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Sensitivity and uncertainty analysis with the ERANOS code system

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Sensitivity and uncertainty analysis has played an important role in nuclear reactor analysis for more than forty years. Based on the pioneer work of Usachev and Gandini in the sixties, extensions of the theory and associated computer codes have been developed in Europe and later on in the US.

Major applications were made for:

- **statistical nuclear data adjustments**, that were at the basis of the adjusted data set, the bias factor and associated uncertainties used for the design (core and shielding) of SUPERPHENIX.
- for the planning of optimized integral experiments, based on the “**representativity factor**” concept introduced by Usachev in the seventies, and developed by Palmiotti and Salvatores to plan integral experiments in support of the European Fast Reactor in the eighties.

The **ERANOS** reactor analysis code system (developed jointly by R&D organizations and Industry of France, UK and Germany) has a wide range of capabilities to perform sensitivity and uncertainty analysis for both fast and thermal neutron systems, and has been extensively used both for reactor physics and reactor design analysis.

A number of algorithms for very different applications (critical and sub critical reactors, fuel cycle physics etc) will be presented.

For any integral parameter:

$$\mathbf{I}_s = \langle \sigma_s \Phi \rangle$$

sensitivity coefficients to nuclear data variations can be calculated using **GPT (Generalized Perturbation Theory)**:

$$\frac{\sigma}{\langle \sigma_s \Phi \rangle} \frac{d\langle \sigma_s \Phi \rangle}{d\sigma} = \sigma \left\{ \frac{\left\langle \left(\frac{\partial \sigma_s}{\partial \sigma} \right) \Phi \right\rangle}{\langle \sigma_s \Phi \rangle} - \left\langle \tilde{\Psi}^*, \left(\frac{\partial \mathbf{A}}{\partial \sigma} - \frac{\partial \mathbf{F}}{\partial \sigma} \right) \Phi \right\rangle \right\}$$

This approach, developed theoretically by L.Usachev in the '60s, and further developed by Gandini et al., has been widely used for a variety of applications.

The Generalized Importance Function Ψ^* satisfies the inhomogeneous equation:

$$\left(\mathbf{A}^* - \frac{\mathbf{F}^*}{\mathbf{K}_{\text{eff}}} \right) \tilde{\Psi}^* = \frac{1}{\mathbf{I}_S} \frac{\partial \mathbf{I}_S}{\partial \Phi} = \frac{\sigma_f(\mathbf{r}, \mathbf{E})}{\langle \sigma_f \Phi \rangle}$$

Φ (and Φ^*) are the solutions of the real (and adjoint) Boltzman equations:

$$A\Phi = \frac{F\Phi}{K_{\text{eff}}} \quad A^* \Phi^* = \frac{F^* \Phi^*}{K_{\text{eff}}}$$

The **ERANOS** code systems calculates sensitivity coefficients (by isotope, nuclear reaction, energy group, space region etc) for:

- Criticality (multiplication factor)
- Any type of reaction rate or any type of adjoint flux functional
- Doppler Reactivity Coefficient
- Coolant Void Reactivity Coefficient
- Any other reactivity coefficient
- Effective Delayed Neutron Fraction
- External neutron source importance
- Reactivity Loss during Irradiation
- Transmutation Potential
- Peak Power Value
- Control Rod Reactivity Worth
- Decay Heat
- Radiation Source at Fuel Discharge or in a Repository
- Radiotoxicity in a Repository
- Shielding related parameters
- ...and more

Sensitivity coefficients: the case of Reaction Rates

Case of e.g. damage rate or He-production in structures, or to the power peak factor in the core (linear functionals of the flux):

$$R = \langle \underline{\Phi}, \underline{\Sigma}_R \rangle$$

The sensitivity coefficients are given by:

$$S_j^R = \langle \underline{\Psi}_R^*, \sigma_j \underline{\Phi} \rangle$$

$\underline{\Psi}_R^*$ is the solution of:

$$M^* \underline{\Psi}_R^* = \underline{\Sigma}_R$$

and M^* is the adjoint of the operator M .

