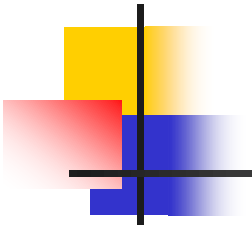
UK Atomic Energy Authority

FISPACT II Workshop

Shielding and application to inventory calculations

- **Ivo Kodeli**

FISPACT II Workshop, Nov. 30, 2020



- **Bateman-Boltzmann coupling (quasy-static)**
- **Boltzmann equation – direct/adjoint**
- **Sensitivity analysis**

BATEMAN equation

$$\frac{\partial N_i(t)}{\partial t} = N_f \sigma_f \Phi Y_{fi} + \sum_{j=1}^{i-1} N_j(t)\left(\lambda_{ij} + \sigma_{ij}\Phi\right) - N_i(t)\left(\lambda_i + \sigma_i \Phi\right)$$

$$\frac{\partial N(t)}{\partial t} = MN(t)$$

Material composition of a nuclear materials changes constantly:

- nuclear fission → lighter nuclides, + secondary particles + energy.
- neutron-induced transmutation reactions
- radioactive decay

Designing new reactor concepts and when optimizing the reactor core loading, waste storage.

BATEMAN equation

$$\frac{\partial N(t)}{\partial t} = MN(t);$$

$$M(\Phi, x)$$

Nuclear data needs:

- Activation cross sections
- Fission product yields
- Decay data (half-lives, decay energies, spectra of decay products (neutrons, α, β^-, β^+, γ, x-rays)

- Inventory calculation codes: time-dependent coupling between nuclide concentrations and neutron density distribution

BATEMAN – BOLTZMANN equation coupling: Quasy-static approximation

$$\Phi(r, E, t_i) = \Phi(t_i)\psi(r, E, t_i)$$

- Isotopic composition and transmutation rates of neutron-induced reactions ←→ neutron density distribution in the system
- Assumption: slow variation of nuclide concentrations ➔ assumed constant when solving the neutron density distribution
- Time-independent eigenvalue problem (*criticality)*
- Rates at which nuclides transform to other nuclides are computed based on the neutron density distribution solution. These reaction rates can be used in Bateman equation, which governs the changes in nuclide concentrations over time.
- Bateman & Boltzmann calculations form a cyclic process: system is modeled forward in time by solving the Boltzmann and Bateman equations sequentially in a cyclic manner.

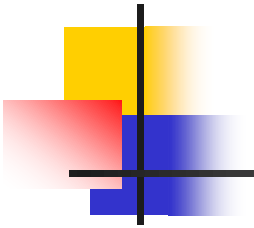
BATEMAN – BOLTZMANN equation coupling

$$N(t) = e^{At} N_0$$

- Matrix exponential of the burnup

Challenges:

- Matrix half-lives of different nuclides vary dramatically, making the system extremely stiff. The time steps used in burnup calculations generally vary from less than a day at the beginning of the irradiation cycle to a few hundred days at the end.
- Predicting the most representative averages for the reaction rates approximated as constants during the solution of burnup equations



- Bateman-Boltzmann coupling (quasy-static)
- **Boltzmann equation – direct/adjoint**
- Sensitivity analysis

BOLTZMANN transport equation

- *Rate of particle gain = Rate of particle loss*

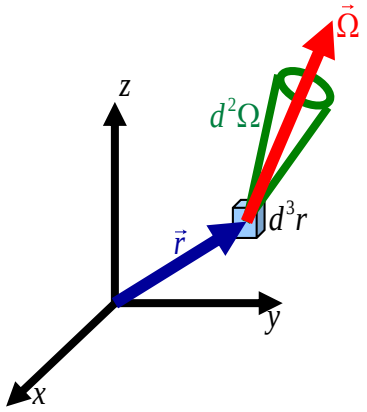
- or:
- *Inscattering gain + Source production gain = Leakage loss + Outscattering loss*

Neutron transport – Boltzmann equation

$$\Phi\left(\vec{r},\vec{\Omega},E,t\right)=vn\left(\vec{r},\vec{\Omega},E,t\right)$$

$$\frac{1}{v}\frac{d\phi\left(\bar{r},E,\bar{\Omega},t\right)}{dt}+\bar{\nabla}\cdot\bar{\Omega}\phi\left(\bar{r},E,\bar{\Omega},t\right)+\Sigma_T\left(\bar{r},E\right)\phi$$
$$=S\left(\bar{r},E,\bar{\Omega},t\right)+\int dE'\int\Sigma_S\left(\bar{r},E'\to E,\bar{\Omega}'\to\bar{\Omega}\right)\phi\left(\bar{r},E',\bar{\Omega}',t\right)d\bar{\Omega}'$$

Statistical approach: n = average particle density in a particular region of phase space at a certain time t



1932 James Chadwick

Ludwig Boltzmann

Ludwig Boltzmann

Born	Ludwig Eduard Boltzmann February 20, 1844 Vienna, Austrian Empire (present-day Austria)
Died	September 5, 1906 (aged 62) Tybein near Trieste, Austria-Hungary (present-day Duino, Italy) Suicide
Residence	Austria, Germany
Nationality	Austrian
Fields	Physics
Institutions	University of Graz University of Vienna University of Munich University of Leipzig
Alma mater	University of Vienna
Doctoral advisor	Josef Stefan
Doctoral students	Paul Ehrenfest Philipp Frank Gustav Herglotz Franc Hočevar Ignacij Klemenčič
Other notable students	Lise Meitner
Known for	Boltzmann constant Boltzmann equation Boltzmann distribution H-theorem

Boltzmann equation for diluted gas atoms

Rate of change of gas atom density in $(d\vec{r}\cdot d\vec{v}\cdot dt)$:

$$\left(\frac{\partial}{\partial t}+\vec{v}_1\cdot\nabla_{\vec{r}}+\vec{a}\cdot\nabla_{\vec{v}_1}\right)f(\vec{r},\vec{v}_1,t)=$$

$$=\int d\vec{v}_1^{\,'}\int d\vec{v}_2^{\,'}\int d\vec{v}_2 W(\vec{v}_1\to\vec{v}_1^{\,'},\vec{v}_2\to\vec{v}_2^{\,'})\left[f(\vec{r},\vec{v}_1^{\,'},t)f(\vec{r},\vec{v}_2^{\,'},t)-f(\vec{r},\vec{v}_1,t)f(\vec{r},\vec{v}_2,t)\right]$$

Mixture of different gases:

$$\left(\frac{\partial}{\partial t}+\vec{v}_i\cdot\nabla_{\vec{r}}+\vec{a}_i\cdot\nabla_{\vec{v}_i}\right)f_i(\vec{r},\vec{v}_i,t)=$$

$$=\sum_j\int d\vec{v}_1^{\,'}\int d\vec{v}_2^{\,'}\int d\vec{v}_2 W_{ij}(\vec{v}_i\to\vec{v}_1^{\,'},\vec{v}_2\to\vec{v}_2^{\,'})\left[f_i(\vec{r},\vec{v}_1^{\,'},t)f_j(\vec{r},\vec{v}_2^{\,'},t)-f_i(\vec{r},\vec{v}_i,t)f_j(\vec{r},\vec{v}_2,t)\right]$$

Density:
Neutrons: $\sim 10^{10}/\mathrm{cm}^3$
Nuclei: $\sim 10^{23}/\mathrm{cm}^3$

Boltzmann equation for diluted gas atoms

Mixture of 2 different gases

$f_1 << f_2 \Rightarrow$

1

$$\left(\frac{\partial}{\partial t} + \vec{v}_1 \cdot \nabla_{\vec{r}} + \vec{a}_1 \cdot \nabla_{\vec{v}_1}\right) f_1(\vec{r}, \vec{v}_i, t) =$$

$$= \int d\vec{v}_1' \int d\vec{v}_2' \int d\vec{v}_2 W_{11}(\vec{v}_1 \to \vec{v}_1', \vec{v}_2 \to \vec{v}_2') \left[f_1(\vec{r}, \vec{v}_1', t) f_1(\vec{r}, \vec{v}_2', t) - f_1(\vec{r}, \vec{v}_1, t) f_1(\vec{r}, \vec{v}_2, t) \right]$$

$$+ \int d\vec{v}_1' \int d\vec{v}_2' \int d\vec{v}_2 W_{12}(\vec{v}_1 \to \vec{v}_1', \vec{v}_2 \to \vec{v}_2') \left[f_1(\vec{r}, \vec{v}_1', t) f_2(\vec{r}, \vec{v}_2', t) - f_1(\vec{r}, \vec{v}_1, t) f_2(\vec{r}, \vec{v}_2, t) \right]$$

