial x_1}{\partial x_2} \frac{\partial x_2}{\partial x_1} & \left( \frac{\partial x_2}{\partial x_2} \right)^2 & \frac{\partial x_1}{\partial x_2} \frac{\partial x_2}{\partial x_2} \\ \frac{\partial y_1}{\partial x_1} \frac{\partial y_2}{\partial x_1} & \frac{\partial y_1}{\partial x_2} \frac{\partial y_2}{\partial x_2} & \frac{\partial y_1}{\partial x_1} \frac{\partial y_2}{\partial x_2} \end{vmatrix} = \begin{vmatrix} x \frac{\partial y_1}{\partial y_1} & x \frac{\partial y_2}{\partial y_1} \\ y \frac{\partial y_1}{\partial y_1} & y \frac{\partial y_2}{\partial y_1} \end{vmatrix} \begin{vmatrix} \left( \frac{\partial x_1}{\partial y_1} \right)^2 & \frac{\partial x_1}{\partial y_1} \frac{\partial x_2}{\partial y_1} & \frac{\partial x_1}{\partial y_1} \frac{\partial x_2}{\partial y_1} \\ \frac{\partial x_1}{\partial y_2} \frac{\partial x_2}{\partial y_1} & \left( \frac{\partial x_2}{\partial y_2} \right)^2 & \frac{\partial x_1}{\partial y_2} \frac{\partial x_2}{\partial y_2} \\ \frac{\partial y_1}{\partial y_1} \frac{\partial y_2}{\partial y_1} & \frac{\partial y_1}{\partial y_2} \frac{\partial y_2}{\partial y_1} & \frac{\partial y_1}{\partial y_1} \frac{\partial y_2}{\partial y_1} \end{vmatrix} \begin{vmatrix} x \frac{\partial y_1}{\partial y_1} & x \frac{\partial y_2}{\partial y_2} \\ y \frac{\partial y_1}{\partial y_1} & y \frac{\partial y_2}{\partial y_2} \end{vmatrix} \]
Peelle’s Pertinent Puzzle

\[ \sigma = Na \]

\[ a_1 = 1.50(1 \pm 0.10) \]

\[ a_2 = 1.00(1 \pm 0.10) \]

\[ N = 1.00(1 \pm 0.20) \]

\[ \bar{a} \pm \Delta a = \frac{\sum a_i}{\sum \frac{1}{\delta a_i^2}} \pm \frac{1}{\sqrt{\sum \frac{1}{\delta a_i^2}}} = 1.15 \pm 0.08 \]

\[ \bar{\sigma} \pm \Delta \sigma = 1.15 \pm 0.25 \]

\[ \delta(Na) = N \delta a + a \delta N \]

\[ \langle \delta N \delta a \rangle = 0 \Rightarrow (\delta(Na))^2 = (N \delta a)^2 + (a \delta N)^2 \]
Peelle’s Pertinent Puzzle

\[ V = \begin{bmatrix} \langle \delta \sigma_1 \rangle^2 & \langle \delta \sigma_1 \delta \sigma_2 \rangle \\ \langle \delta \sigma_1 \delta \sigma_2 \rangle & \langle \delta \sigma_2 \rangle^2 \end{bmatrix} = \begin{bmatrix} 0.1125 & 0.06 \\ 0.06 & 0.05 \end{bmatrix} \]

\[ \langle \delta \sigma_1 \rangle^2 = \langle \delta(Na_1) \rangle^2 = N^2 \langle \delta a_1 \rangle^2 + a_1^2 \langle \delta N \rangle^2 \]

\[ \langle \delta \sigma_1 \delta \sigma_2 \rangle = \langle \delta(Na_1) \delta(Na_2) \rangle = a_1 a_2 \langle \delta N \rangle^2 \]

\[ \bar{\sigma} \pm \Delta \sigma = \frac{\sum_{i,j} Na_j(V^{-1})_{ij}}{\sum_{i,j} (V^{-1})_{ij}} \pm \frac{1}{\sqrt{\sum_{i,j} (V^{-1})_{ij}}} = 0.88 \pm 0.22 \]
Another Puzzle

