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Abstract: Sensitivity coefficients can be used for different objectives like uncertainty estimates, design optimization, determination of target accuracy requirements, adjustment of input parameters, and evaluations of the representativity of an experiment with respect to a reference design configuration. In this paper the theory, based on the adjoint approach, that is implemented in the ERANOS fast reactor code system is presented along with some unique tools and features related to specific types of problems as is the case for nuclide transmutation, reactivity loss during the cycle, decay heat, neutron source associated to fuel fabrication, and experiment representativity.

Introduction

Sensitivity analysis and uncertainty evaluation are the main instruments for dealing with the sometimes scarce knowledge of the input parameters used in simulation tools. For sensitivity analysis, sensitivity coefficients are the key quantities that have to be evaluated. They are determined and assembled, using different methodologies, in a way that when multiplied by the variation of the corresponding input parameter they will quantify the impact on the targeted quantities whose sensitivity is referred to. Sensitivity coefficients can be used for different objectives like uncertainty estimates, design optimization, determination of target accuracy requirements, adjustment of input parameters, and evaluations of the representativity of an experiment with respect to a reference design configuration.

In uncertainty evaluation, the sensitivity coefficients are multiplied by the uncertainties of the input parameters in order to obtain the uncertainty of the targeted parameter of interest. The origin and quality of the uncertainties of the input parameters can be different and vary quite a lot. In some cases, they are provided by the expert judgment of qualified designer. In some other cases more useful information is available, for instance from experimental values, and they are cast in more rigorous formalism. This is the case, for instance, of covariance matrix for neutron cross-sections, where correlations in energy and among the different input parameters (reactions, isotopes) are also provided.

Target accuracy assessments are the inverse problem of the uncertainty evaluation. To establish priorities and target accuracies on data uncertainty reduction, a formal approach can be adopted by defining target accuracy on design parameter and finding out required accuracy on data. In fact, the unknown uncertainty data requirements can be obtained by solving a minimization problem where the sensitivity coefficients in conjunction with the existing constraints provide the needed quantities to find the solutions.

Sensitivity coefficients are also used in input parameter adjustments. In this case, the coefficients are used within a fitting methodology (e.g. least square fit, Lagrange multipliers with most likelihood function, etc.) in order to reduce the discrepancies between measured and calculational results. The resulting adjusted input parameters can be subsequently used, sometimes in combination with bias factors, to obtain calculational results to which a reduced uncertainty will be associated.

A further use of sensitivity coefficients is, in conjunction with a covariance matrix, a representativity analysis of proposed or existing experiments. In this case the calculation of correlations among the design and experiments allow to determine how representative is the

latter of the former, and consequently, to optimize the experiments and to reduce their numbers. Formally one can reduce the estimated uncertainty on a design parameter by a quantity that represents the knowledge gained by performing the experiment.

In this paper we will briefly summarize the sensitivity methodology that has been implemented in the ERANOS [1] code system and associated tools, and that make use of the so-called adjoint approach. The adjoint approach is based on the perturbation theory originally developed in the quantum mechanics field.

The ERANOS code system has been widely validated in the past and recently, it has been used for a very comprehensive analysis of the impact of cross-section uncertainties on the integral parameters of the selected GEN-IV systems, in order to define target accuracy requirement to meet expected design needs. The flexibility of the ERANOS systems has allowed to account for integral parameters related to the core neutronics (like reactivity coefficients, etc) and to the fuel cycle (neutron sources, decay heat, reactivity loss during the cycle, transmutation rates etc).

The present paper will summarize some of the most original features of the ERANOS system.

Historical notes

The perturbation theory has been introduced in reactor physics in the 50' and one can find a classical presentation in the Weinberg and Wigner book [2]. This is the perturbation theory applied to the k_{eff} of the critical reactor and L. N. Usachev gave a comprehensive development in an article published at the Geneva conference of 1955 [3].

It is interesting to note that the the perturbation theory applied to reactor makes use of a definition of a function (the adjoint flux), that has a specific physical meaning if one is dealing with a non-conservative system as in the case of a nuclear reactor. This physical interpretation of the adjoint flux has been the focus of extensive studies, during the 60', in particular by J. Lewins [4, 5].

The perturbation theory, mostly developed and applied for reactivity coefficient studies, was readily used [6] for an application, sensitivity studies, that had a spectacular development in the 70' and 80'. This development was made possible by a generalization of the perturbation theory (thanks again to Usachev), that deals with the general problem of a variation of any kind of a neutron flux functional. Usachev derived an explicit formulation that relates the functional variation to any change of the Boltzmann operator [7].

