

## New Approaches and Applications for Monte Carlo Perturbation Theory

Manuele Aufiero <sup>a,\*</sup>, Adrien Bidaud <sup>b</sup>, Dan Kotlyar <sup>c</sup>, Jaakko Leppänen <sup>d</sup>, Giuseppe Palmiotti <sup>e</sup>, Massimo Salvatores <sup>e</sup>, Sonat Sen <sup>e</sup>, Eugene Shwageraus <sup>f</sup>, Massimiliano Fratoni <sup>a</sup>

<sup>a</sup>University of California, Berkeley, Department of Nuclear Engineering, Berkeley, CA 94720-1730 USA

<sup>b</sup>LPSC, CNRS-IN2P3/UJF/INPG, France

<sup>c</sup>Georgia Institute of Technology, George W. Woodruff School, Nuclear and Radiological Engineering, Atlanta, GA, USA

<sup>d</sup>VTT Technical Research Centre of Finland Ltd., Kivimiehentie 3 Espoo, FI-02044 VTT, Finland

<sup>e</sup>NSDA Division, Idaho National Laboratory, P.O. Box 1625, Idaho Falls, ID 83415-3860, USA

<sup>f</sup>Department of Engineering, University of Cambridge, CB2 1PZ Cambridge, United Kingdom

\*manuele.aufiero@berkeley.edu

**Abstract** - This paper presents some of the recent and new advancements in the extension of Monte Carlo Perturbation Theory methodologies and applications. In particular, the discussed problems involve Brunup calculation, perturbation calculation based on continuous energy functions, and Monte Carlo Perturbation Theory in loosely coupled systems.

### I. INTRODUCTION

In the last few years, interest in perturbation calculations in Monte Carlo has risen, and several codes now are capable of accurate calculation of multi-group cross-section sensitivities for  $k_{\text{eff}}$  and reaction rate ratios (e.g., see [1, 2, 3, 4, 5, 6]). Those capabilities have been available in deterministic codes for a long time [7, 8].

Recently, benefiting from the flexibility of modern Continuous Energy Monte Carlo codes, new perturbation/sensitivity capabilities are being tested and implemented. The present work gives an overview of the ongoing research activities of the authors related to applications that require advanced Monte Carlo Perturbation Theory capabilities. These new capabilities were implemented and tested in the Monte Carlo code SERPENT [9].

#### 1. Monte Carlo Generalized Perturbation Theory (GPT)

In linear perturbation analysis, the effect of a perturbation of the parameter  $x$  on the response  $R$  is often expressed in terms of sensitivity coefficient [8]:

$$S_x^R \equiv \frac{dR/R}{dx/x} \quad (1)$$

Commonly, the considered responses  $R$  are the effective multiplication factor

$$(R = k_{\text{eff}}) \quad (2)$$

reaction rate ratios

$$\left( R = \frac{\langle \Sigma_1, \phi \rangle}{\langle \Sigma_2, \phi \rangle} \right) \quad (3)$$

and bilinear ratios

$$\left( R = \frac{\langle \phi^\dagger, \Sigma_1 \phi \rangle}{\langle \phi^\dagger, \Sigma_2 \phi \rangle} \right) \quad (4)$$

Most of the Monte Carlo Perturbation Theory implementations are limited to the calculation of multi-group nuclear data sensitivities for the first two response functions. A collision history-based approach has been proposed for the calculation of sensitivities for a broad range of response functions, and has been at first demonstrated for responses in the form of bilinear ratios [5, 6]. The method is based on the rather simple concept of computing the statistical correlations between the terms of any generic response function  $R$  and the collision events in the particles history, and will be briefly recalled in the full paper. Considering a response function  $R$  defined as the ratio of two Monte Carlo estimators  $e_1$  and  $e_2$ :

$$R = \frac{E[e_1]}{E[e_2]} \quad (5)$$

The sensitivity of  $R$  to the generic reaction cross-section  $x$  can be obtained as [5]:

$$S_x^R = \frac{\text{COV} \left[ e_1, \sum^{\text{history}} (ACC_x - REJ_x) \right]}{E[e_1]} + \frac{\text{COV} \left[ e_2, \sum^{\text{history}} (ACC_x - REJ_x) \right]}{E[e_2]} \quad (6)$$

$ACC_x - REJ_x$  indicates the net number of accepted minus rejected collisions.  $\text{COV}[X, Y]$  represents the covariance between the quantities  $X$  and  $Y$  associated to each particle, estimated over the whole neutron population.

The sum  $\sum^{\text{history}} (ACC_x - REJ_x)$  of the collisions on the reaction  $x$  for which the sensitivity is being calculated is performed over a number of latent generations that ensures the convergence of the perturbed fission source distribution for the adjoint-weighted estimators. The required number of latent generations is a problem specific to the particular configuration

under investigation, and has to be selected accurately.<sup>1</sup>

This approach made possible to perform sensitivity/uncertainty analysis for adjoint-weighted quantities (e.g., effective prompt lifetime and reactivity coefficients), which is not possible with previously available Monte Carlo Perturbation Theory implementations.

