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# SMALL SAMPLE REACTIVITY WORTHS CALCULATION: EXACT PERTURBATION THEORY AND MONTE CARLO TRANSPORT

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## ABSTRACT

The goal of this work is to calculate with a decent precision and accuracy the effect induced by the oscillation – or the substitution – of a pure sample of material at the center of a critical nuclear reactor core. The difference between the calculated and measured reactivity worth might hopefully be used to feedback nuclear data. Frequently, Monte Carlo transport codes fail in that task due to their inefficiency to reach convergence on such small reactivity differences (*e.g.* measured effects are sometimes lower than 1 pcm). Various deterministic and stochastic approaches have been used in the past, but they failed to provide unquestionable results for all isotopes.

In this paper, we present a new methodology that allows exact calculation (*i.e.* not limited to first order) of these effects using Monte Carlo Neutron Transport codes. This method has several advantages: (1) It does not require significant code developments and it can be applied with almost any standard Monte Carlo codes. (2) It does not rely on any assumptions other than standard assumptions made by these codes: thus, it can be used to calculate any kinds of perturbation (*e.g.* concentration, geometry, medium, cross-sections) with a variable degree of effectiveness; still, it converges to the true value obtained from the difference of two independent runs. (3) In contrary of direct Monte Carlo perturbation technics, the more perturbations are small and locally contained, the more it performs. Validation cases confirm the numerical good behavior of the method named *Black Body Exact Perturbation*.

KEYWORDS: Perturbation Theory ; Small Sample Reactivity Worth ; Sensitivity ; Iterated Fission Probability

## 1. INTRODUCTION

Until 2017, the CEA had the opportunity to lead valuable measurement programs (*e.g.* the CERES program [1,2]) in the pool reactor MINERVE at the middle of which a rod enclosing a small sample could be moved up and down alternatively. The reactivity induced by the oscillating sample was

measured with high accuracy according to the movement of an automatic and calibrated control rod. A lot of work has been dedicated to the development of tools in order to perform reliable interpretation calculations in that context: it includes the development of a dedicated hybrid schema [3] using both deterministic code APOLLO2 [4] and Monte Carlo code TRIPOLI-4 [5] and its validation through an OECD benchmark [6]. More recently and inspired by the renewal of the iterated fissions principle [7,8], the Exact Perturbation Theory (i.e. not limited to a first order approximation) has been successfully used for the first time in the Monte Carlo TRIPOLI-4 [9,10]. Get things back to the computation problem, if one wants to calculate a reactivity worth (i.e. a reactivity perturbation induced by a change in core configuration from a reference configuration), one can apply three main strategies:

- Calculate reactivities in both reference and perturbed states and make the difference. This method is designated as the “eigenvalue difference method” and constitutes the reference calculation. It will encounter convergence issues as reactivity worth gets smaller. In the case of the MINERVE oscillation experiments, it would require millions of cpus hours to get as precise as the experiment.
- Apply Perturbation Theory [11]. Topic has been well study these years and several efficient methods has raised in the field of keff-sensitivity calculations – without being exhaustive [12,13]. Limitation to 1st order Perturbation Theory (or even second order) may raise very precise results that unfortunately are sometime slightly inaccurate as well. Inaccuracy will depend on the nature of the perturbation. It must be kept in mind that a very small perturbation at the scale of a nuclear core might be associated with a large local change in neutron flux.
- Introduce correlations between calculations of both states. The best way is to calculate both reactor states at the same time and get reactivity difference directly from neutron paths that differ: splitting [14] or weights technics [15] can be used. In the later, weights should be used carefully as it seems to be mathematically correct, give precise results, but can raise convergence issues linked to very rare events (i.e. phase space need to be more or less evenly explored in order to fit all kinds of perturbations.).

Hereafter, a new method belonging to the second category is introduced. The *Black Body Exact Perturbation* method provide both confidence and precision in order to estimate small reactivity differences of any kinds with Monte Carlo codes – provided that Monte Carlo best practices are applied. In the first Section of this paper, the method and its equations are introduced before being applied to small validation cases in a second Section.