This development, and its further generalization by Gandini, to the case of any kind of linear and bilinear functional of the real and adjoint flux [8], opened a new territory for the perturbation theory. It was now possible to relate explicitly the variation of any type of integral parameter (multiplication factor, reaction rates, reactivity coefficients, source values, etc.) to any kind of change of the operator that characterizes the system.

The application of the generalized perturbation theory to real life problems lead to new interesting developments that allowed to clarify specific characteristics of the new theory with implications for the computation of the generalized importance functions introduced by the theory [9].

Starting from the early 70' the generalized perturbation methods, which were essentially developed and used in Europe, became popular also in the rest of the world and in particular with new developments in several U. S. laboratories, ANL [10] and ORNL [11], and in Japan [12].

The perturbation methods, and their main application in the field of sensitivity analysis, have been used mostly in their first order formulation. Actually, as for any perturbation theory, the power of the method is particularly evident when one considers small perturbations (for instance for cross-sections σ) that therefore induce little changes of the functions (e. g. the neutron flux ϕ), that characterize the system, and for whom one can neglect the second order product (for instance $\delta\sigma\delta\phi$). However, there have been theoretical developments that take into accounts higher order effects without losing all the advantages typical of the first order formulations [13, 14, and 15].

Among the theoretical developments after the 70' that had significant practical impact, one has to mention the extension of the perturbation theory to the nuclide field that allows to study the burn up due to irradiation in the reactor at the first order [16], and to higher orders [17]. Subsequently a new formulation, the "equivalent Generalized Perturbation Theory" EGPT [18], allowed to treat in a very simple and efficient way the perturbation and sensitivity analyses for reactivity coefficients.

Among the most recent development it is worth to mention those related to the ADS case with functionals that allow to calculate the sensitivity of the source importance (ϕ^*) and the inhomogeneous reactivity [19].

Finally, one should remind that, besides the neutronic field, there have been several studies for extending the perturbation theory developed for reactor physics to other domains (thermal-hydraulics, safety, etc.) with very interesting theoretical developments [20, 21, and 22].

Theory

Sensitivity coefficients and perturbation theories

The variations of any integral parameter Q due to variations of cross-sections σ can be expressed using perturbation theories [23], to evaluate sensitivity coefficients S :

$$\delta Q/Q = \sum_j S_j \frac{\delta \sigma_j}{\sigma_j} \quad (1)$$

where the sensitivity coefficients S_j are formally given by:

$$S_j = \frac{\partial Q}{\partial \sigma_j} \cdot \frac{\sigma_j}{Q} \quad (2)$$

For practical purposes, in the general expression of any integral parameter Q , the explicit dependence from some cross-sections (e.g. σ_i^e) and the implicit dependence from some other cross-sections (e.g. σ_j^{im}) are kept separated:

$$Q = f(\sigma_j^{im}, \sigma_i^e). \quad (3)$$

As an example, we consider a reaction rate:

$$R = \langle \underline{\sigma}^e, \underline{\Phi} \rangle \quad (4)$$

where brackets $\langle \cdot \rangle$ indicate integration over the phase space. In the case of a source-driven system, $\underline{\Phi}$ is the inhomogeneous flux driven by the external source, and the homogeneous flux in the case of critical core studies. In Eq. (4), $\underline{\sigma}^e$ can be an energy dependent detector cross-section; R is “explicitly” dependent on the $\underline{\sigma}^e$ and “implicitly” dependent on the cross-sections which characterize the system, described by the flux $\underline{\Phi}$. In other terms, R depends on the system cross-sections via $\underline{\Phi}$. Eq. (1) can be rewritten as follows:

$$\delta Q/Q = \sum_j S_j \frac{\delta \sigma_j^{im}}{\sigma_j^{im}} + \left(\frac{\partial Q}{\partial \sigma^e} \cdot \frac{\sigma^e}{Q} \right) \cdot \frac{\delta \sigma^e}{\sigma^e} \quad (5)$$

where we have the hypothesis of an explicit dependence of Q on only one σ^e . If we drop the index “im”:

$$\delta Q/Q = \sum_j S_j \frac{\delta \sigma_j}{\sigma_j} + \left(\frac{\partial Q}{\partial \sigma^e} \cdot \frac{\sigma^e}{Q} \right) \cdot \frac{\delta \sigma^e}{\sigma^e} = I + D \quad (6)$$

where the term I is generally called “indirect” effect, and the term D is called “direct” effect. While the direct effects can be obtained with explicit expressions of the derivatives of Q , the indirect effect (i.e. the sensitivity coefficients S), can be obtained with perturbation expression, most frequently at the first order [23].