In the next section, innovative applications of Monte Carlo Generalized Perturbation Theory for coupled transport/depletion problem in ongoing research activities are presented.

Equation (6) has been generalized in order to consider responses beyond those that are in the form of bilinear functions of the flux and adjoint flux, and sensitivity functions not in the form of multi-group cross sections. These advanced Perturbation Theory approaches are specifically tailored to continuous-energy Monte Carlo transport, and the new applications under investigation are hardly treated via deterministic codes. In the following sections, these approaches are presented and discussed.

## II. MONTE CARLO GPT IN BURNUP CALCULATIONS

Coupled depletion/transport perturbation theory has been developed and described in the 1970s (e.g., see [11, 12, 13, 14]). In this Section we focus on recent developments related to the adoption of Monte Carlo Perturbation Theory. A very interesting work in this direction, based on the correlated sampling method, has been proposed in the past by [15].

### 1. Improving the accuracy of burnup calculations via GPT

The problem of fuel isotopic evolution in burnup calculation is usually presented through the Bateman equations describing the rate of change of a generic nuclide  $i$ :

$$\frac{dN_i}{dt} = \sum_j N_j \phi \cdot \sigma_{j \rightarrow i} - \sum_j N_i \phi \cdot \sigma_{i \rightarrow j} + \sum_j N_j \lambda_j b_{j \rightarrow i} - N_i \lambda_i \quad (7)$$

In matrix notation, the burnup equations are expressed as:

$$\frac{d\bar{\mathbf{N}}}{dt} = \bar{\mathbf{A}} \bar{\mathbf{N}}, \quad \bar{\mathbf{N}}(0) = \bar{\mathbf{N}}_0 \quad (8)$$

where  $\bar{\mathbf{N}}$  is the vector of atomic densities for the  $n$  isotopes considered in the problem, and  $\bar{\mathbf{A}}$  is the burnup matrix, accounting for both the transmutation and decay terms of Eq. (7).

In Monte Carlo burnup calculations, the one-group transmutation cross sections  $\sigma_{j \rightarrow i}$  are computed during criticality source simulations, along with the flux  $\phi$  in each depleted region.

Assuming  $\bar{\mathbf{A}}$  constant with time, the solution of Eq. (8) is:

$$\bar{\mathbf{N}}(t) = e^{\bar{\mathbf{A}}t} \bar{\mathbf{N}}_0 \quad (9)$$

<sup>1</sup>[10] offers an interesting analysis of the perturbed fission source convergence in simple problems, considering  $k_{\text{eff}}$  as response function.

The exponential matrix  $e^{\bar{\mathbf{A}}t}$  can be efficiently computed numerically [16, 17]. Unfortunately, in common reactor physics applications, the one-group transmutation cross sections  $\sigma_{j \rightarrow i}$  changes with time as effect of the impact of the isotopic composition evolution on the neutron spectrum. In this view, the burnup matrix  $\bar{\mathbf{A}}$  depends on the vector of isotopic compositions  $\bar{\mathbf{N}}$  through spectrum and flux normalization effects (i.e.,  $\bar{\mathbf{A}} = \bar{\mathbf{A}}(\bar{\mathbf{N}})$ ). For this reason, to achieve accurate depletion calculations, the evolution is often divided in several burnup steps for which one or more criticality source Monte Carlo simulations are required.

To reduce the number of required steps and Monte Carlo calculations, [18] proposed to use MC GPT to compute  $\frac{d\bar{\mathbf{A}}}{d\bar{\mathbf{N}}}$  at each burnup step, to approximate the evolution of  $\bar{\mathbf{A}}$  in the intervals between the transport simulations and reduce the computational requirements.

Adopting the collision history framework for Generalized Perturbation Theory presented in the previous section,  $\frac{d\bar{\mathbf{A}}}{d\bar{\mathbf{N}}}$  is obtained by computing the sensitivities of each response function  $R = \frac{\langle \sigma_{j \rightarrow i}, \phi \rangle}{\langle \phi \rangle}$  to each nuclide density  $N_k$ .

In [18], a simple 2D PWR pin cell is adopted as case study to investigate the possible improvements obtained by the estimation of  $\frac{d\bar{\mathbf{A}}}{d\bar{\mathbf{N}}}$  during burnup calculations. The selected oxide fuel has 3.5w% initial <sup>235</sup>U enrichment and contains 0.5w% Gd<sub>2</sub>O<sub>3</sub>.

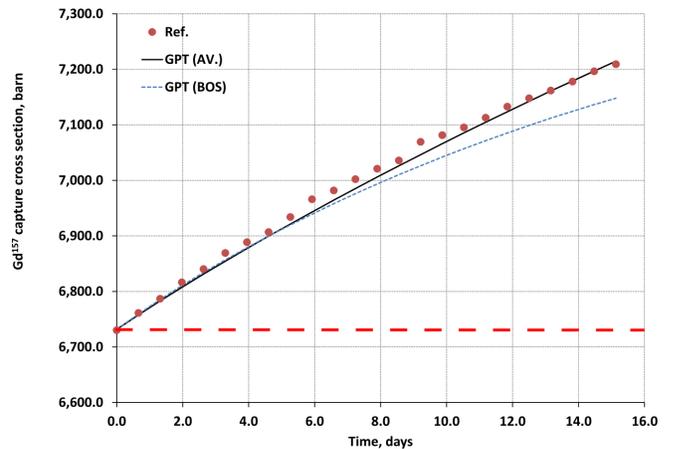


Fig. 1. Evolution of the <sup>157</sup>Gd effective one-group capture cross section during the first 15 days of burnup. (from [18]).