\[ 0.5 < \frac{V_{\text{wine}}}{V_{\text{water}}} < 1 \Rightarrow \left\langle \frac{V_{\text{wine}}}{V_{\text{water}}} \right\rangle = \frac{3}{4} = 0.75 \]

\[ 1 < \frac{V_{\text{water}}}{V_{\text{wine}}} < 2 \Rightarrow \left\langle \frac{V_{\text{water}}}{V_{\text{wine}}} \right\rangle = \frac{3}{2} = 1.5 \]

\[ V_{\text{water}} + V_{\text{wine}} = 1 \]

\[ \left\langle \frac{V_{\text{wine}}}{V_{\text{water}}} \right\rangle = \frac{5}{7} = 0.71 \]
Cross-section Generation

Measurement & Theory (EXFOR)

Evaluation
n(ENDF/B-VI.8, JEFF-3, JENDL 3.3, CENDL-2, BROND-2.2)
γ(EPDL)
e-(EEDL)

Processing (NJOY, AMPX/SCALE)

Testing against integral experiments
Cross Section Covariance Matrix Evaluation

**Measurements**: least square fitting of measured data sets: cross section error consists of statistical uncertainty (representing scatter among data) and systematic error.

**Nuclear models**: model approximations and deficiencies; expressed in terms of covariances of input parameters and sensitivities (uncertainty propagation law), uncertainty in input parameters is deduced by the comparison with the experimental data using Bayesian analysis.
Data Formats for Cross Section Covariances in Evaluated Files

- **MF=30**: Covariance of a set of important parameters and parameter sensitivities
- **MF=31**: Covariances of average number of neutrons per fission ($\nu$)
- **MF=32**: Shape and area of individual resonances
- **MF=33**: Cov. of energy dependent cross-sections
- **MF=34**: SAD covariances
- **MF=35**: SED covariances
- **MF=36**: Proposed for energy-angle covariances
- **MF=40**: Covariances for production of radioactive nuclei
Cross-section Covariance Data in BROND-2.2

- File types are
  - MF= 33 (cross sections)

- The Nuclides are:
  - C-0, Au-197, Pb-0
Cross-section Covariance Data in CENDL-2.1

• File types are
  – MF=31 (\(\nu\)), 32 (resonances),
    33 (cross sections), 34 (angular distributions)

• The Nuclides are:
  – H-2, H-3, O-16, F-19, Mn-55, Fe-56, U-235, U-238,
    Pu-240, Am-241
Cross-section Covariance Data in ENDF/B-VI.7

- File types are
  - MF=31 (ν), 32 (resonances), 33 (cross sections)
- The Nuclides are:
Cross-section Covariance Data in ENDF/B-V

- File types are
  - MF=31 (ν), 32 (resonances), 33 (cross sections),
- The Nuclides are:
Cross-section Covariance Data in JEFF-3.0

• File types are
  – MF=31 (ν), 33 (cross sections), 
    34 (angular distributions)
• The Nuclides are:
  – H-3, C-0, Be-9, F-19, Si-28, V-0, Cr-50, Cr-53, Cr-54 
    Mn-55, Fe-54, Fe-56, Co-59, Ni-58, Ni-60, Ni-61, Ni-62, 
    Ni-64, Cu-63, Cu-65, Y-89, Nb-93, Re-185, Re-187, 
    Au-197, Bi-209, Th-232, (U-238)
Cross-section Covariance Data in JEF-2.2

- File types are
  - MF=31 (ν), 33 (cross sections)
- The Nuclides are:
  - H-1, Li-6, Li-7, Be-9, C-0, Co-59, Ni-58, Ni-60, Ni-61, Ni-62, Ni-64, Y-89, Au-197, U-235, (U-238)
Cross-section Covariance Data in EFF-2.4

• File types are
  – MF= 33 (cross sections), 34 (angular distributions)

• The Nuclides are:
  – H-1, Li-6, C-0, F-19, Al-27, V-0, Cr-52, Mn-55, Fe-56,
    Co-59, Ni-58, Ni-60, Ni-61, Ni-62, Ni-64, Cu-63, Cu-65,
    Nb-93, Re-185, Re-187
Cross-section Covariance Data in JENDL-3.3