In what follows, we will explicit the formulations used by the ERANOS code system for the sensitivity coefficients at the first order for the indirect effects related to reactivity coefficients [18], reaction rates [23], nuclide transmutation (i.e., evolution in time [16]). The formulations related to other parameters of interest for critical or sub-critical systems will also be described (e.g. the reactivity loss during the irradiation, the decay heat etc). These examples are provided in order to highlight the wide extent of capabilities of the sensitivity algorithms of the ERANOS code system.

Reactivity coefficients [18]

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 Boltzman operator M , a flux $\underline{\Phi}$ and an adjoint flux $\underline{\Phi}^*$):

$$\Delta\rho = \left(1 - \frac{1}{K_p}\right) - \left(1 - \frac{1}{K}\right) = \frac{1}{K} - \frac{1}{K_p} \quad (7)$$

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

$$\begin{aligned} M &\rightarrow M_p (= M + \delta M_p) & \underline{\Phi} &\rightarrow \underline{\Phi}_p (= \underline{\Phi} + \delta \underline{\Phi}_p) \\ \underline{\Phi}^* &\rightarrow \underline{\Phi}_p^* (= \underline{\Phi}^* + \delta \underline{\Phi}_p^*) & K &\rightarrow K_p (= K + \delta K_p) \end{aligned} \quad (8)$$

The sensitivity coefficients (at first order) for $\Delta\rho$ to variations of the σ_j are given as in [3]:

$$S_j^{\Delta\rho} = \frac{\partial(\Delta\rho)}{\partial\sigma_j} \cdot \frac{\sigma_j}{\Delta\rho} = \left\{ \frac{1}{I_f^p} \langle \underline{\Phi}_p^*, \sigma_j \underline{\Phi}_p \rangle - \frac{1}{I_f} \langle \underline{\Phi}^*, \sigma_j \underline{\Phi} \rangle \right\} \quad (9)$$

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.

Reaction rates

The classical formulations found e.g. in [23] can be applied to the case of e.g., damage rate or He-production in the structures, or to the power peak factor in the core:

$$R = \langle \underline{\Phi}, \underline{\Sigma}_R \rangle \quad (10)$$

The sensitivity coefficients are given by:

$$S_j^R = \langle \underline{\Psi}_R^*, \sigma_j \underline{\Phi} \rangle \quad (11)$$

where $\underline{\Phi}$ has been defined above, and $\underline{\Psi}_R^*$ is the solution of:

$$M^* \underline{\Psi}_R^* = \underline{\Sigma}_R \quad (12)$$

and M^* is the adjoint of the operator M . In the specific case of the power peak, this parameter can be expressed as the ratio:

$$R = \frac{\langle \underline{\Sigma}_p \underline{\Phi} \rangle_{MAX}}{\langle \underline{\Sigma}_p \underline{\Phi} \rangle_{Reactor}} \quad (13)$$

with $\underline{\Sigma}_p$ the power cross-section, essentially represented by $E_f \cdot \underline{\Sigma}_f$, E_f being the average energy released per fission. The sensitivity coefficients are defined as:

$$S_j = \langle \underline{\Psi}^*, \sigma_j \underline{\Phi} \rangle \quad (14)$$

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

$$M^* \underline{\Psi}^* = \frac{\underline{\Sigma}_{p,MAX}}{\langle \underline{\Sigma}_p \underline{\Phi} \rangle_{MAX}} - \frac{\underline{\Sigma}_{p,Reactor}}{\langle \underline{\Sigma}_p \underline{\Phi} \rangle_{Reactor}} \quad (15)$$

where $\underline{\Sigma}_{p,MAX}$ is the $\underline{\Sigma}_p$ value at the spatial point where $\langle \underline{\Sigma}_p \underline{\Phi} \rangle \equiv \langle \underline{\Sigma}_p \underline{\Phi} \rangle_{MAX}$, and $\underline{\Sigma}_{p,Reactor}$ is the $\underline{\Sigma}_p$ value at each spatial point of the reactor. In Eq. (15) effects due to $\underline{\Sigma}_{p,MAX}$ and $\underline{\Sigma}_{p,Reactor}$ variations are assumed to be negligible.