Fig. 1 shows the evolution of the <sup>157</sup>Gd one-group capture cross section during the first 15 days of burnup. While <sup>157</sup>Gd is depleted in the first few days, important spectral changes arise, and change the effective value of the <sup>157</sup>Gd cross section. For this reason, the common approach to the simulation of this problem involves the adoption of small burnup steps and

several Monte Carlo transport simulation, to correctly track the cross sections evolution. The red dots show the reference cross sections estimates, obtained adopting 0.5 days burnup intervals, with a total of 30 Monte Carlo calculations in the first 15 days of evolution. The blue dashed line shows the estimated evolution of the  $^{157}\text{Gd}$  one-group capture cross section obtained adopting a single Monte Carlo run, and adopting the GPT  $\frac{d\bar{A}}{dN}$  calculation. GPT calculations approximate very well reference results for most part of the 15 days burnup interval.

## 2. Uncertainty propagation in burnup calculation

The last few years have seen the Total Monte Carlo (TMC) approach becoming a popular method for uncertainty propagation in burn up calculations. TMC proved to be very useful in uncertainty quantification studies, but it is not efficient in explaining how the reactor physics and fuel evolution equations are connected to nuclear data uncertainty.

Coupled nuclide and neutron fields perturbation theory offers a theoretical framework to explain those connections [11, 12, 13, 14]. Nonetheless, the complexity of the full implementation of coupled perturbation theory and of the interpretation of the results posed severe limitations to the use of this approach.

An attempt to separate and understand the different effects of the perturbations of  $^{239}\text{Pu}$  nuclear data on the end of cycle fuel composition in a fast reactor assembly case study was presented in [19]. In that work, Monte Carlo Perturbation Theory and Total Monte Carlo approaches were combined and compared successfully.

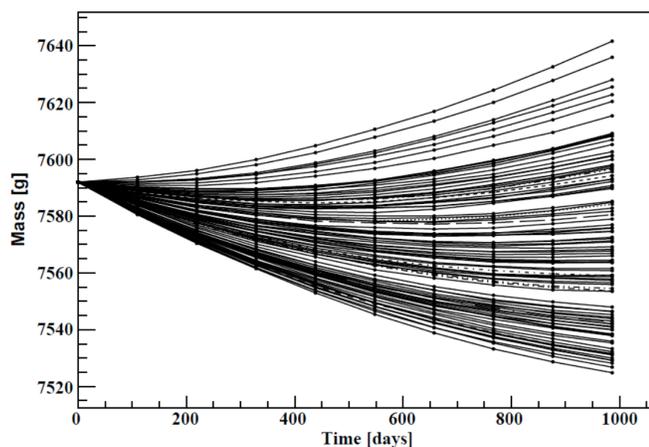


Fig. 2. Evolution of the  $^{240}\text{Pu}$  mass with burn up using 100 different random  $^{239}\text{Pu}$  evaluations (from [19]).

To highlight the importance of these investigations, it is useful to discuss some of the obtained results. In particular, the study showed that  $^{239}\text{Pu}$  nuclear data uncertainties have a stronger impact on higher mass nuclides than the impact on  $^{239}\text{Pu}$  itself. This means that the “direct” effect [12] of one cross section in the evolution matrix is not sufficient to

accurately explain the propagation of uncertainties. Fig. 2 presents the results of 100 evolutions of  $^{240}\text{Pu}$  as a function of time, obtained with 100 independent burnup calculations, starting from random  $^{239}\text{Pu}$  evaluations.

In [19], using formalism from [12], it was demonstrated that the “indirect” effects can be calculated by integrating the product of the adjoint and direct nuclide densities. As for the “direct” effect but with adapted factors and using extended covariance matrices and not only those of  $^{239}\text{Pu}$  nuclear data. Approximately half of the effect of  $^{239}\text{Pu}$  nuclear data uncertainties derives from its impact on the flux normalization, when assuming burnup evolution at constant power. The second important effect is related to the impact of  $^{239}\text{Pu}$  nuclear data perturbations on the effective transmutation cross sections of other actinides, due to spectral effects. The different effects can’t be efficiently studied via TMC alone. On the other hand, both contributions can be easily evaluated with Serpent extended GPT capabilities.

The results presented in [19] show that the amplitude and general shape of the observed covariance matrices of the one-group cross sections observed in TMC could be reproduced via the convolution of sensitivities calculated in Serpent GPT and  $^{239}\text{Pu}$  nuclear data covariances.