## 2. THEORY

The Exact Perturbation Theory expression of a reactivity difference is briefly recalled below in order to derived the equations needed by the Standard *Black Body Exact Perturbation* \*. Defining reactor states 1 and 2 respectively as the perturbed and reference states, forward and adjoint

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\*The equations for the *Generalized* version of the method (i.e. that deals with other parameters than the reactivity) are for now only written down in French [16].

equations can lead after some manipulations [11] to an expression of the reactivity difference  $\Delta\rho = \lambda_2 - \lambda_1$  as a function of  $\Delta\mathcal{P} = \mathcal{P}_2 - \mathcal{P}_1$  and  $\Delta\mathcal{K} = \mathcal{K}_2 - \mathcal{K}_1$ :

$$\Delta\rho = \frac{\langle \Phi_1^\dagger, [\lambda_1 \Delta\mathcal{P} - \Delta\mathcal{K}] \Phi_2 \rangle}{\langle \Phi_1^\dagger, \mathcal{P}_2 \Phi_2 \rangle} \quad (1)$$

Where for state  $i$  of the reactor,  $\Phi_i$  and  $\Phi_i^\dagger$  stand for the fundamental forward and adjoint neutron flux modes of the transport equation. Where  $\lambda_i$  is the highest eigenvalue (proven to be the same in both forward and adjoint equations). Where  $\mathcal{K}_i$  stands for the transport, multiplicity reactions, leakage and disappearing operator and  $\mathcal{P}_i$  stands for the production by fission operator.

## 2.1. (Standard) Black Body Exact Perturbation

Say that the operator variations between state 1 and 2 is limited to a subspace of the phase space  $V_{\text{Pert}}$  (e.g. in the case of small sample experiment, the physical volume of the sample), the Black Body Exact Perturbation method will estimate the reactivity difference as follow,

$$\Delta\rho = [\lambda_2 - \lambda_{\text{BB}}] - [\lambda_1 - \lambda_{\text{BB}}] = \Delta\rho_2 - \Delta\rho_1 \quad (2)$$

introducing a new state (labeled BB) where  $V_{\text{Pert}}$  is replaced by a black body, non-emissive medium, that will absorb all incoming neutrons reaching the surface  $S_{\text{Pert}}^+$ . Coming from the Exact Perturbation Theory expression, each reactivity effect relative to the BB state can be expressed as:

$$\Delta\rho_i = \frac{\langle \Phi_i^\dagger, \Phi_{\text{BB}} |_{\vec{r} \in S_{\text{Pert}}^+} \rangle}{\langle \Phi_i^\dagger, S_{\text{BB}} \rangle} \quad (3)$$

Where,

- $\Phi_{\text{BB}} |_{\vec{r} \in S_{\text{Pert}}^+}$  corresponds to all neutrons entering the black medium. These neutrons can be saved by Monte Carlo codes while running the simulation of the BB state as they reach the surface of the black body with their position, direction and stochastic weight.
- $S_{\text{BB}}$  corresponds to the fission production of the power iteration process, that can also be saved by Monte Carlo codes while running the simulation of the BB state.
- Ponderation and integration on phase space of these neutrons by  $\Phi_i^\dagger$  can be obtained using the Iterated Fission Probability principle. Basically, this principle [7,8] states that if a source  $S$  initiates a power iterations algorithm, the asymptotic number of fissions produced will correspond to the importance of that source in the fundamental mode. This number can be approach by the product of successive renormalization factors  $k_g$ ,  $\langle \Phi^\dagger S \rangle = \sum_{g=1}^L k_g$ , up to a number  $L$  usually designated as the IFP (cycle) length<sup>†</sup>.

Note that (3) had already been established in a more general case by K. Smith [14],

$$\Delta\rho = \frac{\langle \Phi_1^\dagger, \Phi_2 |_{\vec{r} \in S_{\text{Pert}}^+} \rangle - \langle \Phi_1^\dagger, \Phi_2 |_{\vec{r} \in S_{\text{Pert}}^-} \rangle}{\langle \Phi_1^\dagger, S_2 \rangle} \quad (4)$$

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<sup>†</sup>More precisely, for the series to converge, it would be better to write  $\langle \Phi^\dagger S \rangle = \sum_{g=1}^L \frac{k_g}{k_\infty}$ , where  $k_\infty$  is the effective multiplication factor. In the next expression, this factor appears both to the numerator and the denominator and is therefore omitted.