2

$$\left(\frac{\partial}{\partial t} + \vec{v}_2 \cdot \nabla_{\vec{r}} + \vec{a}_2 \cdot \nabla_{\vec{v}_2}\right) f_2(\vec{r}, \vec{v}_2, t) =$$

f_2 in equilibrium

$$= \int d\vec{v}_1' \int d\vec{v}_2' \int d\vec{v}_2'' W_{21}(\vec{v}_2 \to \vec{v}_1', \vec{v}_2'' \to \vec{v}_2') \left[f_2(\vec{r}, \vec{v}_1', t) f_1(\vec{r}, \vec{v}_2', t) - f_2(\vec{r}, \vec{v}_2, t) f_1(\vec{r}, \vec{v}_2'', t) \right]$$

$$+ \int d\vec{v}_1' \int d\vec{v}_2' \int d\vec{v}_2'' W_{22}(\vec{v}_2 \to \vec{v}_1', \vec{v}_2'' \to \vec{v}_2') \left[f_2(\vec{r}, \vec{v}_1', t) f_2(\vec{r}, \vec{v}_2', t) - f_2(\vec{r}, \vec{v}_2, t) f_2(\vec{r}, \vec{v}_2'', t) \right]$$

BOLTZMANN transport equation: assumptions

$$\frac{1}{\mathrm{v}}\frac{\partial}{\partial \mathrm{t}}\Phi = B\Phi + Q = \left(P - L\right)\Phi + Q$$

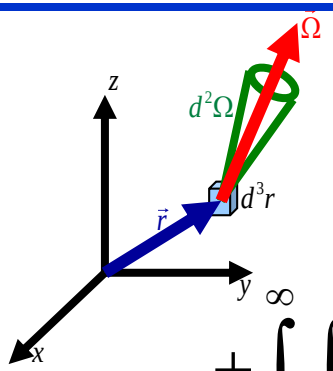
- **Diluted gas approximation:** only collisions between 2 particles are considered, 3-body collisions are assumed to be very rare
- **Molecular chaos approx.:** no correlation between colliding particles, so that the movement is fully chaotic; ($W_{12}=W_1\ W_2$)
- The **collision time is much shorter** than the time that elapses between collisions; time rate of change of W_1 and W_2 can be neglected.
- Over the range of the forces of interaction, the **gradient of inhomogeneities in the transport medium may be ignored**. This assumption effectively makes W a function of (r_1-r_2) only, and allows gradients of W to be neglected over a distance of the range of molecular forces.

Neutron transport – Boltzmann equation

Rate of change of mean neutron density in $(d\vec{r}\cdot d\vec{\Omega}\cdot dE\cdot dt)$

$$\frac{\partial}{\partial t}N(\vec{r},\vec{\Omega},E,t)d\vec{r}\cdot d\vec{\Omega}\cdot dE=\left[gains-losses\right]d\vec{r}\cdot d\vec{\Omega}\cdot dE$$

$$\Phi(\vec{r},\vec{\Omega},E,t)=vN(\vec{r},\vec{\Omega},E,t)$$



$$\frac{1}{v}\frac{\partial}{\partial t}\Phi=-(\vec{\Omega}\cdot\vec{\nabla})\cdot\Phi$$ — Streaming

$$-\Sigma_t\cdot\Phi$$ — Removal (abs. + scattering

$$+\int_0^\infty\int_{4\pi}\Sigma_s(E'\rightarrow E,\vec{\Omega}'\rightarrow\vec{\Omega})\Phi dE'\,d\vec{\Omega}'$$ — Scattering source

$$\left(A-\lambda F\right)\Phi=0$$

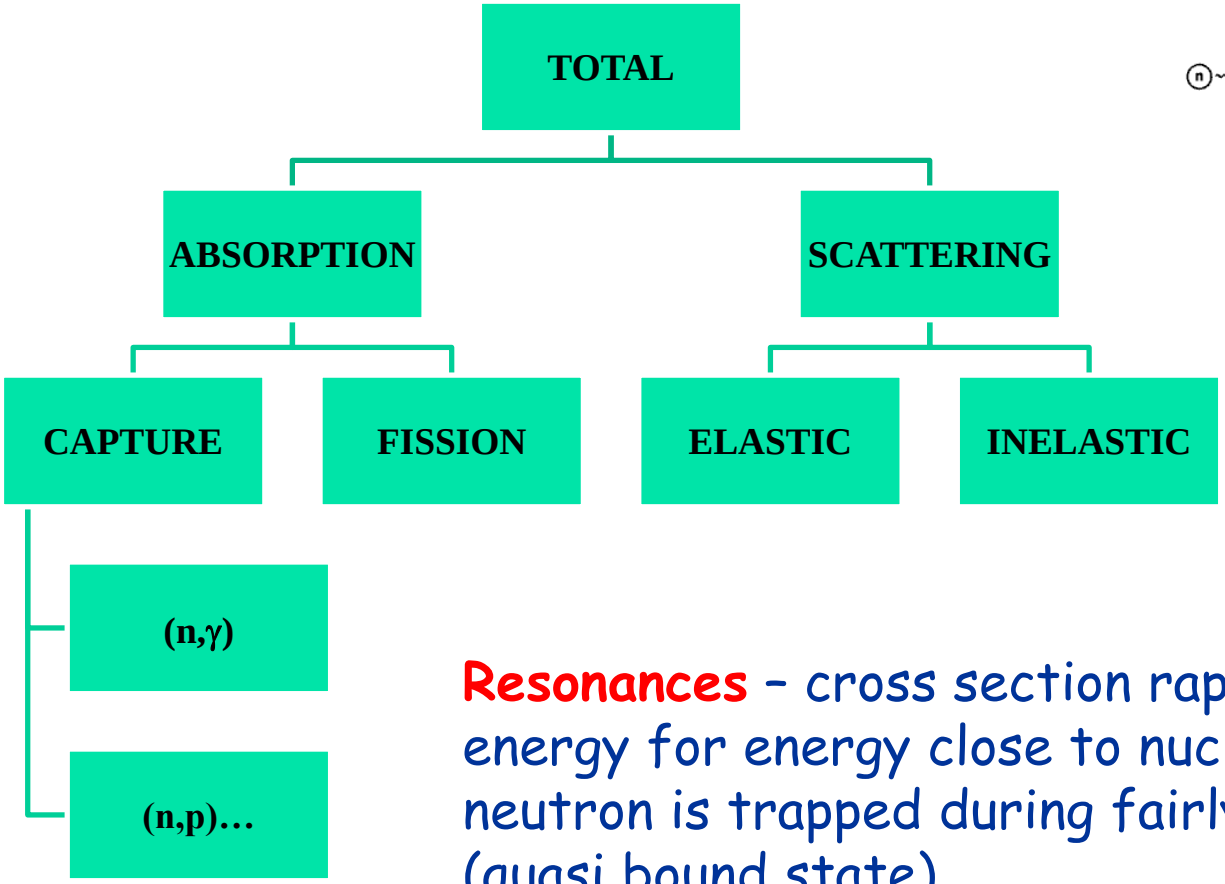
$$+\frac{1}{4\pi}\chi\int_0^\infty\int_{4\pi}\overline{\nu}\Sigma_f\Phi dE'\,d\vec{\Omega}'$$ — Fission source

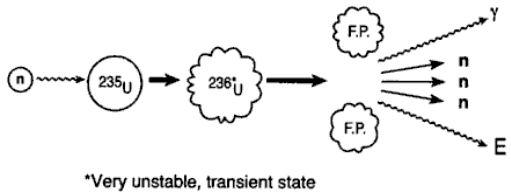
$$+Q_{ext}$$ — Other sources

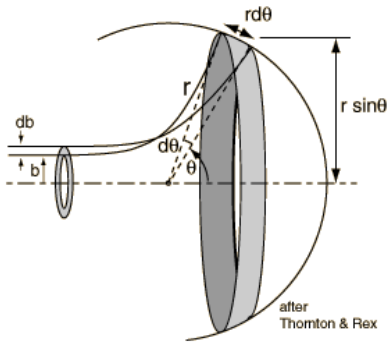
$$\frac{1}{v}\frac{\partial}{\partial t}\Phi=B\Phi+Q=\left(P-L\right)\Phi+Q$$

Neutron cross sections

A neutron is absorbed to form a "compound nucleus": $n + {}^{A}Z \rightarrow {}^{A+1}Z^{*}$ which lives for a short time and decays:



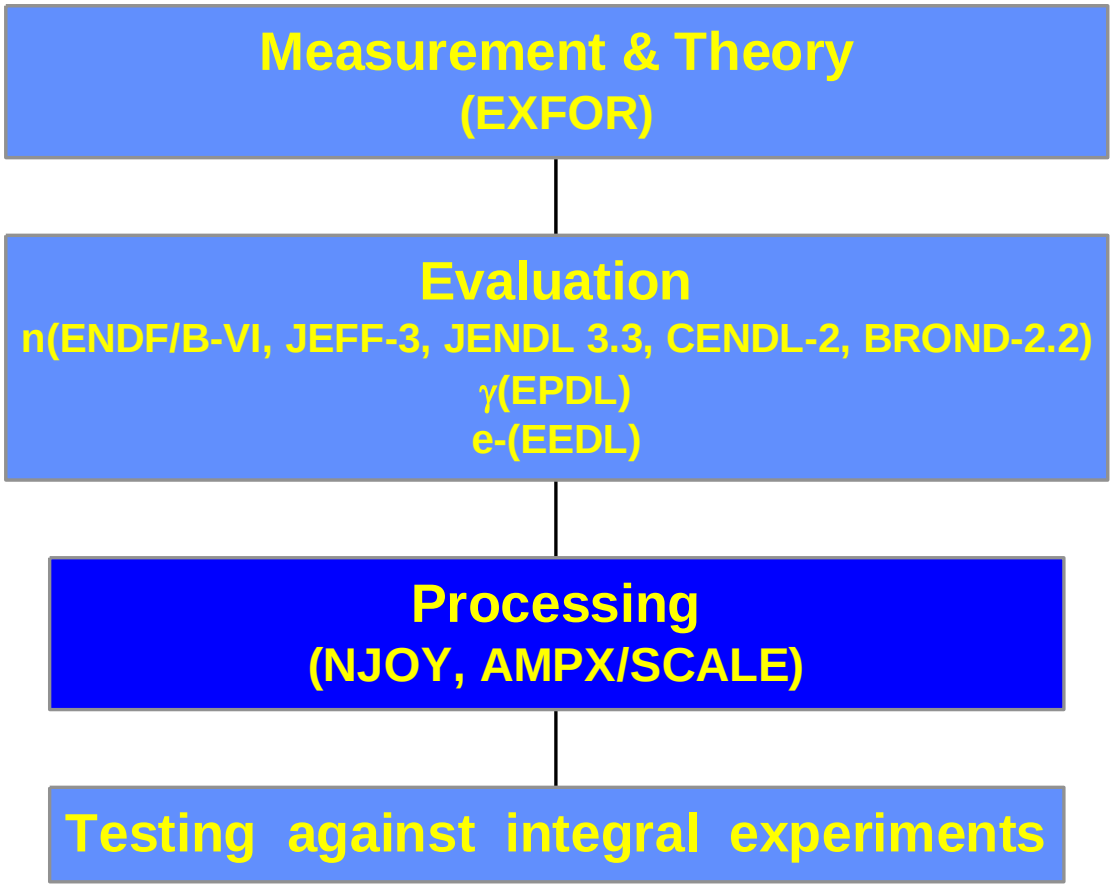




Resonances – cross section rapidly varying with energy for energy close to nuclear excitation level; neutron is trapped during fairly long time interval (quasi bound state).

Cross-section Generation Process

- **Basic nuclear data**
- **Evaluated data libraries**
- **Application libraries**
  - **- pointwise data**
  - **- multigroup data (fine- / few-group)**



Evaluated Cross Section Files Data and Formats

General purpose lib.

- **BROND-3.1**
- **CENDL-3.1**
- **ENDF/B-VIII**
- **JEFF-3.3**
- **JENDL-4.0**
- **RUSFOND-2010**
- **TENDL-2019**

E ~ 10^{-5} eV – 150 MeV

- **MF=1**: description text
- **MF=2**: resonances parameters
- **MF=3**: energy cross-sections
- **MF=4**: angular Distributions
- **MF=5**: energy Distributions
- **MF=6**: energy-angle distributions
- **MF=7**: thermal scattering data
- **MF=8**: radioactive data
- **MF=9-10**: nuclide production data
- **MF=12-15**: photon production data
- **MF=30-40**: covariance data

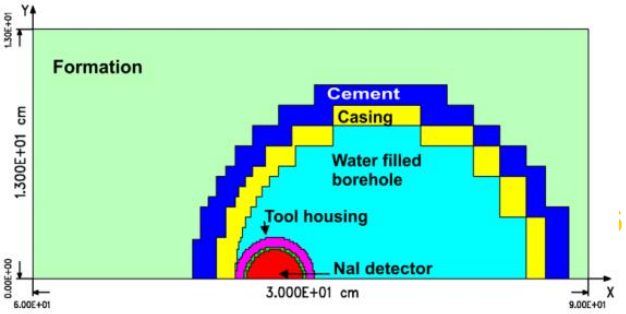
Boltzmann – Louville equations

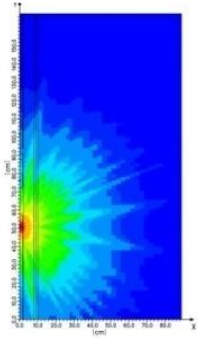
$$\frac{1}{\mathrm{v}}\frac{\partial}{\partial \mathrm{t}}\Phi = B\Phi + Q = \left(P - L\right)\Phi + Q$$

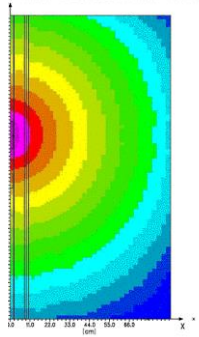
- $f_1(r,v,t)$, as defined in Louville equation, is the probability (averaged over phase space) that particle number one is at position *r* with velocity *v* at time *t*. The Boltzmann equation, however, is a balance equation for $f(r,v,t)$, where $f(r,v,t)dr\,dv$ is the average number of particles in the volume element *dr* with velocity lying between *v* and *v+dv* at time *t*.

Deterministic vs. Monte Carlo Methods

	Deterministic (Discrete ordinates S_N)	Monte Carlo
+	• Low CPU time • Detailed flux distributions • Suitable for sensitivity and uncertainty analyses	• Exact geometry description • Pointwise cross section treatment
-	• Discretisation ➔approximate representation in space, energy, angle • Case dependent multigroup cross sections (self-shielding, weighting spectra) • Memory needs	• Long CPU time • Statistical uncertainties, difficulty in using variance reduction • "Limited" information (integral quantities)







Particle transport methods

- ***Monte Carlo (→ continuus energy or multigroup XS):*** MCNP, KENO, McBEND, TRIPOLI, SERPENT, MORSE, EGS4, PENELOPE, MONK, ITS, FLUKA, LAHET, GEANT
- ***Deterministic transport or diffusion codes (→ multigroup XS):*** ANISN, DOORS, DANTSYS, PARTISN, TWOTRAN, CEPXS/ONELD, WIMS, APOLLO, CASMO, DRAGON, ATTILA, DENOVO

Group averaged cross sections

$$\langle \sigma_x \rangle_g = \frac{\int_{E_{g+1}}^{E_g} \sigma_x(E)\Phi(E)dE}{\int_{E_{g+1}}^{E_g} \Phi(E)dE}$$

σ_x = cross section

$\Phi(E)$ = weighting function

E_g = energy group boundaries

Example of weighting function: fission + 1/E + Maxwellian

Multigroup cross sections (XS) are obtained by weighting point-wise XS with a flux spectrum. As the spectrum used depends on the application, generated XS are problem dependent.

In resonance region Bondarenko method can be used.

Bondarenko self - shielding correction

$$\Phi(E) = \frac{C(E)}{\sigma_t(E) + \sigma_0}$$

σ_0 = background cross section

Group averaged cross sections

Multigroup data libraries:

- **General purpose libraries - several hundred (>200) energy groups for several self-shielding factors (self-shielding of resonances reconstructed depending on material composition and geometry.**
- **Problem dependent few-group XS: 2-step procedure: 1D calculation of zone spectra used to collapse to coarse energy group structure. Further space homogenization and group collapsing to few groups for 3D core design, transient and fuel management analysis.**