	Error	Rel. Diff. vs TMC (%)		
	TMC	NPT	XS Cov	Flux +XS
$^{239}\text{Pu}$	0,3%	22	10	6
$^{240}\text{Pu}$	0,4%	1	1	3
$^{241}\text{Pu}$	0,1%	18	1	15
$^{241}\text{Am}$	0,1%	93	69	8
$^{243}\text{Am}$	0,6%	100	50	4
$^{243}\text{Cm}$	1,3%	100	41	14
$^{244}\text{Cm}$	1,4%	100	55	5
$^{245}\text{Cm}$	2,0%	100	55	13

Fig. 3. Comparison of TMC and perturbation-based results for the end of cycle fuel assembly composition, considering random  $^{239}\text{Pu}$  evaluations (from [19]).

Fig. 3 shows a comparison of TMC and perturbation-based results for the end of cycle fuel assembly composition, considering random  $^{239}\text{Pu}$  evaluations. The “TMC” column represents the reference estimates for the fuel composition uncertainties, obtained via the Total Monte Carlo method. The following columns show the EOC uncertainty composition estimated obtained adopting different perturbation theory approximation, and expressed as relative difference from the reference TMC results. When all the separate effects described above are considered, GPT-based results are within 5-15% difference from TMC estimates for the most important isotopes.

### III. CONTINUOUS ENERGY SENSITIVITY FUNCTIONS

The standard approach to Perturbation Theory in deterministic codes involved the calculation of multi-group sensitivities for (generalized) response functions. This path has been followed as well by previous implementation of Perturbation Theory in continuous energy Monte Carlo codes.

Recently it has been shown that Eq. (6) can be extended to continuous-energy sensitivity functions [20]. These Monte Carlo eXtended Generalized Perturbation Theory capabilities (XGPT) have been tested and demonstrated for two different applications, that are presented in this section.

#### 1. Resonance parameters sensitivity

The first application of XGPT consists in the direct calculation of response sensitivities to cross-section resonance parameters perturbation, without intermediate multi-group collapsing steps.

In deterministic GPT calculations, the impact of resonance parameters uncertainty could only be calculated indirectly through their impact on multi-group cross sections, for which the sensitivities can be obtained. For this reason, resonance parameters covariances (i.e., MF32 ENDF files) are commonly propagated into multi-group covariances, which are used in the uncertainty quantification process.

In the Monte Carlo continuous-energy sensitivity functions approach proposed in [21], resonance parameters perturbations are obtained computing the covariances between the scores for the terms of  $R$  (Eq. (5)) and the collisions in the event history of the neutron population, weighted by a continuous energy sensitivity function  $G_f(E)$  [20]:

$$S_{b_{s,j}}^R = \frac{COV \left[ e_1, \sum^{history} G_f \right]}{E[e_1]} - \frac{COV \left[ e_2, \sum^{history} G_f \right]}{E[e_2]} \quad (10)$$

where  $G_f$  represents a score equal to the generic function  $f(E)$ , evaluated at the collision energy  $E$ , which is added to the particle history buffer in case of accepted collisions, and subtracted in case of rejected collisions.<sup>2</sup>

In case of resonance parameter perturbations, the continuous-energy sensitivity functions are defined as the derivatives of the cross sections with respect to the perturbed parameters. Figure 4 shows the  $^{238}\text{U}$  capture cross section sensitivity to the  $\Gamma_\gamma$  (radiative width) parameter perturbation in the 6.67 eV resonance:  $\frac{d\sigma_\gamma}{d\Gamma_\gamma}(E)$ .

In the present work, the continuous sensitivity functions were computed numerically via NJOY, and adopted for the XGPT calculation of the effect of resonance parameters perturbation on  $k_{\text{eff}}$  in a PWR MOX pincell, and compared to direct perturbations. Results are presented in Table I and Table II.

<sup>2</sup>See [20] for the details of the continuous energy sensitivity implementation.

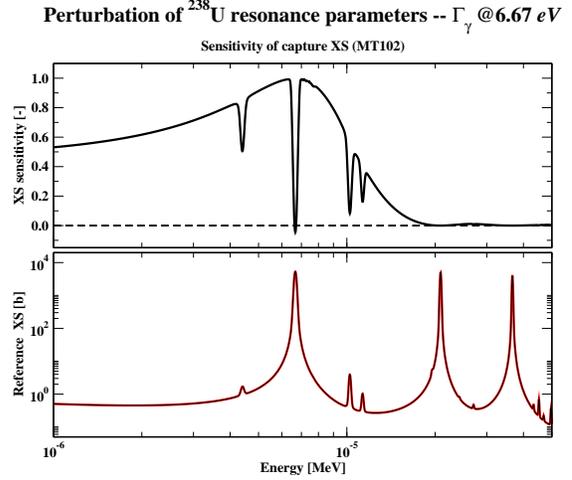


Fig. 4. Continuous-energy sensitivity function for  $\Gamma_\gamma$  parameter perturbation in the 6.67 eV resonance of  $^{238}\text{U}$ .