but it's evaluation was not relying on the IFP principle what lead to simplification hypothesis and hypothetic inaccuracy. The equation was more general in the sense that it does not necessarily implies a black body, what would require storing out-coming neutrons  $S_{\text{Pert}}^-$  from the perturbed subspace volume. In the specific case of a small sample, neutrons coming out of the perturbed volume will not seen their importance changed so much compared to neutrons coming in. Therefore, it is much more efficient to use a black body so as not to calculate the importance of neutrons coming out. If the perturbed volume is larger, the method as it is will not be as efficient and one should prefer using the eigenvalue difference method.

### 3. APPLICATION AND VALIDATION

#### 3.1. Calculation Scheme

In practice, (3) is rewritten to take special care of normalisations:

$$\Delta\rho_i^L = \frac{W|_{S_{\text{Pert}}^+} \sum_{g=1}^L k_{i,g}^{(3)}}{\mathcal{N} k_{\infty}^{\text{BB}} \sum_{g=1}^L k_{i,g}^{(2)}} \quad (5)$$

1. First, a critical simulation is conducted in the BB state with  $\mathcal{N}$  neutrons per generation <sup>‡</sup>. After fission source convergence, neutrons touching the surface are stored during  $n$  generations. At the end of the simulation, the sum of all statistical weights of neutrons stored,  $W|_{S_{\text{Pert}}^+}$ , is calculated while the last fission source is also stored. In TRIPOLI-4, fission source weight is normalized to the number of neutrons per generation  $\mathcal{N}$  and must be multiplied by the mean effective multiplication factor  $k_{\infty}^{\text{BB}}$  to get the actual production weight.
2. Fission sources are used as initial sources of a simulation in state  $i$  for  $L$  generations. Each renormalization factor  $k_{i,g}^{(2)}$  of generation  $g$  is saved in order to compute  $\sum_{g=1}^L k_{i,g}^{(2)}$  later on (*i.e.* the importance of the fission source according to the IFP).
3. Particles stored on the surface of the black body are used as initial sources of a simulation in state  $i$  for  $L$  generations. Each renormalization factor  $k_{i,g}^{(3)}$  of generation  $g$  is saved in order to compute  $\sum_{g=1}^L k_{i,g}^{(3)}$  later on (*i.e.* the importance of neutrons entering the perturbed volume according to the IFP).

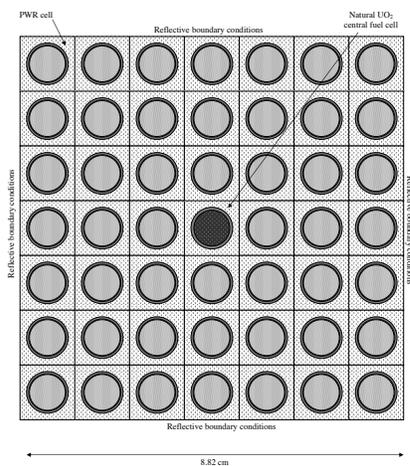
To compute rigorous uncertainty estimation, the binding of these three steps is carried on individually a high number of times on multicore cpus for each state  $i$ . Mean and standard deviation can then be derived from result distributions. If one has access to Monte Carlo source code, it is of great interest to track neutrons through generations to gather steps 2 and 3 in the same IFP simulation (*i.e.* importances will thus be correlated and it will increase convergence rate). It could be achieved by distinguishing which source (fission or neutrons entering the perturbed volume) has produced which portion of the asymptotic generation.