In the case of the power peak:

$$R = \frac{\langle \Sigma_p \underline{\Phi} \rangle_{MAX}}{\langle \Sigma_p \underline{\Phi} \rangle_{Reactor}}$$

Σ_p = power cross-section, defined as $E_f \cdot \Sigma_f$, E_f being the average energy released per fission.

The sensitivity coefficients are defined as:

$$S_j = \langle \underline{\Psi}^*, \sigma_j \underline{\Phi} \rangle$$

$\underline{\Psi}^*$ is the importance function solution of:

$$M^* \underline{\Psi}^* = \frac{\Sigma_{p,MAX}}{\langle \Sigma_p \underline{\Phi} \rangle_{MAX}} - \frac{\Sigma_{p,Reactor}}{\langle \Sigma_p \underline{\Phi} \rangle_{Reactor}}$$

where $\Sigma_{p,MAX}$ is the Σ_p value at the spatial point where $\langle \Sigma_p \underline{\Phi} \rangle \equiv \langle \Sigma_p \underline{\Phi} \rangle_{MAX}$, and $\Sigma_{p,Reactor}$ is the Σ_p value at each spatial point of the reactor

Sensitivity Coefficients for Reactivity Coefficients, EGPT: Equivalent Generalized Perturbation Theory (Gandini, Palmiotti, Salvatores)

A reactivity coefficient (like the Doppler effect) can be expressed as a variation of the reactivity of the unperturbed system (characterized by a value K of the multiplication factor, a Boltzmann operator M , a flux $\underline{\Phi}$ and an adjoint flux $\underline{\Phi}^*$) :

$$\Delta\rho = \left(1 - \frac{1}{K_p}\right) - \left(1 - \frac{1}{K}\right) = \frac{1}{K} - \frac{1}{K_p}$$

where K_p corresponds to a variation of the Boltzmann operator such that :

$$\begin{aligned} M &\rightarrow M_p (= M + \delta M_p) & \underline{\Phi} &\rightarrow \underline{\Phi}_p (= \underline{\Phi} + \delta \underline{\Phi}_p) \\ \underline{\Phi}^* &\rightarrow \underline{\Phi}_p^* (= \underline{\Phi}^* + \delta \underline{\Phi}_p^*) & K &\rightarrow K_p (= K + \delta K_p) \end{aligned}$$

The sensitivity coefficients (at first order) for $\Delta\rho$ to variations of the σ_j are given as :

$$S_j = \frac{\partial(\Delta\rho)}{\partial\sigma_j} \cdot \frac{\sigma_j}{\Delta\rho} = \left\{ \frac{1}{I_f^p} \langle \underline{\Phi}_p^*, \sigma_j \underline{\Phi}_p \rangle - \frac{1}{I_f} \langle \underline{\Phi}^*, \sigma_j \underline{\Phi} \rangle \right\}$$

where $I_f = \langle \underline{\Phi}^*, F \underline{\Phi} \rangle$ and $I_f^p = \langle \underline{\Phi}_p^*, F \underline{\Phi}_p \rangle$

F being the neutron fission production part of the M ($= F - A$) operator.

Sensitivity Coefficients : The Case of Nuclide Transmutation (i.e. nuclide densities at end of irradiation)

The generic nuclide K transmutation during irradiation can be represented as the nuclide density variation between time t_0 and t_F . If we denote n_F^K the “final” density, the appropriate sensitivity coefficients are given by :

$$S_j^K = \frac{\partial n_F^K}{\partial \sigma_j} \cdot \frac{\sigma_j}{n_F^K} = \frac{1}{n_F^K} \int_{t_0}^{t_F} \underline{n}^* \sigma_j \underline{n} dt$$

where the time dependent equations to obtain \underline{n}^* and \underline{n} are the classical Bateman equation and its adjoint equation, with appropriate boundary conditions (Gandini et al).

Sensitivity Coefficients : The Case of the Reactivity Loss during Irradiation, $\Delta\rho^{\text{cycle}}$

At first order :

$$\Delta\rho^{\text{cycle}} = \sum_K \Delta n^K \rho_K \qquad \Delta n^K = n_F^K - n_0^K$$

and ρ_K is the reactivity per unit mass associated to the isotope K.