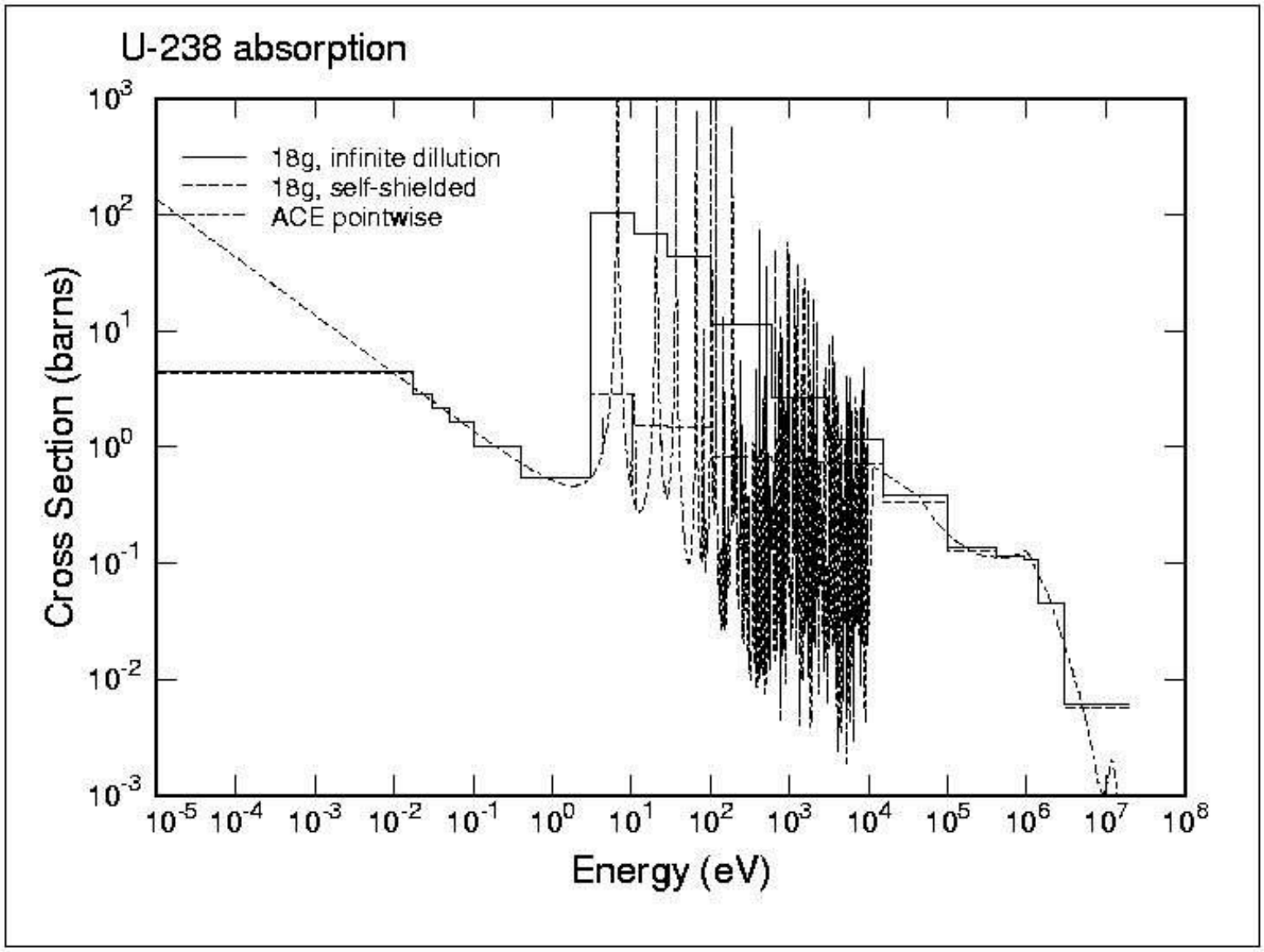
Energy group collapsing

$$\langle \sigma_x \rangle_g = \frac{\sum_{g' \in g} \sigma_{x,g'} \Phi_{g'}}{\sum_{g' \in g} \Phi_{g'}}$$

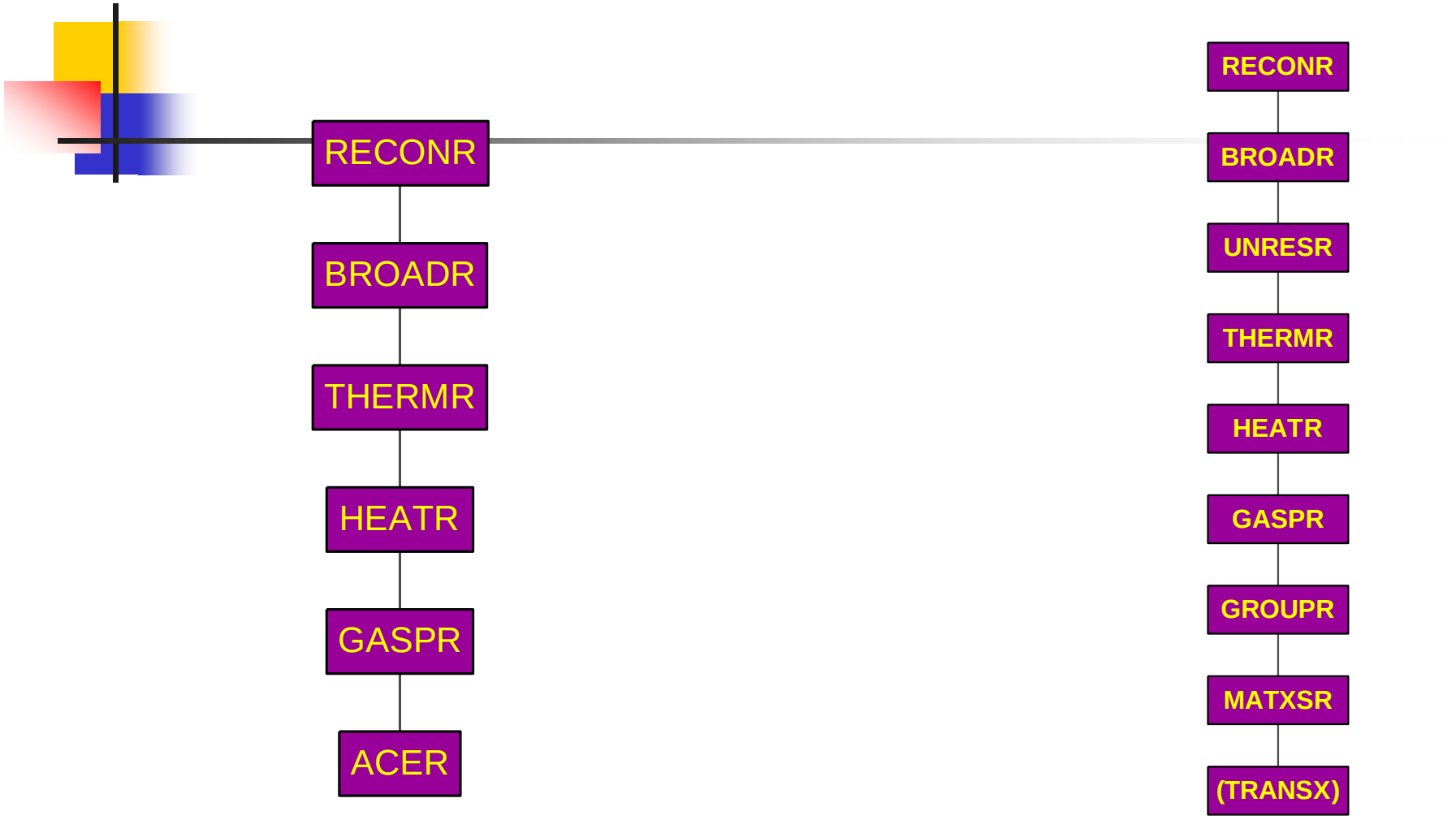
Spatial homogenization

$$\langle \sigma_x \rangle = \frac{\sum_V \sigma_{x,V_i} \Phi_{V_i} V_i}{\sum_V \Phi_{V_i} V_i}$$

U-238 absorption cross-sections in point-wise and 18 group structure



NJOY Flowchart of Cross-section Processing



MCNP ACE format

Multigroup Cross-sections

Types of cross-section data for MCNP

- **c – continuous-energy neutron**
- **d – discrete reaction neutron**
- **p – photon interaction data**
- **y – neutron dosimetry**
- **t – neutron S(α,β) thermal data**
- **m – multigroup neutron, coupled neutron/photon, and charged particles**
- **g – multigroup photon**
- **e – electron data**

Direct and adjoint transport equation – importance fonction

- Solution of the Boltzmann equation: $B \cdot \Phi = Q$

- Each bounded linear operator on a complex Hilbert space has a corresponding adjoint operator.
- Fondamental propriety of the adjoint function

$$\left\langle B^* \cdot \Phi^* \middle| \Phi \right\rangle = \left\langle \Phi^* \middle| B \cdot \Phi \right\rangle$$
$$\left\langle Q^* \middle| \Phi \right\rangle = \left\langle \Phi^* \middle| Q \right\rangle$$

If the transport operator *B* is not self-adjoint an adjoint operator can be defined as:

$$B^* \cdot \Phi^* = Q^*$$

Direct and adjoint transport equation – importance fonction

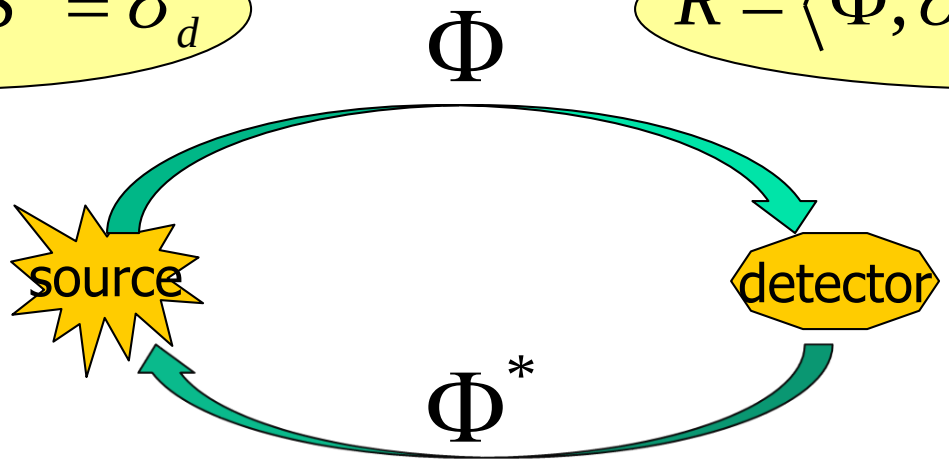
Calculation of the reaction rates:

$$R = \left\langle \sigma_d \cdot \Phi \right\rangle = \int_V \int_0^{E_{\max}} \int_{4\pi} \Phi\left(\vec{r}, \vec{\Omega}, E\right) \sigma_d\left(\vec{r}, \vec{\Omega}, E\right) d\vec{r} dE d\vec{\Omega}$$