	Direct perturbation	XGPT
$S_{\Gamma_\gamma}^{k_{\text{eff}}}$	$-4.603 \times 10^{-2}$ $\pm 9.9 \times 10^{-4}$	$-4.469 \times 10^{-2}$ $\pm 1.4 \times 10^{-4}$
$S_{\Gamma_n}^{k_{\text{eff}}}$	$-4.392 \times 10^{-2}$ $\pm 9.9 \times 10^{-4}$	$-4.512 \times 10^{-2}$ $\pm 1.6 \times 10^{-4}$

TABLE I.  $k_{\text{eff}}$  sensitivity to the  $\Gamma_\gamma$  parameter perturbation in the 6.67 eV resonance of  $^{238}\text{U}$ . XGPT vs. Direct Perturbation.

#### 2. XGPT as a reduced order approximation for Total Monte Carlo analysis

The Total Monte Carlo (TMC) method [22] is stochastic approach to nuclear data uncertainty propagation. A large number of independent ENDF files are randomly generated starting from resonances and nuclear models parameters and their uncertainties. These files are then processed with NJOY to produce a set of formatted continuous-energy cross sections (i.e., ACE files), and independent Monte Carlo neutron transport simulations are run with these different ACE files as input, to estimate the uncertain distribution of the considered

	Direct perturbation	XGPT
$S_{\Gamma_\gamma}^{k_{\text{eff}}}$	$-1.832 \times 10^{-2}$ $\pm 9.9 \times 10^{-4}$	$-1.835 \times 10^{-2}$ $\pm 3.8 \times 10^{-4}$
$S_{\Gamma_n}^{k_{\text{eff}}}$	$1.495 \times 10^{-2}$ $\pm 9.9 \times 10^{-4}$	$1.495 \times 10^{-2}$ $\pm 1.6 \times 10^{-4}$
$S_{\Gamma_f}^{k_{\text{eff}}}$	$1.859 \times 10^{-2}$ $\pm 9.9 \times 10^{-4}$	$1.857 \times 10^{-2}$ $\pm 4.1 \times 10^{-4}$

TABLE II.  $k_{\text{eff}}$  sensitivity to the  $\Gamma_\gamma$ ,  $\Gamma_f$  and  $\Gamma_n$  parameters perturbation in the 0.295 eV resonance of  $^{239}\text{Pu}$ . XGPT vs. Direct Perturbation.

response functions.

TMC makes use of minimum approximations for the propagation of nuclear data uncertainties, and it is often considered as a reference approach in the framework of UQ studies. Nonetheless, running thousands of independent Monte Carlo simulations might lead to large computational requirements. For this reason, in [20] XGPT has been proposed as a reduced order model approximation to the full TMC calculation, to be adopted in combination with the Proper Orthogonal Decomposition (POD) of the random nuclear data.

The POD of the nuclear data set, allows each random cross section  $\Sigma_i$  to be expressed as a linear combination of basis functions  $b_{\Sigma,j}$ :

$$\Sigma_i(E) \approx \widetilde{\Sigma}_i(E) = \Sigma_0(E) \cdot \left( 1 + \sum_{j=1}^n \alpha_i^j \cdot b_{\Sigma,j}(E) \right) \quad (11)$$

This way, adopting the XGPT continuous-energy sensitivity calculation of Eq. (10), the response  $R$  corresponding to each random cross section  $\Sigma_i$  is approximated as:

$$R_{\Sigma_i} \approx \widetilde{R}_{\Sigma_i} = R_{\Sigma_0} \cdot \left( 1 + \sum_{j=1}^n \alpha_i^j \cdot S_{b_{\Sigma,j}}^R \right) \quad (12)$$

$S_{b_{\Sigma,j}}^R$  represents the relative change in the response function  $R$  due to a perturbation of the cross section  $\Sigma(E)$  equal to the relative basis function  $b_{\Sigma,j}(E)$ , and can be expressed as:

$$S_{b_{\Sigma,j}}^R = \int_{E_{min}}^{E_{max}} b_{\Sigma,j}(E) \cdot S_{\Sigma}^R(E) dE \quad (13)$$

In Fig. 5, the  $\ell_{eff}$  distribution due to TENDL-2013  $^{208}\text{Pb}$  uncertainties is presented for the criticality benchmark HMF-64. XGPT and TMC results are compared. As it can be observed, the XGPT/POD, single-run results closely match those obtained with 3000 independent TMC calculations.

For a better understanding of the data adopted for producing the uncertainty propagation results in Fig. 5, Fig. 6 shows 50 of the 3000 random cross sections from the TENDL-2013  $^{208}\text{Pb}$  evaluation, focusing on the elastic scattering cross sections in two specific energy regions.

#### IV. MC PERTURBATION THEORY FOR LARGE AND LOOSELY-COUPLED SYSTEMS

The different implementations of Perturbation Theory in Continuous Energy Monte Carlo codes require information or scores to be propagated over multiple generations, to correctly account for the effect of perturbations on the fission source spatial distribution.