Nuclide transmutation [16]

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_{Fi}^K the “final” density, the appropriate sensitivity coefficient is given by:

$$S_j^K = \frac{\partial n_F^K}{\partial \sigma_j} \cdot \frac{\sigma_j}{n_F^K} = \frac{1}{n_F^K} \int_{t_0}^{t_F} \underline{n}^* \sigma_j \underline{n} \, dt \quad (16)$$

where the time dependent equations to obtain \underline{n}^* and \underline{n} , together with their boundary conditions, are defined in [16].

Reactivity loss during irradiation, $\Delta \rho^{\text{cycle}}$

At the first order, and neglecting the cross-section variation during irradiation (which is a good approximation for fast neutron systems), we can write:

$$\Delta \rho^{\text{cycle}} = \sum_K \Delta n^K \rho_K \quad (17)$$

where:

$$\Delta n^K = n_F^K - n_0^K \quad (18)$$

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

The related sensitivity coefficients S_j^{cycle} associated to the variation of a σ_j , are given by:

$$S_j^{\text{cycle}} = \frac{\sigma_j}{\Delta \rho^{\text{cycle}}} \frac{\partial \Delta \rho^{\text{cycle}}}{\partial \sigma_j} = \frac{\sigma_j}{\Delta \rho^{\text{cycle}}} \left(\sum_K \frac{\partial n^K}{\partial \sigma_j} \cdot \rho_K + \sum_K \Delta n^K \frac{\partial \rho_K}{\partial \sigma_j} \right) \quad (19)$$

Using the formulations previously indicated., we obtain:

$$S_j^{\text{cycle}} = \sum_K \frac{\rho_K}{\Delta \rho^{\text{cycle}}} \int_{t_0}^{t_F} \underline{n}^* \sigma_j \underline{n} \, dt + \left\{ \frac{1}{I_f^p} \langle \Phi_p^*, \sigma_j \Phi_p \rangle - \frac{1}{I_f} \langle \Phi^*, \sigma_j \Phi \rangle \right\} \quad (20)$$

where the index “p” refers to the core state at $t = t_F$.

Case of a neutron source (e.g. at fuel fabrication)

A neutron source $NS_{t=t_F}$ at $t = t_F$ can be defined as:

$$NS_{t=t_F} = \sum_i P_i n_{i,t=t_F} \quad (21)$$

where P_i is the neutron production cross-section (e.g. by spontaneous fissions). The sensitivity coefficients are:

$$S_j^i = P_i \cdot \frac{\partial n_F^i}{\partial \sigma_j} \cdot \frac{\sigma_j}{n_F^i} = \frac{P_i}{n_F^i} \int_{t_0}^{t_F} \underline{n}^* \sigma_j \underline{n} \, dt \quad (22)$$

where effects due to P_i cross-section variations are supposed to be negligible.

Decay heat

The decay heat is defined as:

$$H(t) = \sum_K \lambda_K Q_K n^K(t) \quad (23)$$

where for each isotope K, λ_K are the decay constants, Q_K the heat released in decay reaction and $n^K(t)$ are the nuclide densities at time t. The equations for $n^K(t)$ are the classical ones:

$$\frac{dn^K(t)}{dt} = \sum_F \gamma_{K,f} \tau_f + \sum_j n^K(t) \tau_j b_{j \rightarrow K} + \sum_i n^i(t) \lambda_i b_{i \rightarrow K} - \tau_K n^K(t) - \lambda_K n^K(t) \quad (24)$$

Or in a more compact form:

$$\frac{dn^K(t)}{dt} = b_K + \sum_{j=1}^{K-1} C_{kj} n^j(t) - C_{kK} n^K(t) \quad (25)$$

where $\gamma_{K,f}$ are the fission yields for fissionable isotope f, τ are microscopic reaction rates and $b_{j \rightarrow K}$ are branching ratios. This is an inhomogeneous Bateman-type equation that defines the appropriate nuclide field. The uncertainty on $H(t)$ is obtained by combining the appropriate derivatives of H with respect to λ , Q and n , and accounting for possible correlations. As far as variations of the n^K terms, they can be evaluated using the perturbation techniques previously

indicated. A specific feature is represented by the variation of the fission yields γ , i.e., by the variation of the “source” term b_K in Eq. (25).

The relative sensitivity coefficients corresponding to the decay heat at $t = t_x$ are given by:

$$S_K^\gamma = \tau_f \frac{\partial n_{t=t_x}^K}{\partial \gamma_{K,f}} \cdot \frac{\gamma_{K,f}}{n_{t=t_x}^K} = \frac{\tau_f}{n_{t=t_x}^K} \int_0^{t_x} \underline{n}^* \gamma_{K,f} dt \quad (26)$$

Calculational tools in the ERANOS code system

All the sensitivity calculations described above can be performed with the ERANOS code system, which allows to calculate homogeneous and inhomogeneous solutions of the Boltzmann equation and generalized importance functions, and to perform perturbation and uncertainty analysis. Specific modules in ERANOS allow generation of the source terms of the generalized importance equations and solution in two or three-dimensional 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. Procedures that manipulate different perturbation modules are used to generate the sensitivity coefficients related to reactivity coefficients.