- Corresponding adjoint operator can be defined as:

$$B^* \cdot \Phi^* = S^* = \sigma_d$$

$$R = \left\langle \Phi, \sigma_d \right\rangle = \left\langle \Phi^*, Q \right\rangle$$

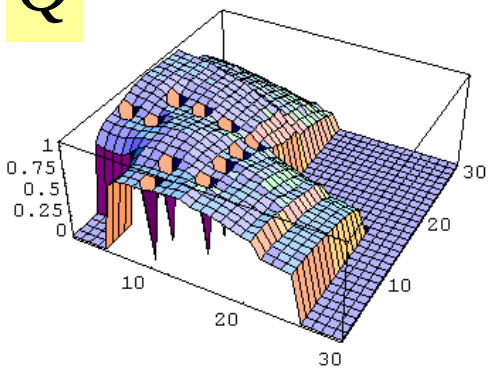


VENUS-3 reactor

core barrel:

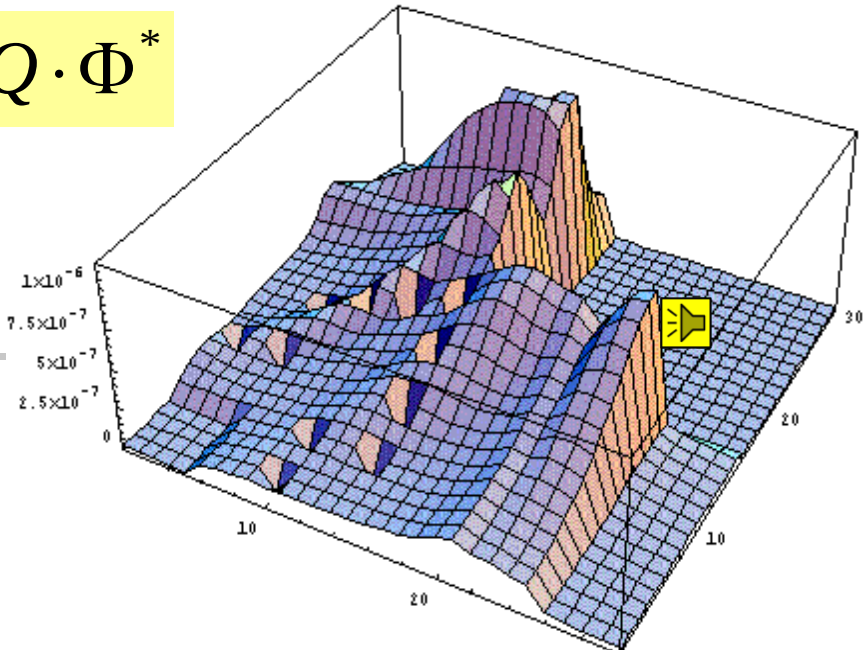
$Q^* = \sigma_{Al27(n,\alpha)}$

Q



Actual neutron source (mid-plane)

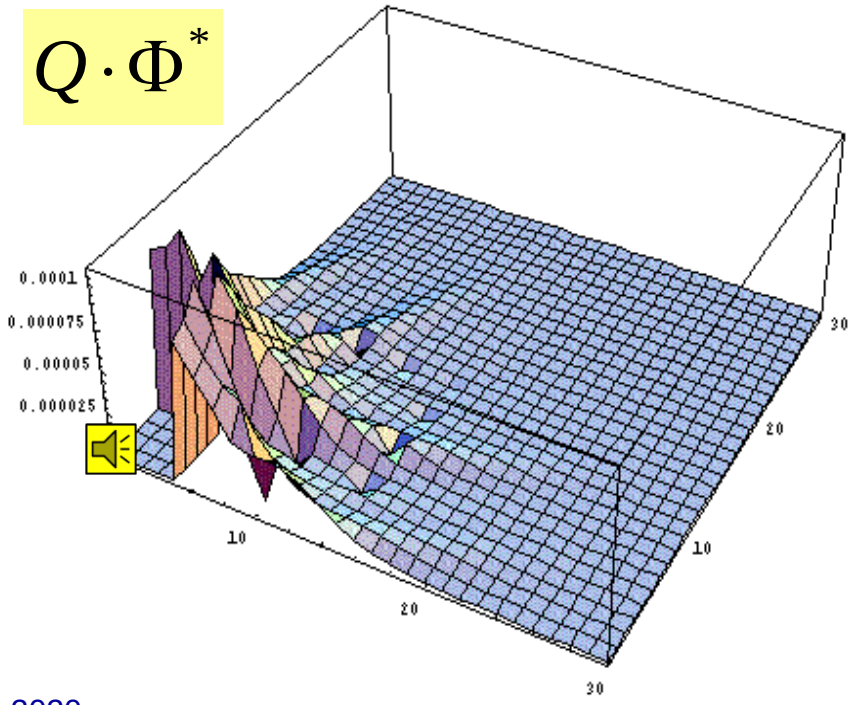
$Q \cdot \Phi^*$



inner buffle:

$Q^* = \sigma_{Ni58(n,p)}$

$Q \cdot \Phi^*$



Nuclide adjoint fonction

$$\frac{\partial N(t)}{\partial t} = MN(t)$$

$$\frac{\partial N^*(t_a)}{\partial t} = -M^* N^*(t_a)$$

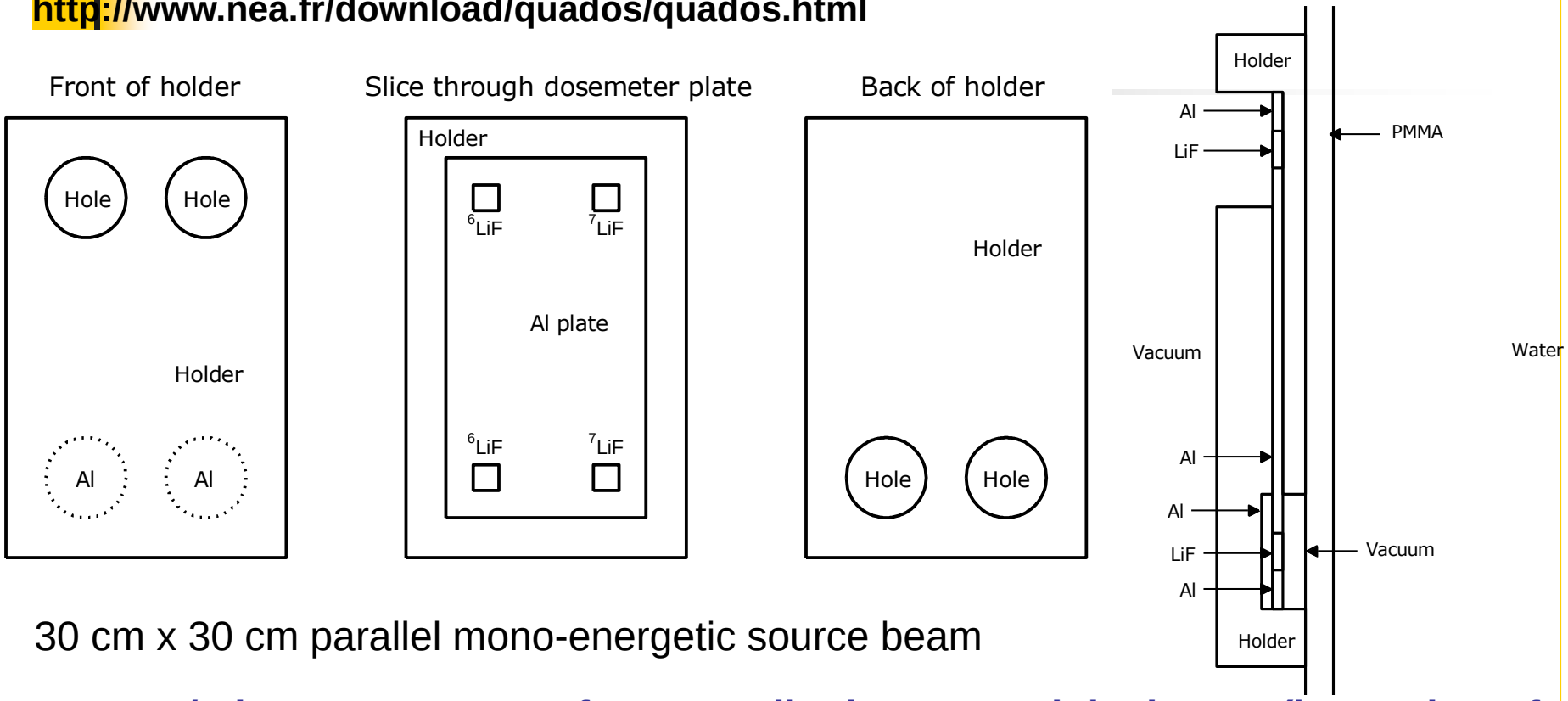
$$t_a = t_F - t$$

Nuclide adjoint functions represent the time-dependent importances of the various nuclides in the reactor for producing the response nuclide.