The related sensitivity coefficients associated to the variation of a σ_j , are given by :

$$S_j^{\text{cycle}} = \frac{\sigma_j}{\Delta\rho^{\text{cycle}}} \frac{\partial \Delta\rho^{\text{cycle}}}{\partial \sigma_j} = \frac{\sigma_j}{\Delta\rho^{\text{cycle}}} \left(\sum_K \frac{\partial n^K}{\partial \sigma_j} \cdot \rho_K + \sum_K \Delta n^K \frac{\partial \rho_K}{\partial \sigma_j} \right)$$

or:

$$S_j^{\text{cycle}} = \sum_K \frac{\rho_K}{\Delta\rho^{\text{cycle}}} \int_{t_0}^{t_F} \underline{n}^* \sigma_j \underline{n} \, dt + \left\{ \frac{1}{I_p} \langle \underline{\Phi}_p^*, \sigma_j \underline{\Phi}_p \rangle - \frac{1}{I_f} \langle \underline{\Phi}^*, \sigma_j \underline{\Phi} \rangle \right\}$$

Perturbation of the source term

An example is related to the γ -heating of a material j :

$$\mathbf{H}_{\gamma}^j = \langle \underline{\mathbf{K}}_{\gamma}^j \underline{\phi}_{\gamma} \rangle$$

The photon flux $\underline{\phi}_{\gamma}$ is the solution of the inhomogeneous equation :

$$\mathbf{M}_{\gamma} \underline{\phi}_{\gamma} = \underline{\mathbf{G}}_{(n \rightarrow \gamma)}$$

where M_{γ} is the Boltzmann operator for the transport of γ , and $\underline{\mathbf{G}}_{(n \rightarrow \gamma)}$ is the photon source due to neutron reactions which, at a photon energy E_{γ} , S is given by :

$$\mathbf{G}(\mathbf{E}_{\gamma}) = \sum_{\mathbf{K}} \int \sigma_{\mathbf{k}}(\mathbf{E}_{\mathbf{n}}) \mathbf{P}_{\mathbf{k}}(\mathbf{E}_{\mathbf{n}} \rightarrow \mathbf{E}_{\gamma}) \phi_{\mathbf{n}}(\mathbf{E}_{\mathbf{n}}) d\mathbf{E}_{\mathbf{n}}$$

To compute the **sensitivity of \mathbf{H}_{γ}^j to uncertainties in the γ -source $\underline{\mathbf{G}}_{(n \rightarrow \gamma)}$** it is necessary to

define an "adjoint" equation :

$$\mathbf{M}_{\gamma}^* \underline{\phi}_{\gamma,j}^* = \underline{\mathbf{K}}_{\gamma}^j$$

$\underline{\mathbf{K}}_{\gamma}^j$ being the photon KERMA for material j

The sensitivity coefficients are of the type :

$$\mathbf{S} = \frac{\partial \mathbf{H}_{\gamma}^j}{\partial \underline{\mathbf{G}}_{(n \rightarrow \gamma)}} \bigg/ \frac{\partial \underline{\mathbf{G}}_{(n \rightarrow \gamma)}}{\underline{\mathbf{G}}_{(n \rightarrow \gamma)}} = \left\langle \underline{\phi}_{\gamma,j}^* \cdot \underline{\mathbf{G}}_{(n \rightarrow \gamma)} \right\rangle$$

Experiment “representativity factors”