In case of neutronically large or loosely coupled systems, the number of latent generation required to correctly describe the impact of localized perturbations on the asymptotic power

HMF-64 -  $\ell_{eff}$  uncertainty - XGPT + POD vs. TMC

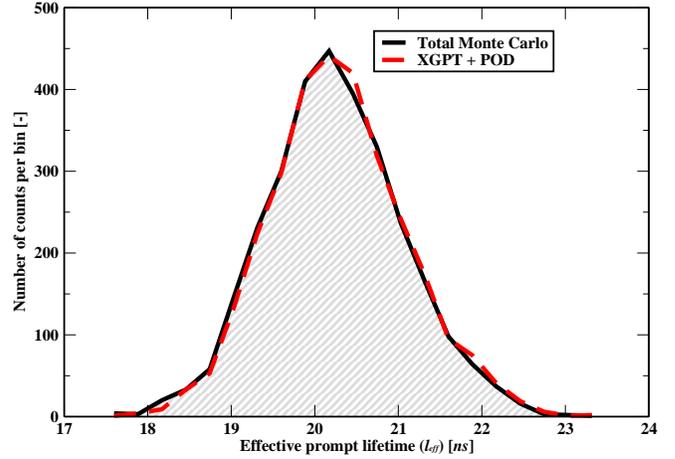


Fig. 5. HMF-64  $\ell_{eff}$  distribution from TENDL-2013  $^{208}\text{Pb}$  cross section data.

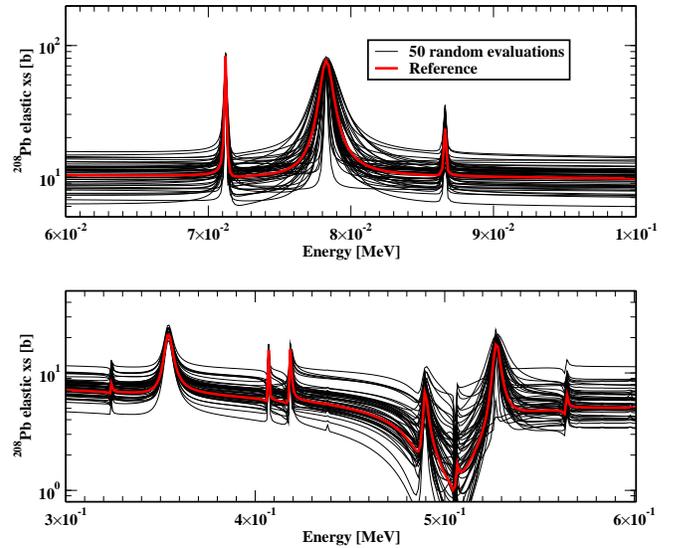


Fig. 6. TENDL-2013  $^{208}\text{Pb}$  random scattering cross section. Top: 60 keV to 100 keV interval. Bottom: 300 keV to 600 keV interval. Red curve represents the reference TENDL-2013 value.

distribution might become highly inefficient. This issue is correlated to the number of skip cycles required to reach a converged initial fission source distribution in standard Monte Carlo simulations.

To overcome this problem, new perturbation capabilities have been developed, and are presented in the following sections. In particular, the new approaches required the calculation of sensitivities for response functions that do not fall in the standard Generalized Perturbation Theory cases of reaction rate ratios (Eq. (3)) or ratios of bilinear functions of  $\phi$  and  $\phi^\dagger$  (Eq. (4)).

## 1. Calculation of perturbation on Avery's coefficients for coupled reactor theory

“Coupled” reactors are reactors in which two or more core regions with different neutron spectra are present. These regions might be neutronicly coupled to each other through neutron filters or geometric barriers, to achieve desired features for the reactor core (e.g., see [23]).

A powerful tool for the analysis of “coupled” reactors' behavior is provided by Avery's theory [24]. In particular, the point kinetics equations for a core with  $N$  regions are given by:

$$\begin{aligned} l_{jk} \frac{dS_{jk}}{dt} &= k_{jk}(1 - \beta) \sum_{m=1}^N S_{km} - S_{jk} + k_{jk} \sum_{i=1}^D C_{ki} \\ \frac{dC_{ki}}{dt} &= \beta_i \sum_{m=1}^N S_{km} - \lambda_i C_{ki} \end{aligned} \quad (14)$$

where  $S_k = \sum_{m=1}^N S_{km}$  is the fission rate in the region  $k$ .  $S_{km}$  is the rate of fissions produced in  $k$  from neutrons originating in  $m$ .  $k_{jk}$  represents the average number of fission neutrons produced in  $j$  from neutrons originating in  $k$ .  $l_{jk}$  is the adjoint-weighted time constant associated to this process.

Calculating the effect of perturbations in loosely coupled systems via Monte Carlo GPT might require a large number of latent generations. Avery's theory allows the calculation of important perturbation effects to be obtained from the sensitivities of  $k_{jk}$  and  $l_{jk}$  parameters.

$C_{ki}$  represents the quantity of delayed neutron precursors belonging to the  $i^{th}$  family, in the region  $k$ .  $\beta_i$  is the  $i^{th}$  effective delayed neutron fraction, which is assumed constant over the different regions, for simplicity.

In [25], the implementation of Monte Carlo estimators for Avery's coefficients and their sensitivities in the Serpent code was presented, along with code-to-code comparisons against ERANOS and verification against direct perturbation results.