$$\Delta R = \left\langle N^* \middle| \Delta MN \right\rangle$$

QUADOS Problem 4: TLD response function

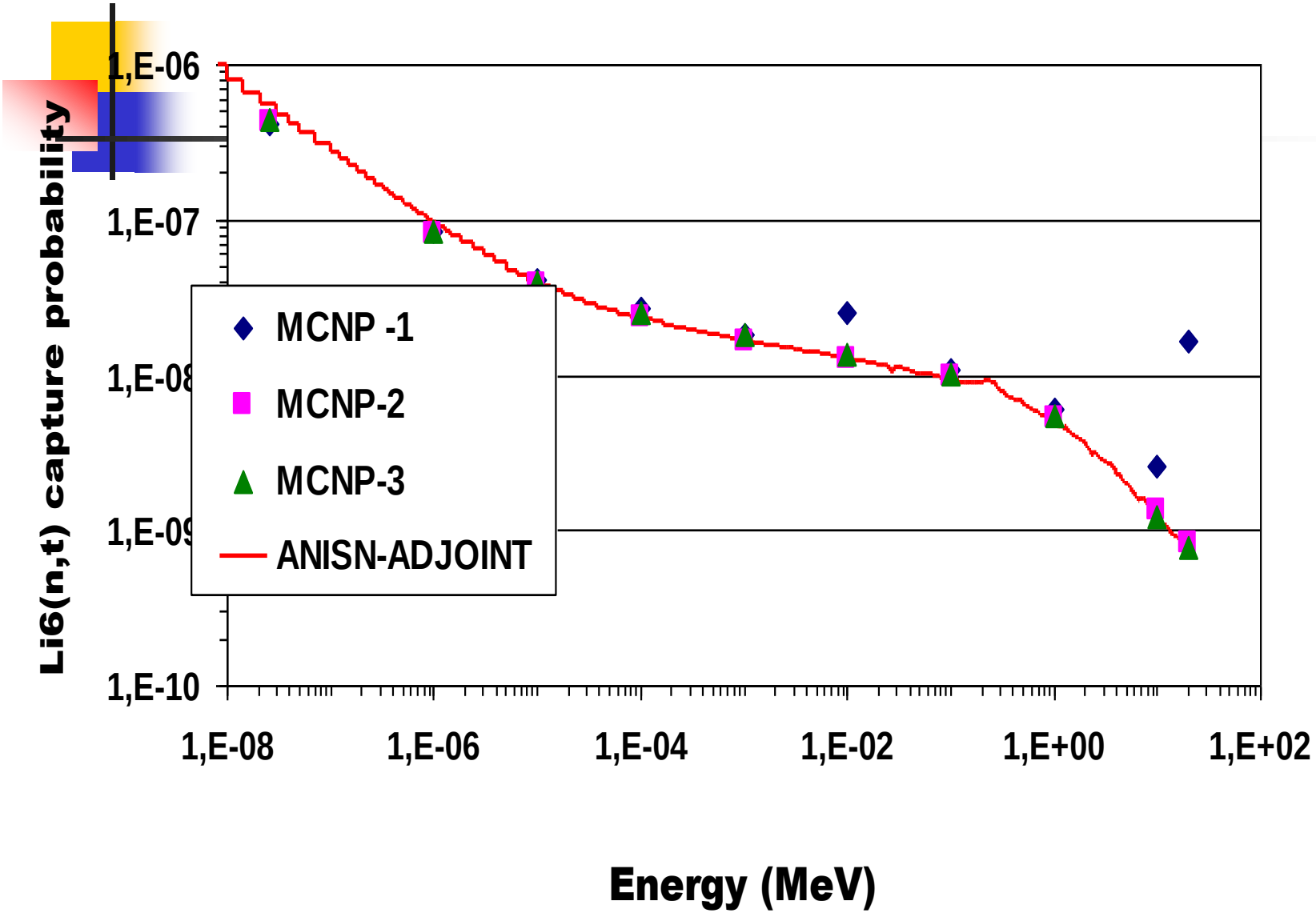
http://www.nea.fr/download/quados/quados.html



30 cm x 30 cm parallel mono-energetic source beam

Neutron / photon response of a TLD - albedo personal dosimeter (in number of Li6(n,t) reactions) for the four elements at normal incidence and at different energies.

QUADOS - TLD


Detector 2
Li6(n,t) capture probability
1,E-06
1,E-07
1,E-08
1,E-09
1,E-10
MCNP -1
MCNP-2
MCNP-3
ANISN-ADJOINT
1,E-08
1,E-06
1,E-04
1,E-02
1,E+00
1,E+02
Energy (MeV)

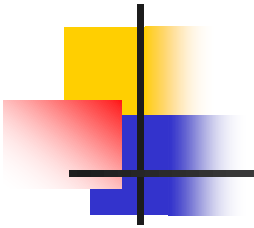
Monte Carlo adjoint calculations

Difficulty of M/C methods to provide adjoint fluxes with good statistics:

- Inversion of pointwise cross section tables
- Statistical difficulties due to varying weights of adjoint „particles“ arriving at the adjoint source:

$$\sigma \cong \frac{1}{N}\sum_{i=1}^{N} x_i^2 - \left(\frac{1}{N}\sum_{i=1}^{N} x_i\right)^2$$

- Multigroup adjoint M/C available in MCBEND, MCNP
- Iterated fission probability approach, MCNP6 (Kiedrowski), Serpent (Aufiero).



- Bateman-Boltzmann coupling (quasy-static)
- Boltzmann equation – direct/adjoint
- **Sensitivity analysis**

Sources of Uncertainty in Neutronics Calculations

- **Mathematical methods and simplifications:** e.g. M/C statistics, S_N space/energy/angular discretization, anisotropic scattering order, convergence criteria, diffusion equation
- **Nuclear data uncertainties**: nuclear cross-sections, fission spectra (U, Pu), standards, response functions (kerma, dpa)
- **Radiation source description** (space, energy distribution)
- **Geometry modelling, material compositions, conditions** (1D / 2D / 3D, temperature, dosimeter locations...)
- **"Human factor"**

Verification of results:

- **Sensitivity and uncertainty analysis**
- **Benchmark experiments analysis**

Verification of results

- **Sensitivity and uncertainty analysis**
- **Benchmark experiments analysis**

  NEA/NSC sponsored projects on integral experiments:

  - SINBAD - Radiation Shielding Experiments
  - ICSBEP - International Handbook of Evaluated Criticality Safety Benchmark Experiments
  - IRPhEP - Reactor Physics Experiments
  - IFPE - Fuel Performance Experiments

Methods for Cross-section Sensitivity Analysis

- Analytical method
- **Several independent calculations (brute force)** – time consuming but possible with todays computers (**total M/C-** TENDL, XSUSA)
- **Perturbation methods: sensitivity of a small number of responses to a very large number of uncertain inputs;**
  - forward and adjoint (deterministic, Monte Carlo) flux calculations; 1st order perturbations;
  - Monte Carlo differential operator perturbation method, correlated sampling;
- Examples of available computer codes:

  ERANOS, TSUNAMI, SUSD3D, SERPENT, MCSEN, MCNP-6, XSUSA, TENDL based code systems

SHORT CHRONOLOGY OF WORKS

on the Perturbation *theory and the sensitivity & uncertainty analyses in reactor physics*

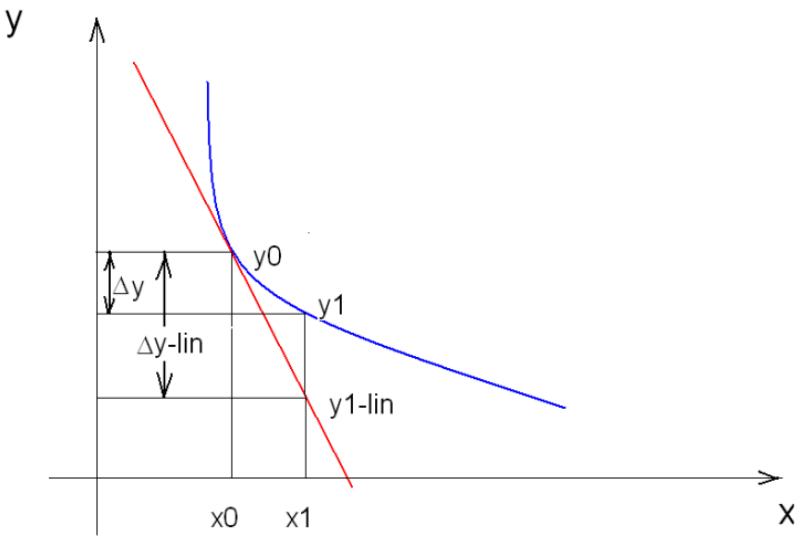
Perturbations are used for describing real systems which cannot be solved exactly (e.g. Schrödinger equation for Hamiltonians other than hydrogen atom, the quantum harmonic oscillator and the particle in a box, known solutions of simple Hamiltonians are used to generate solutions for more complicated systems **Eugène P. WIGNER « Effect of Small Perturbations on Pile Period » classified document of Manhattan Project (CP 3048, 13 june 1945). A.M WEINBERG and E.P. WIGNER,** « *The Physical Theory of Neutron chain Reactors* » University Press Chicago (1958).