• File types are
  – MF=31 (ν), 32 (resonances), 33 (cross sections), 34 (angular distributions) & 35 (spectra)
• The Nuclides are:

ERRORR-J module required for processing of some materials
Processed Multigroup Covariance Data Libraries

- **ZZ-COVFILS**: 30-Group Neutron Cross-Section Covariance Library from ENDF/B-V (in BOXER format)
- **ZZ-COVFILS-2**: 74-Group Covariances for Fusion Reactors (ENDF/B-V)
- **PUFF-2**: Multigroup Covariances from ENDF/B-V & processing code (COVERX for.)
- **ZZ-DOSCOV**: 24-Group Covariance Library from ENDF/B-V for Dosimetry Calcul.
- **ZZ-COVERV**: Multigroup Cross-Section Covariance Matrices from ENDF/B-V
- **ZZ-VITAMIN-J/COVA**: Covariance Matrix Library based on JEF-1, ENDF/B-IV & -V data; processing & verification codes
- **ZZ-VITAMIN-J/COVA/EFF2**: EFF-2.3 covariance matrices for 18 materials, detector response function covariances from IRDF 90.2
- **ZZ-VITAMIN-J/COVA/EFF3**: EFF-3 covariance matrices for Be-9, Si-28, Fe-56, Ni-58, Ni-60; processing & verification utilities
- **ERRORJ**: processing code & JENDL-3.2 covariance matrices
U-235(n,f)

JEF-2.2 (ENDF/B-V)  IRDF-90  JENDL-3.2
U-235(n,γ)

JEF-2.2 (ENDF/B-V)

JENDL-3.2
U-238\((n, \gamma)\)

JEF-2.2/JEFF-3

IRDF-90

JENDL-3.2
Fe-56(n,inel)

Eff-3.1

JENDL-3.2
Cross Section Uncertainties

Cross section processing uncertainties

- *Conversion to MCNP ACE format*: reproduction tolerance, conversion of Legendre moments to equally-probable cosine bins, self-shielding in unresolved resonances

- *Conversion to multigroup format*: flux weighting, multigroup collapsing, self-shielding. Problem dependent libraries.

- Linearisation and Doppler broadening (negligible)
Iron total cross-section - point data
Iron total cross-sections in 640 group structure
Cross Section Sensitivity Analysis

- Several independent calculations (brute force) - unpractical
- **Perturbation method based on forward and adjoint flux**: first order perturbations (deterministic & M/C methods):
  - SN: SWANLAKE (1D), SENSIT&SUSD (1D, 2D, SED/SAD)
  - McBEND (M/C 1st order perturbations)
  - SUSD3D (1D, 2D, 3D SN uncertainty including SED/SAD);
  - TSUNAMI (SCALE-5): 1D SN, 3D M/C (KENO5)
- **Monte Carlo methods**: (correlated sampling, first and second order perturbations)
  - MCNP4C differential operator perturbation method (material density, composition, cross sections)
Discrete Ordinates (S\textsubscript{N}) Method

Discretisation of all independent variables, i.e. space, energy, and direction:

- The space mesh size comparable to the mean free path of the particle.
- Discrete angular direction quadrature set. The number of directions in the quadrature set depends on the the S\textsubscript{N} order and the number of dimensions. If anisotropy is important higher S\textsubscript{N} order and therefore larger number of directions are needed.
- Preparation of nuclear data: self-shielding, weighting spectra.
Advantages of Discrete Ordinates Codes

- **Relatively low CPU** time requirements as compared to M/C;
- Provide detailed particle **flux distribution**;
- Suitable for **sensitivity/uncertainty analysis**.
Disadvantages of Discrete Ordinates Codes

- Phase space is divided into \textit{energy-space-angular intervals}.