## 2. Iterated Fission Matrix and XGPT for eigenmode perturbation theory

The Iterated Fission Matrix (IFM) approach allows calculating higher forward and adjoint eigenmodes of the  $l^{th}$  iterated fission kernel  ${}^{(l)}\mathbf{F}(r' \leftarrow r)$ , defined as the expected number of neutron descendents produced in  $r'$  after  $l$  generations from a neutron born in  $r$  [26]. Higher eigenmodes are obtained after spatial discretization of the continuous  ${}^{(l)}\mathbf{F}(r' \leftarrow r)$ , and the solution of the discretized eigenproblem, as in the Fission Matrix method:

$$\overline{\mathbf{S}}_{\mathbf{n}} = \left( \frac{1}{k_n} \right)^l \cdot {}^{(l)}\overline{\mathbf{F}} \cdot \overline{\mathbf{S}}_{\mathbf{n}} \quad (15)$$

If the forward and adjoint discretized eigenmodes are biorthonormalized such that  $\overline{\mathbf{S}}_{\mathbf{n}}^T \overline{\mathbf{S}} = \overline{\mathbf{I}}$ , the effect of pertur-

bations on the fundamental fission source distribution can be obtained as [27]:

$$\frac{d\overline{\mathbf{S}}_0}{dx} = \sum_{i=0}^{\infty} \overline{\mathbf{S}}_i \cdot \frac{\overline{\mathbf{S}}_i^T \frac{d{}^{(l)}\overline{\mathbf{F}}}{dx} \overline{\mathbf{S}}_0}{(k_0)^l - (k_i)^l} \quad (16)$$

where  $\frac{d\overline{\mathbf{S}}_0}{dx}$  represents the derivative of the fission source distributions  $\overline{\mathbf{S}}_0$  with respect to the perturbed parameter  $x$ .  $\frac{d{}^{(l)}\overline{\mathbf{F}}}{dx}$  is the effect of the perturbation on the fission kernel  ${}^{(l)}\overline{\mathbf{F}}$ .  $\overline{\mathbf{S}}_i$ ,  $\overline{\mathbf{S}}_i^T$  and  $\left(\frac{1}{k_i}\right)^l$  form the  $i^{th}$  eigentriplet of the discretized  $l^{th}$  iterated eigenproblem.

Adopting Eq. (16), fission distribution perturbations can be easily projected into the fission kernel eigenmode expansion, provided that the derivatives  $\frac{d{}^{(l)}\overline{\mathbf{F}}}{dx}$  can be obtained.

Via the collision history-based approach, the effects of a perturbation of the parameter  $x$  on the  $F_{I \leftarrow J}$  element of the discretized fission kernel are estimated from the average number of accepted and rejected collisions  $x$  in the history of the particles producing a fission neutron in  $I$ , and whose  $l^{th}$  ancestor was born in  $J$ :

$$\frac{d({}^{(l)}F_{I \leftarrow J})}{dx} = \frac{\sum_{p \in \alpha} w_p \cdot \delta_{(\text{cell}), I} \cdot \delta_{(l^{th} \text{ ancestor cell}), J} \sum_{g=\alpha-l}^{\alpha} (ACC_x - REJ_x)}{\sum_{s \in \alpha-l} w_s \cdot \delta_{(\text{cell}), J}} \quad (17)$$

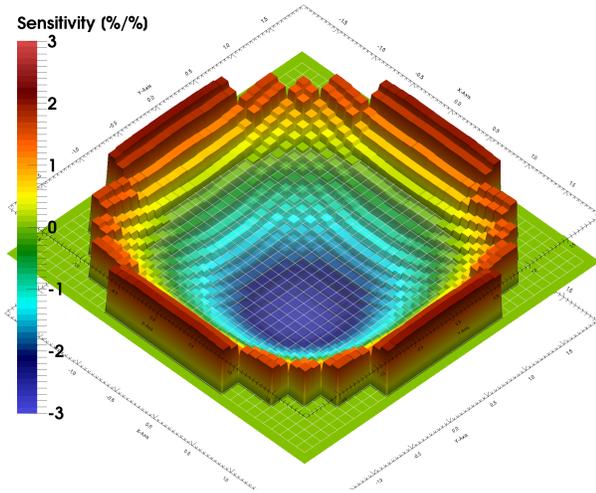
$\alpha$  represents the present generation, at which the fission in  $I$  is being recorded.

Eq. (17) derives from the application of Eq. (6) to a very peculiar response function, that is the estimator of the  $(I, J)$  element of the  $l^{th}$  Iterated Fission Matrix  ${}^{(l)}F_{I \leftarrow J}$ . Thanks to the flexibility of the XGPT implementation, based on the collision history approach, perturbation calculations can be performed considering virtually any response function. Usually, response functions as  $k_{\text{eff}}$ , reaction rate ratios and bilinear ratios are considered. In this case, to obtain the IFM eigenvector perturbation, the considered response function can not be expressed as a simple function of the critical forward and adjoint fluxes. Nonetheless, sensitivity calculations remain relatively straightforward thanks to the available methods.