L. N. USACHEV: Equations for the Importance of neutrons, reactor kinetics and the theory of perturbations, Int. Conf. Peaceful Uses of Atomic Energy 5, 503-510, UN, N.Y. (1955).

- **L.N. USACHEV,** *« Perturbations theory for the breeding ratio and for other number ratios pertaining to various reactor processes »*, J. Nucl. Energy, 18 p.571 (1964)
- **A.GANDINI,** *« A generalized perturbation method for bilinear fuctionals of the real and adjoint fluxes »* J. Nucl. Energy, 21, 735-745, 1967.

M. L. Williams, Perturbation Theory for Nuclear Reactor Analysis, CRC Press, 1986.

- Multiplication factor
- BOC peak to average power
- Control rod worth
- Breeding ratio
- Moderator void coefficient
- Absorbed radiation dose
- Material damage
- Detector reading, ex core
- Peak transient power
- EOC fuel inventory
- EOC reactivity and EOC neutron flux



Classical Perturbation Theory (CPT): sensitivity of k_{eff} to basic data:

- Perturbation of stationary Boltzmann equation:

$$\lambda = \frac{1}{k}$$

$$A \cdot \Phi = \lambda F \cdot \Phi$$

$$(A+\Delta A)\cdot(\Phi+\Delta\Phi) = (\lambda+\Delta\lambda)(F+\Delta F)\cdot(\Phi$$

Simplification due to the fundamental property of the adjoint!

- **1er order** perturbation (sensitivity independent of the perturbation):

$$\frac{\Delta\lambda}{\lambda} = \frac{\left\langle \Phi^* \middle| (\frac{\partial A}{\partial \alpha} - \lambda \frac{\partial F}{\partial \alpha}) \cdot \Phi \Delta\alpha \right\rangle - \left\langle \Phi^* \middle| (A-\lambda F) \cdot \frac{\partial \Phi}{\partial \alpha} \Delta\alpha \right\rangle}{\lambda \left\langle \Phi^* \middle| F \cdot \Phi \right\rangle}$$

=0

$$\Delta A = \frac{\partial A}{\partial \alpha} \Delta\alpha$$

- **2 calculations provide all the sensitivities**

$$\frac{\Delta\lambda}{\lambda} = \sum_{\alpha} S_\alpha \frac{\Delta\alpha}{\alpha}$$

$$S_\alpha = \frac{\alpha}{\lambda}\frac{\partial\lambda}{\partial\alpha}$$

Generalised Perturbation Theory (GPT)

- Sensitivity to parameters other than k_{eff}: reaction rates, reaction rate ratio, T coefficients, breeding ratio, linear functions of flux with flux normalisation.
- Boltzmann stationary eq. for fixed source problem:

$$B \cdot \Phi = Q$$

$$B^* \cdot \Phi^* = \sigma_D$$

$$\left\langle B^* \cdot \Phi^* \middle| \Phi \right\rangle = \left\langle \Phi^* \middle| B \cdot \Phi \right\rangle$$

$$\left\langle Q^* \middle| \Phi \right\rangle = \left\langle \Phi^* \middle| Q \right\rangle$$

Definition of a perturbation:

$$B' = B + \Delta B; Q' = Q + \Delta Q$$

$$\Phi' = \Phi + \Delta\Phi; \sigma' = \sigma + \Delta\sigma$$

$$\Delta R = \left\langle \Phi^* \Delta Q \right\rangle$$

$$(B + \Delta B)(\Phi + \Delta\Phi) = Q \Rightarrow B\Phi - Q + B\Delta\Phi + \Delta B\Phi + \Delta B\Delta\Phi = 0 \Rightarrow B\Delta\Phi = -\Delta B\Phi$$

$$\left\langle \Phi^* B\Delta\Phi \right\rangle = -\left\langle \Phi^* \Delta B\Phi \right\rangle \Rightarrow \left\langle \Delta\Phi B^* \Phi^* \right\rangle = -\left\langle \Phi^* \Delta B\Phi \right\rangle \Rightarrow \left\langle \Delta\Phi \sigma_D \right\rangle = \Delta R_\phi = -\left\langle \Phi^* \Delta B\Phi \right\rangle$$

=0

=0

Linear order simplification

$$\frac{\Delta R}{R} = \frac{\left\langle \Phi^* \Delta Q \right\rangle}{R} + \frac{\left\langle \Phi \Delta\sigma_D \right\rangle}{R} - \left\langle S_\sigma \frac{\Delta\sigma}{\sigma} \right\rangle$$

$$S_\sigma = \frac{\sigma}{R} \Phi^* \frac{\partial B}{\partial \sigma} \Phi$$

- Fixed source equation for perturbed system to **1st order** (sensitivity is independant of the perturbation) :
- **2 calculations provide all the sensitivities.**

$$S_\sigma = \frac{\sigma}{R} \frac{\partial R}{\partial \sigma}$$

Time-dependent Perturbation Theory – Coupled neutron-nuclide evolution (nonlinear systems of equations with feedback)

$$\frac{\partial N(t)}{\partial t} = MN(t) \quad \Longleftrightarrow \quad \frac{1}{v}\frac{\partial}{\partial t}\Phi = B\Phi + Q$$

Depletion greatly increases the adjoint formulation complexity.

Constraints:

$$\Phi(r, E, t_i) = \Phi(t_i)\psi(r, E, t_i)$$

Functional using Lagrange multipliers:

Flux shape $\left(A - \lambda F\right)\psi = 0$

Flux amplitude $\mathrm{P}_i = \int_{E,r} C\Phi_i\Sigma_f \, dEdx$

Bateman $\frac{\partial N(t)}{\partial t} = MN(t)$

$$\begin{aligned}
K[\underline{N},\psi_i,\Phi_i,\lambda_i,\underline{N}^*,\Gamma_i^*,P_i^*,A_i^*] = \\
R[\underline{N},\psi_i,\Phi_i] \\
+ \sum_{i=1}^{T}\int_{t_i}^{t_{i+1}}\int_X \underline{N}^{*T}(x,t)\left(\underline{\underline{M}} - \frac{\partial}{\partial t}\underline{\underline{I}}\right)\underline{N}(x,t)dxdt \\
- \sum_{i=1}^{T}\int_X\int_E \Gamma_i^*(x,E)(L - \lambda_i P)\psi_i(x,E)dEdx \\
- \sum_{i=1}^{T} P_i^*\left(\Phi_i\int_X\int_E \Sigma_{F,i}\psi_i(x,E)dEdx - P_i\right) \\
- \sum_{i=1}^{T} A_i^*\left(\int_X\int_E \psi_i(x,E)dEdx - 1\right)
\end{aligned}$$

UNCERTAINTY ANALYSIS OF MODELING (UAM)

Phase I (Neutronics Phase)

Exercise I-1: "Cell Physics" - focused on the derivation of the multi-group microscopic cross-section libraries

Exercise I-2: "Lattice Physics" - focused on the derivation of the few-group macroscopic cross-section libraries

Exercise I-3: "Core Physics" - focused on the core steady state stand-alone neutronics calculations

Phase II (Core Phase)

Exercise II-1: Fuel thermal properties relevant for transient performance

Exercise II-2: Neutron kinetics stand-alone performance (kinetics data, space-time dependence treatment, etc.)

Exercise II-3: Thermal-hydraulic fuel bundle performance

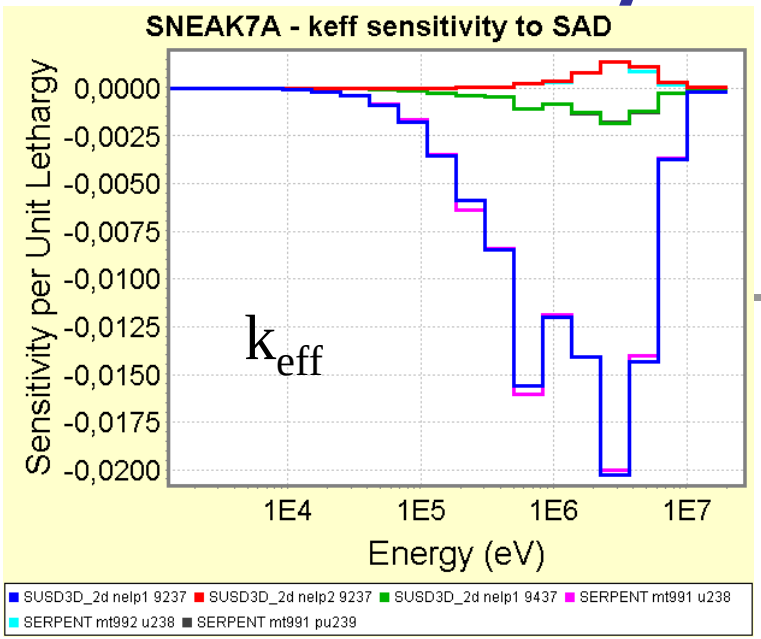
Phase III (System Phase)