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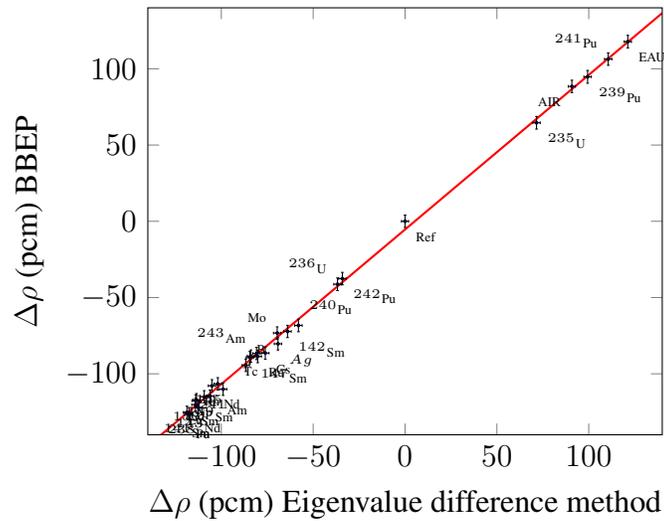
<sup>‡</sup>A fictive isotope with dumb cross sections is created so as to achieve total absorption at the surface of the black body.

### 3.2. Small-sample-like Benchmark

In this validation case, the BBEP method is compared to the eigenvalue difference method on the  $7 \times 7$  cells geometry (*cf.* Fig. 1a) of an OECD benchmark [6] where different isotopes are added successively to the central pin. Although bigger kind of networks are also present in the benchmark definition, the relatively small size of the  $7 \times 7$  cells geometry allows the evaluation of differences directly from the eigenvalue difference method with relatively high precision (and accuracy) for benchmarking the BBEP. Several kinds of isotopes have been tested (absorbents, fissile, diffusive) and all results obtained by Monte Carlo code TRIPOLI-4 in 3D and continuous energy cross sections show great agreement with the reference eigenvalue difference method, see Fig. 1b.



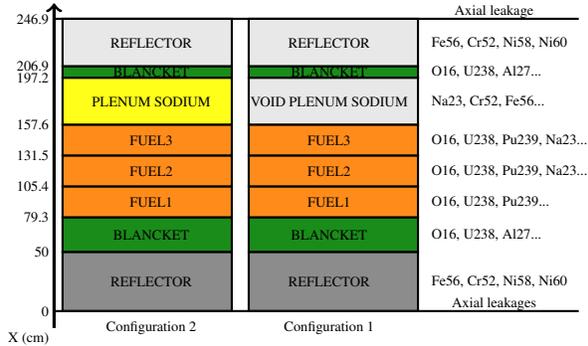
(a) Horizontal cut of CHANDA benchmark:  $7 \times 7$  cells PWR representative, central pin is successively doped with different kinds of isotopes



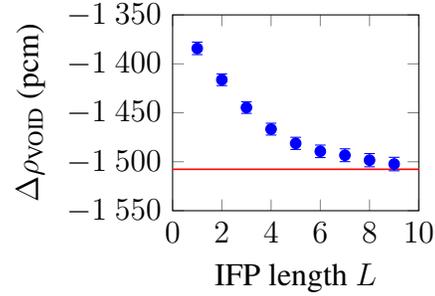
(b) Correlation between the reference and the newly developed BBEP method on a  $7 \times 7$  cells network. Uncertainty bars are given to  $1\sigma$ .

### 3.3. Sodium Void Effect

Another validation test shows the great versatility of the method. A 1D geometry representative of a fast breeder reactor cooled down by sodium is modeled in TRIPOLI-4 and the difference of reactivity induced by the decrease of the sodium level in the plenum area is calculated as a function of the IFP cycle length (*cf.* Fig. 2a). After 10 generations, IFP has converged and strictly give the same reactivity worth than the eigenvalue difference method, see Fig. 2b.



(a) Reactivity perturbation is induced by the void of the plenum in sodium



(b) BBEP void reactivity as a function of the IFP length (in blue). Reactivity obtained by eigenvalue difference method is plot in red.

#### 4. CONCLUSIONS

A new method has been developed and applied in the specific case of small sample worth calculation using Monte Carlo neutron transport code. This method is actually able to evaluate local change of any kind in an exact manner as it does not rely on further hypothesis than those made by Monte Carlo codes in general. In the case of very local changes to the reactor reference state, the BBEP method will perform several orders of magnitudes faster than the traditional eigenvalue difference method. Source codes modifications are not required but an agile handling of Monte Carlo codes inputs and outputs is mandatory, especially to handle IFP calculations and rigorous uncertainty propagations.

Two applications cases has been carried on to show the reliability of the method. The extension of BBEP to Generalized Perturbation Theory is a work in progress.

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