This new XGPT+IFM+Eigenmode expansion approach to fission distribution perturbations has been implemented in Serpent and verified in case of a large 2D PWR core from the GEN-III exercise in [28] (load of UO2 assemblies with an outer ring of MOX assemblies). XGPT+IFM and reference estimates for the effect of perturbation of  ${}^{239}\text{Pu}$  resonance parameter on the fission source distributions are compared in Fig. 7.

The sensitivity is very large (expressed as %/%) . One of the reason for the strong sensitivity is the high dominance ratio of the system (0.995): perturbations are likely to induce large change in the power distribution, without necessarily inducing large changes in  $k_{\text{eff}}$ . Moreover, the selected perturbation

**Fiss. source sensitivity to Pu239  $\Gamma_f$  @ 0.295eV  
Reference (mesh detectors in two Serpent runs)**



**Fiss. source sensitivity to Pu239  $\Gamma_f$  @ 0.295eV  
XGPT + IFM + Eigenvalue perturbation**

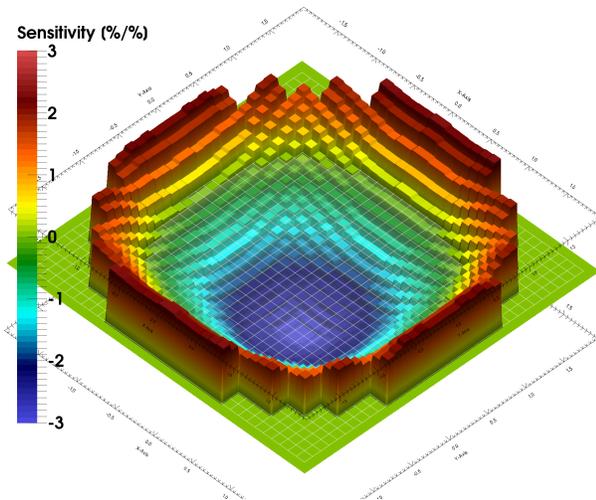


Fig. 7. Sensitivity of the fission source distribution to  $^{239}\text{Pu}$   $\Gamma_f$  at 0.295 eV. Direct perturbation vs. Perturbation Theory

is very localized, acting only in the outer MOX assembly ring. Nonetheless, the agreement between reference results and perturbation-based results is reasonably good. Direct perturbation results were obtained via two separate Serpent runs and a 3%  $\Gamma_f$  perturbation in the  $^{239}\text{Pu}$  resonance at 0.295 eV.

The denominator of the expansion coefficients in Eq. (16) is the eigenvalue separation. For this reason, is reasonable to truncate the eigenvalue expansion to a finite  $i$ : any perturbation is less likely to “excite” eigenmodes with corresponding small eigenvalues.

Fig. 8 shows the most important eigenmodes for the projection of the fission source derivative due to  $^{239}\text{Pu}$   $\Gamma_f$  at 0.295

eV perturbation in the selected case study. The top contributors of the linear expansion are symmetric as the perturbation is symmetric. Nonetheless, non-symmetric modes are excited as well, due to statistical errors in the Monte Carlo GPT calculation. It should be recalled that the normalization of each eigenmode is arbitrary, as long as the bi-orthonormality between forward and adjoint eigenmode is preserved.

## V. CONCLUSIONS

The present paper describes recent applications of the Monte Carlo Perturbation Theory and new development of this methodology. In particular, calculation of continuous-energy function sensitivities, adoption of GPT in burnup simulation, and the adoption of perturbation theory in loosely coupled systems have been described in details.

Monte Carlo Perturbation Theory proved useful in a wide set of applications of interest for computational reactor physics. Further developments in the field of continuous-energy cross section adjustment and nuclear data assimilation are presented in a separate paper.

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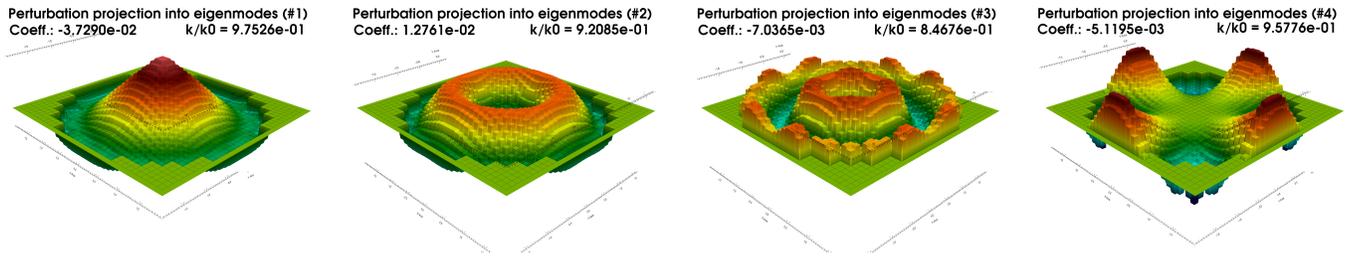


Fig. 8. Linear expansion of the fission source derivative due to  $^{239}\text{Pu } \Gamma_f$  at 0.295 eV perturbation: top eigenmodes contributors.

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