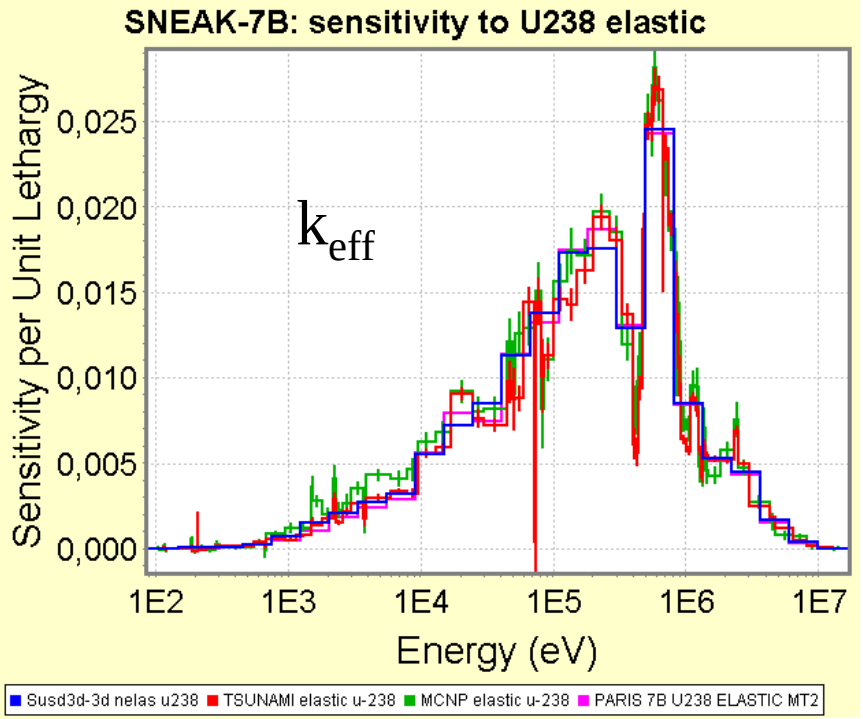
Exercise III-1: Coupled neutronics/thermal-hydraulics core performance (coupled steady state, coupled depletion, and coupled core transient with boundary conditions)

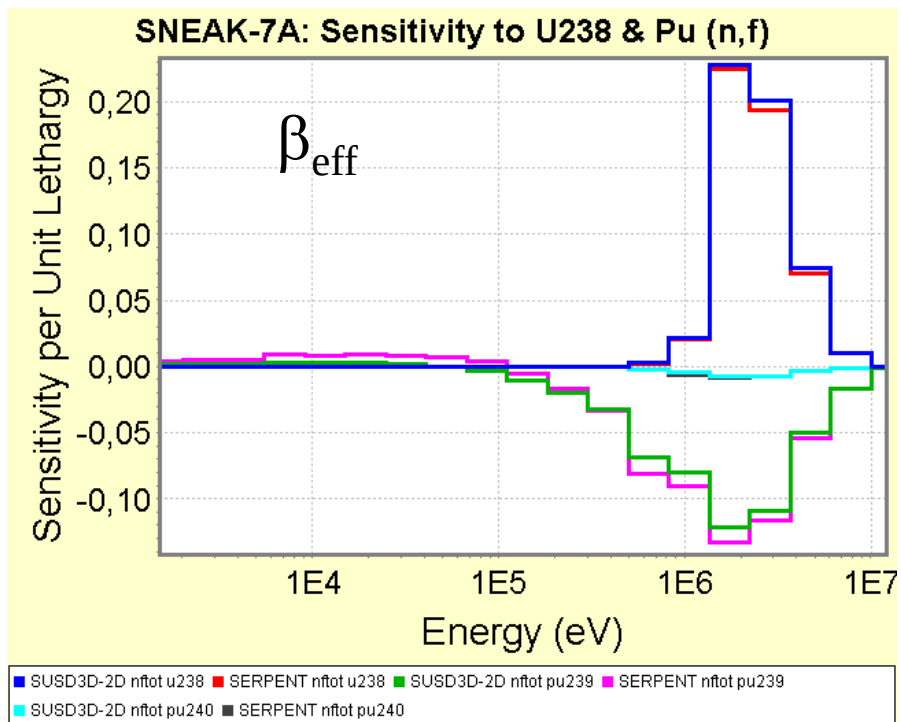
Exercise III-2: Thermal-hydraulics system performance

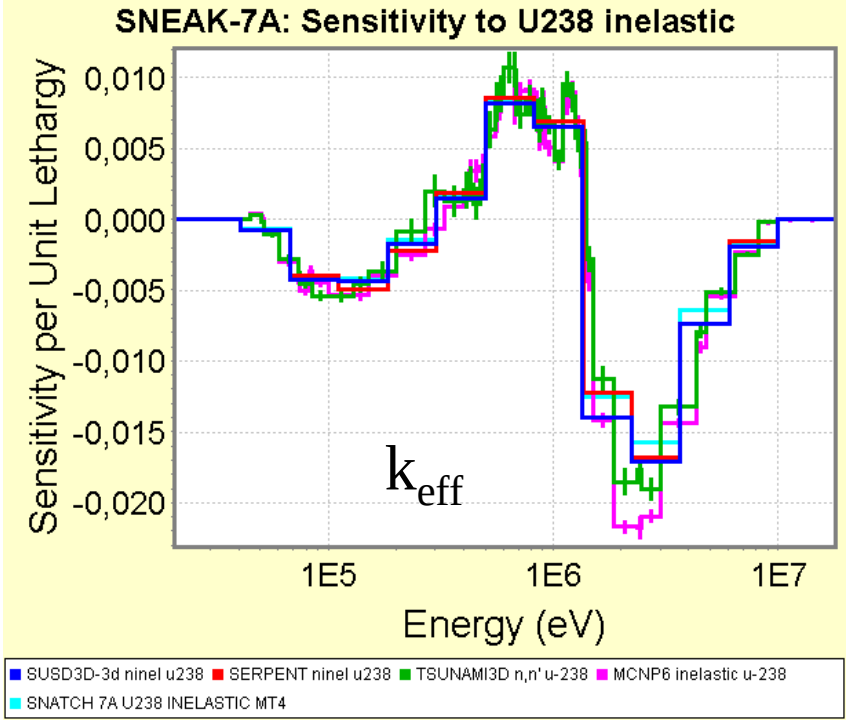
Exercise III-3: Coupled neutron kinetics thermal-hydraulic core/thermal-hydraulic system performance

SNEAK-7-Sensitivity of k_{eff} & β_{eff}









Use of sensitivity / uncertainty analysis

- **Provides uncertainty in the result (physical quantity)**
- **Ranking key parameters (most sensitive, contributing the most to the uncertainty)**
- **Gives confidence in the simulation results**

Use of sensitivity / uncertainty analysis

- ***New project design studies or improved design***: design and safety margins: parameter studies for fusion shielding blanket and its cooling to fulfil constraints imposed by tritium breeding ratio, heating, dose rates, dpa), GEN-IV, ADS. Accuracy of the calculated parameters determines the safety margins attributed to them, and in this way the design, safety and the cost of the project.
- ***General System Performance Assessment, reactor operation & safety analysis*** , ***criticality safety***
- ***Nuclear data evaluations, data adjustment***
- ***Pre- and post-analysis of benchmark experiments***: optimisation of experimental configuration, explain eventual discrepancies, representativity studies, data consistency

Bayes's Theorem and information up-dating

- The probability of a hypothesis A conditional on a given body of data *B* is the ratio of the unconditional probability of the conjunction of the hypothesis with the data to the unconditional probability of the data alone.
- **Bayes theorem: how to use new information?** B representing the new result which depends on A, the updated information about A is calculated as a product of a priori probability and a likelihood function.

$$P(A|C)+P(\overline{A}|C)=1$$

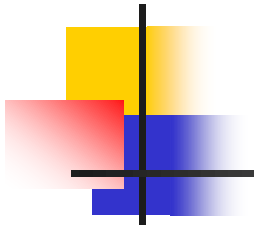
$$P(AB|C)=P(A|BC)P(B|C)=P(B|AC)P(A|C)$$

$$P(A|BC)=P(A|C)\frac{P(B|AC)}{P(B|C)}$$

A posteriori

New measurement

Prior



Thanks for your attention

SINBAD - Radiation Shielding Experiments Scope and Objectives

- Compilation of high quality experiments for validation and benchmarking of computer codes and nuclear data used for radiation transport and shielding problems encompassing:
  - reactor shielding, PV dosimetry **(48)**
  - fusion blanket neutronics **(31)**
  - accelerator shielding **(23)**
- Low and inter-mediate energy particles applications.
- **Contains 102 experiments**
- **Available from OECD/NEA and RSICC.**

https://www.oecd-nea.org/science/wprs/shielding/sinbad/