- \textit{Complex geometry description} more difficult

- \textit{Cross sections preparation}: averaged over discrete energy intervals (weighting function, self-shielding), problem dependent

- \textit{Ray effects} in low-scattering media (air/vacuum) or black bodies (in case of 2D and 3D);
  - first collision source approach.
Direct and Adjoint Transport Solutions

Steady state system with distributed source Q:

\[ L\phi + Q = 0 \]

\[ F = (\phi, \sigma) = \int_{V} \int_{0}^{E_{\text{max}}} \int_{4\pi} d\vec{r} dE d\Omega \phi(\vec{r}, \Omega, E) \sigma_d(\vec{r}, \Omega, E) \]

If transport operator L is not self-adjoint it is possible to define an adjoint operator satisfying:

\[ (\phi^+, L\phi) = (\phi, L^+ \phi^+) \]

\[ L^+ \phi^+ + \sigma_d = 0 \]

\[ F = (\phi, \sigma_d) = (\phi^+, Q) \]
VENUS-3 neutron source in the core * adjoint flux

core barrel: $Q^+ = \sigma_{Al27(n,\alpha)}$
VENUS-3 neutron source in the core * adjoint flux.

Actual neutron source

Inner baffle:

\( Q^+ = \sigma_{Ni58(n,p)} \)
Cross Section Sensitivity Coefficients
Forward/adjoint Flux Approach

\[ P_g^x = \frac{\frac{\delta R}{R}}{\frac{\delta \sigma_g^x}{\sigma_g^x}} \]

\[ = \frac{1}{R} \sum_i \Delta V_i \left( -\rho_i^x \sigma_{T,g,i}^x i \sum_m \Phi_{g,i,m} \Phi_{g,i,m}^* \Delta \Omega_m \right) \]

\[ + \rho_i^x \sum_{g'} \sum_{l=0}^L \sigma_{l,g \rightarrow g'}^x \sum_{n=-l}^l \sum_{M_{g',i}} M_{g',i}^* M_{g,i} \]

\[ + \sigma_{g}^{Dx} \sum_m \Phi_{g,i,m} \Delta \Omega_m \right) \]

**Loss term**
(absorption, scattering)

**Gain term**
(scattering, fission, nu-bar)

**Direct term**
(detector response function)
Sensitivity terms

- Transport cross-section loss term: absorption
- Transport cross-section loss and gain terms: scattering, fission
  \( \hat{\sigma}_{g-g'} = \nu_g \chi_{g'} \sigma_{f,g} \)
- Transport cross-section gain terms: nu-bar (\( \nu \): MT452, 455, 456)
- Direct term: detector response function

Relative variance of \( R \) is obtained from sensitivities and covariance matrices as:

\[
\frac{\Delta R}{R} = \sum_g \sum_{g',x'} P_g^x \cdot R \text{cov}(\sigma_{g,x}^x, \sigma_{g,x'}^{x'}) \cdot P_{g'}^{x'}
\]
Examples of the Use of Sensitivity/Uncertainties Analysis

- **Reactor pressure vessel surveillance**: uncertainty in predicted dosimeter reaction rates and PV exposition, determination of safety margins --> reactor lifetime predictions

- **New project design studies or improved design**: design and safety margins: parameter studies for fusion shielding blanket (tritium breeding ratio, heating, dose rates), ADS

- **Pre- and post-analysis of benchmark experiments**: optimisation of experimental configuration, explain eventual discrepancies, representativity studies, data consistency

- **Criticality safety**

- **Nuclear data evaluations**
Sensitivity/uncertainty code system

DOORS
DANTSYS

Φ, Φ+

GROUPR
GROUPSR

Partial
X-sections

ANGELO
ERRORR

Group
covariances

SEADR
ERRORR34

Group
SAD/SED
covariances

SUSD3D
SUSD3D Analysis Examples

- **PWR pressure vessel dosimetry**
- **Fusion benchmark analysis**: FNG Bulk Shield, FNG Streaming, FNG SiC, FNG Tungsten, preparation of fusion tritium breeding experiment
- **Fission shielding benchmarks**: ASPIS, VENUS-3
- **Criticality benchmarks**: VENUS-2, KRITZ
- **Oil well logging**: C/O (gamma) ratio sensitivity & uncertainty
- **TLD**