The discrete ordinate module BISTRO [24] in ERANOS can be used to perform flux and generalized importance function calculations. In order to avoid problems related to S_n negative solutions that are present for instance in the case of reaction rate ratios importance calculations, ERANOS uses a special procedure that allows separately calculating the generalized importance for the positive and negative contributions and combining them at the level of the perturbation or sensitivity coefficient computation.

Ancillary calculations: uncertainty analysis, experiment representativity, and target accuracy assessment

Uncertainty evaluation and experiment representativity factors are computed in ERANOS with covariance matrices provided in different general formats. The uncertainties associated to the cross-section can be represented in the form of a variance-covariance matrix:

$$D_\sigma = \begin{pmatrix} d_{11} & d_{12} & \cdots & d_{1J} \\ d_{12} & d_{22} & \cdots & d_{2J} \\ \cdots & \cdots & \cdots & \cdots \\ d_{1J} & d_{2J} & \cdots & d_{JJ} \end{pmatrix} \quad (37)$$

where the elements d_{ij} represent the expected values related to the parameters σ_j , and σ_i .

The variance of Q can then be obtained as:

$$\text{var}(Q) = \sum_{j,i} S_j S_i d_{ij}$$

In order to plan for specific experiments able to reduce uncertainties on selected design parameters, a formal approach, initially proposed by L. Usachev [25] has been applied by Palmiotti and Salvatores [26] and further developed in by Gandini [27]).

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:

$$\Delta R_0^2 = S_R^+ D S_R \quad (38)$$

We can consider an integral experiment conceived in order to reduce the uncertainty ΔR_0^2 . Let us indicate by S_E the sensitivity matrix associated with this experiment. If we call “representativity factor” the following expression:

$$r_{RE} = \frac{(S_R^+ D S_E)}{[(S_R^+ D S_R)(S_E^+ D S_E)]^{1/2}}, \quad (39)$$

it can be shown [25] that the uncertainty on the reference parameter R is reduced by:

$$\Delta R_0'^2 = \Delta R_0^2 \cdot (1 - r_{RE}^2) \quad (40)$$

If more than one experiment is available, the Eq. (40) can be generalized. In the case of two experiments, characterized by sensitivity matrices S_{E1} and S_{E2} the following expression [27] can be derived:

$$\Delta R_0'^2 = S_R^+ D' S_R = \Delta R_0^2 \left[1 - \frac{1}{1 - r_{12}^2} (r_{R1} - r_{R2})^2 - \frac{2}{1 + r_{12}} r_{R1} r_{R2} \right] \quad (41)$$

where D' is the new covariance matrix and

$$r_{12} = \frac{(S_{E1}^+ D S_{E2})}{[(S_{E1}^+ D S_{E1})(S_{E2}^+ D S_{E2})]^{1/2}} \quad (42)$$

$$r_{R1} = \frac{(S_R^+ D S_{E1})}{[(S_R^+ D S_R)(S_{E1}^+ D S_{E1})]^{1/2}} \quad (43)$$

$$r_{R2} = \frac{(S_R^+ D S_{E2})}{[(S_R^+ D S_R)(S_{E2}^+ D S_{E2})]^{1/2}} \quad (44)$$

The approach outlined here can be used to plan optimized integral experiments to reduce uncertainties on a set of integral parameters of a reference system.

A successive step is the assessment of target accuracy requirements. To establish priorities and target accuracies on data uncertainty reduction, a formal approach can be adopted by defining target accuracy on design parameter and finding out required accuracy on data. In fact, the unknown uncertainty data requirements d_i can be obtained (e.g. for parameters I not correlated among themselves), by solving the following minimization problem:

$$\sum_I \lambda_I / d_I^2 = \min \quad I = 1 \dots L \quad (45)$$

(L : total number of parameters) with the following constraints:

$$\sum_I S_{ni}^2 d_I^2 < (R_n^T)^2 \quad n = 1 \dots N \quad (46)$$

(N : total number of integral design parameters) where S_{ni} are the sensitivity coefficients for the integral parameter R_n and R_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).

All the formulations shown above can be calculated with specific modules of the ERANOS code system.

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