In the case of a reference parameter R, once the sensitivity coefficient matrix S_R and the covariance matrix D are available, the uncertainty on the integral parameter can be evaluated by the equation:

$$\Delta R_0^2 = S_R^+ D S_R$$

We can consider an integral experiment conceived in order to reduce the uncertainty. If S_E is the sensitivity matrix associated to this experiment, we can call “**representativity factor**” the following expression:

$$r_{RE} = \frac{(S_R^+ D S_E)}{[(S_R^+ D S_R)(S_E^+ D S_E)]^{1/2}}$$

It can be shown that the uncertainty on the reference parameter R is reduced by:

$$\Delta R_0'^2 = \Delta R_0^2 \cdot (1 - r_{RE}^2)$$

If more than one experiment is available, the expression can be generalized. In the case of two experiments, characterized by sensitivity matrices S_{E1} and S_{E2} :

$$\Delta R_0'^2 = S_R^+ D' S_R = \Delta R_0^2 \left[1 - \frac{1}{1 - r_{12}^2} (r_{R1} - r_{R2})^2 - \frac{2}{1 + r_{12}} r_{R1} r_{R2} \right]$$

where D' is the new covariance matrix.

Target accuracy requirements

To establish priorities and target accuracies on data uncertainty reduction, a formal approach can be adopted: define target accuracy on design parameter and find out required accuracy on data (the “inverse” problem).

The unknown uncertainty data requirements \mathbf{d}_i can be obtained solving with ERANOS the following minimization problem :

$$\sum_i \lambda_i / d_i^2 = \min \quad i = 1 \dots I$$

with the following constraints :

$$\sum_i \mathbf{S}_{ni}^2 \mathbf{d}_i^2 < \mathbf{Q}_n^T \quad n = 1 \dots N$$

where \mathbf{S}_{ni} are the sensitivity coefficients for the integral parameter \mathbf{Q}_n , and \mathbf{Q}_n^T are the target accuracies on the N integral parameters.

λ_i are “cost” parameters related to each σ_i and should give a relative figure of merit of the difficulty of improving that parameter (e.g., reducing uncertainties with an appropriate experiment).

Statistical Data Adjustment

When a set of calculated integral parameters Q_i (which are function of nuclear data σ_j) and the corresponding experimental values Q_i^{exp} are available, ERANOS evaluates the best estimates (“adjustments”) of σ_j , given the covariance matrices of the σ and of the experiments Q_i .

If we define: $y_j = (\sigma_j^{\text{adj}} - \sigma_j) / \sigma_j$ and $y_{Q_i}^{\text{exp}} = (Q_i^{\text{exp}} - Q_i) / Q_i$, the y_j are given by:

$$\bar{y} = \left(\mathbf{S}^T \mathbf{D}_Q^{-1} \mathbf{S} + \mathbf{D}^{-1} \right)^{-1} \mathbf{S}^T \mathbf{D}_Q^{-1} \bar{y}_Q^{\text{exp}}$$

where \mathbf{D}_Q is the covariance matrix of the experiments, \mathbf{D} the covariance matrix of the cross sections and \mathbf{S} is the sensitivity matrix.

It will also result an adjusted covariance matrix for the nuclear data:

$$\left(\mathbf{D}^{\text{adj}} \right)^{-1} = \mathbf{D}^{-1} + \mathbf{S}^T \mathbf{D}_Q^{-1} \mathbf{S}$$

This new matrix will replace the initial \mathbf{D} matrix in the data base.

Calculational Tools in the ERANOS code system

All **sensitivity** calculations can be performed with ERANOS which calculates homogeneous and inhomogeneous solutions of the Boltzman equation and generalized importance functions, and performs perturbation and uncertainty analysis.

Modules of ERANOS generate the source terms of the generalized importance equations and provides the solution in two or three-dimensions (e.g. in hexagonal geometry) of the finite-difference diffusion or S_n transport equation, or of nodal variational transport equations.

A fundamental mode removal algorithm is applied when solving the generalized importance equations for sources that are orthogonal to the homogeneous solutions.

The S_n module BISTRO can be used to perform flux and generalized importance function calculations. To avoid S_n negative solutions (e.g. in the case of reaction rate ratios importance calculations), ERANOS uses a special procedure to calculate separately the generalized importance for the positive and negative contributions, combining them at the level of the sensitivity coefficient computation .

Ancillary calculations: uncertainty analysis, experiment representativity factors, target accuracy and nuclear data statistical adjustments.

Integral parameter uncertainty, experiment representativity factors, nuclear data target accuracy and statistical nuclear data adjustments are computed in ERANOS with covariance matrices provided in different general formats.